HGSYSTEM 3.0

Technical Reference Manual

by

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TNER.94.059

Shell Research Limited, Thornton Research Centre,
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The LPOOL model was made available by Exxon Research and Engineering Company.

EXECUTIVE SUMMARY

1. Historical background

As a result of many years in-house research, the gas dispersion group at Shell Research Ltd. Thornton (United Kingdom) has developed a package of mathematical models, called HGSYSTEM, to study the atmospheric dispersion of accidental pollutant releases with emphasis on denser-than-air materials. HGSYSTEM can be simulate different dispersion scenarios (jet dispersion, heavy gas dispersion, passive dispersion). The first version of HGSYSTEM was made freely available for use in November 1990. This version, called NOV90 or version 1.0, was prepared by Shell Research Ltd. for *The Industry Cooperative HF Mitigation/Assessment Program, Ambient Impact Assessment Subcommittee* as one component of a wider programme aimed at a better understanding of atmospheric dispersion, including hydrogen fluoride (HF) releases. HGSYSTEM can model the full HF chemistry and thermodynamics. Most of the modules in the HGSYSTEM package can also be used for more general, non-reactive (ideal gas) releases as well. Validation of the HF-related simulations has been done with the well-known Goldfish Test Series. Full documentation to the 1.0 version was given in the HGSYSTEM Technical Reference Manual and User's Manual.

After release of the 1.0 (NOV90) version, a version 1.1 was made available which contained minor changes to solve some program bugs. Several internal versions were also developed.

2. HGSYSTEM 3.0

HGSYSTEM is in wide use for simulation of atmospheric dispersion scenarios for HF and other pollutant releases. It has been assessed against other models and found to rank amongst the best available atmospheric dispersion models in the world. HGSYSTEM sets the standard for HF dispersion calculations. However, a number of topics were open for improvement and generalisation. With financial support of the *American Petroleum Institute, Air Modelling Task Force*, Shell Research has upgraded and updated the existing HGSYSTEM package, resulting in a new release called HGSYSTEM version 3.0. The following major changes have been made to HGSYSTEM 1.0 to obtain HGSYSTEM 3.0:

- The thermodynamical models available in HGSYSTEM have been extended. The full HF chemistry and thermodynamical model is now suitable for mixtures of HF, water and an inert ideal gas. The non-reactive ideal gas description has been extended to multi-compound liquid-vapour mixtures (aerosols).

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- A database containing physical properties for some 30 compounds has been added to HGSYSTEM. This database is needed when using the new two-phase multi-compound thermodynamical model.

- The PLUME model for pressurised releases has been extended to model jet dispersion of multi-compound, two-phase mixtures and is now called AEROPLUME.

- A new model describing the initial phase of instantaneous releases, HEGABOX, has been added to HGSYSTEM.

- A new model to calculate release rates from pressurised vessels, SPILL, is now available in HGSYSTEM version 3.0.

- The existing evaporating pool model EVAP has been replaced by a better model, LPOOL, for boiling and non-boiling pools and land and water. LPOOL is based on a model developed by Exxon Research and Engineering Company.

- The formulation of the lateral spreading in the heavy gas dispersion model HEGADAS has been reviewed and improved.

- Several options have been added to the time-dependent version of the heavy gas model HEGADAS making it easier to use and to evaluate the results.

- HGSYSTEM now contains three post-processors to generate data for graphical output after a pressurised jet release, steady state heavy gas release and a time-dependent heavy gas release respectively. These post-processors will improve the ease of use of the HGSYSTEM modules.

- Five additional options resulting from work done on HGSYSTEM as sponsored by Martin Marietta Energy Systems Inc (USA) are available to all HGSYSTEM users.

- A new HGSYSTEM 3.0 User's Manual and Technical Reference Manual have been written. These are now up-to-date and their format allows for easy future updating.

3. Modules available in HGSYSTEM 3.0

The following models are available in HGSYSTEM version 3.0:

Database program

DATAPROP	generates physical properties used in other HGSYSTEM models

Source term models

SPILL	transient liquid release from a pressurised vessel
HFSPILL	SPILL version specifically for hydrogen fluoride (HF)
LPOOL	evaporating multi-compound liquid pool model (unpressurised release)

Near-field dispersion models

AEROPLUME	high-momentum jet and elevated plume model
HFPLUME	AEROPLUME version specifically for hydrogen fluoride (HF)
HEGABOX	dispersion of instantaneous heavy gas releases

Far-field dispersion models

HEGADAS	heavy gas dispersion (steady-state and transient version)
PGPLUME	passive Gaussian plume dispersion

Utility programs

HFFLASH	flashing of hydrogen fluoride (HF) from pressurised vessel
POSTHS/POSTHT	post-processing of HEGADAS results (steady state and time-dependent version)
PROFILE	post-processor for concentration contours of air borne plumes
GET2COL	utility for data retrieval

4. Documentation

HGSYSTEM version 3.0 is documented in the following two manuals:

HGSYSTEM 3.0 User's Manual
L. Post
Shell Research Limited, Thornton Research Centre, TNER.94.058
1994

HGSYSTEM 3.0 Technical Reference Manual
L. Post (editor)
Shell Research Limited, Thornton Research Centre, TNER.94.059
1994

The User's Manual is thought to be the main reference document for normal us of the HGSYSTEM modules. It contains all information necessary to run the models and interpret the generated results. The Technical Reference Manual is intended as a source of background information for users who want to know more about the technical/scientific contents of the HGSYSTEM modules.

HGSYSTEM 3.0 Course Notes (TNER.94.060) are also available for use during possible HGSYSTEM training sessions.

HGSYSTEM 3.0 TECHNICAL REFERENCE MODEL

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1. GENERAL INTRODUCTION

1.1. Introduction

This Technical Reference Manual gives technical background information for the HGSYSTEM version 3.0 models. To keep this Manual as concise as possible, in general only that information is supplied which is not available in the open scientific literature.

Of course, for every model detailed descriptions of all input parameters is given in the HGSYSTEM User's Manual. Information in the User's Manual should enable the user to run any HGSYSTEM model.
The information in this Technical Reference Manual is intended as supplementary information for those users who want to know more about the 'technical' contents of an HGSYSTEM model.

In this paragraph, an overview of the main new features available in HGSYSTEM version 3.0 is given, as compared to the first public domain release of HGSYSTEM, version 1.0 which is also called the NOV90 version.

1.2. Main new features in HGSYSTEM version 3.0

Compared to the first public domain version of HGSYSTEM (version 1.0 or NOV90), many changes have been made to the separate models. Apart from several minor changes (additional input parameters, removed bugs etc.), the following new *major features* are now available in version 3.0 of HGSYSTEM.

- A new thermodynamical model describing *multi-compound, two-phase fluids* has been implemented. This model is also called the HGSYSTEM aerosol model. It is described in full detail in Chapter 2.A. It is available in all main and non-HF specific HGSYSTEM models.

- To generate the physical compound properties need by the new two-phase model, a *database program* called DATAPROP has been added to HGSYSTEM. DATAPROP generates link files containing all relevant data, for all HGSYSTEM models using the two-phase description.

- The new PLUME version using the new two-phase thermodynamical model is renamed to *AEROPLUME*. AEROPLUME describes near-field jet dispersion for multi-compound, two-phase releases from pressurised vessels. AEROPLUME has a built-in discharge model

to give estimates for release rates, that is, it calculates a source term for the dispersion calculation.
The AEROPLUME implementation in HGSYSTEM is described in detail in Chapter 5.A.

- The *hydrogen fluoride (HF) chemistry and thermodynamical model* has been extended to describe mixtures of HF, water and an inert ideal gas. This model is now available in the HGSYSTEM modules HFPLUME, HEGADAS and the new HEGABOX model. The new HF model is described in full detail in Chapter 2.B.

- A new model describing the initial gravity slumping behaviour for *instantaneous releases* is now available in HGSYSTEM. This model is called HEGABOX. More details are given in Chapter 8.

- A new model calculating the *transient* (time-dependent) *release rate* of a multi-compound, two-phase fluid from a pressurised vessel is now available in HGSYSTEM. This model is called SPILL and can be seen as the counterpart of the HF-specific model HFSPILL. The new SPILL model is discussed in full detail in Chapter 3.

- The EVAP model describing *evaporating liquid pools*, as used in HGSYSTEM 1.0, has been replaced be a completely new model called LPOOL. LPOOL is based on the LSM90 model as made available by Exxon Research & Engineering Company. LPOOL can be used for boiling and non-boiling pools of multi-compound mixtures on land or on water. More information on the LPOOL model is given in Chapter 4.

- The HEGADAS algorithm has been revised to prevent unrealistic concentration profiles. A detailed description of these changes is given in Chapter 7.B.

- Several new options have been added to the transient (time-dependent) version of the heavy gas model, HEGADAS-T. These new features are:
  - An algorithm to automatically generate an 'optimal' set of output times. See User's Manual, Chapter on HEGADAS, input block AUTOTIM.
  - A similar algorithm to automatically generate an 'optimal' step size in the downwind direction. See User's Manual, Chapter on HEGADAS, input block CLOUD, parameters XSFACT and XSEPS.
  - The possibility to specify a change in surface roughness at given downwind distances. See User's Manual, Chapter on HEGADAS, input block TRANSIT, parameter ZRS.

  Technical documentation on these new HEGADAS-T features are given in Chapter 7.C.

- The post-processors for HEGADAS results have been updated and can now be used in 'batch' mode like all other main HGSYSTEM modules. Capabilities for dosage calculations were added. Time-averaging is now done in a better way. These new models are called POSTHS and POSTHT. See the relevant chapter in the HGSYSTEM User's Manual.

- A utility program to generate concentration contours for airborne plumes as calculated by AEROPLUME and PGPLUME, is now available. The utility is called PROFILE. See the relevant chapter in the HGSYSTEM User's Manual.

- The model HFJET, which was a strongly simplified version of the HFPLUME model, is no longer part of HGSYSTEM, as its use is very limited.

- Following work done on a specific HGSYSTEM version by The Earth Technology Corporation, U.S.A., several new options are now available to all users of HGSYSTEM version 3.0. This work was sponsored by Martin Marietta Energy Systems and the added options are therefore available in an MMESOPT input block. The technical descriptions of options are given in Chapter 9. The corresponding input parameters are discussed in the HGSYSTEM 3.0 User's Manual for the relevant models (AEROPLUME, HEGADAS, HEGABOX and HFPLUME). General guidance is given in Chapter 18 of the HGSYSTEM 3.0 User's Manual.

2. THERMODYNAMICAL DESCRIPTIONS IN HGSYSTEM

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2. THERMODYNAMICAL DESCRIPTIONS IN HGSYSTEM

There are two thermodynamical descriptions for fluids available in HGSYSTEM:

1. A *multi-compound, two-phase model* which calculates the two-phase liquid-vapour state of a mixture. The user can specify the mixture composition, choosing compounds as available in the HGSYSTEM database program DATAPROP. This thermodynamical description is quite general, but does *not* include the effect of any chemical reactions. The two-phase model is also sometimes called the *aerosol* model. It is described in full detail in Chapter 2.A.

   All HGSYSTEM models using this thermodynamical model need specific physical properties, like saturated vapour pressures, liquid densities, specific heats and so on, for all specified compounds in the mixture. It is strongly recommended to generate these properties using the database program DATAPROP and transfer the results to HGSYSTEM to be used via a link file. For details on this, see the DATAPROP chapter and Chapter 4 in the HGSYSTEM User's Manual. HGSYSTEM models using this aerosol model are: SPILL, AEROPLUME, HEGABOX and HEGADAS. LPOOL does use the compound properties as generated by DATAPROP but its pool description does not need a full thermodynamical model.

2. A *hydrogen fluoride (HF) chemistry and thermodynamical* model. This model is suitable for mixtures of HF, water and an inert ideal gas. It includes the effect of chemical reactions (reaction of HF and water, polymerisation of HF) and gives a full thermodynamical description based on the empirical relations of the so-called Schotte model. This very specific model is available because originally HGSYSTEM was developed to simulate the dispersion of HF releases only. The HF chemistry and thermodynamical model is discussed in full detail in Chapter 2.B. HGSYSTEM contains several HF-specific models: HFSPILL (only pure HF) and HFPLUME. Other models can optionally use the HF-model: HEGABOX and HEGADAS. LPOOL can use the physical properties of HF but does not need the full HF chemistry and thermodynamics.

The following two chapters (2.A and 2.B) give detailed descriptions of each of the two thermodynamical models mentioned above.

2.A. THE MULTI-COMPOUND, TWO-PHASE MODEL

2.A.1. Introduction

In accidental releases, the released pollutant often does *not* consist of a single inert gas in the vapour phase, but it consists of a mixture of inert gases and possibly water with possible accompanying aerosols. Following mixing of the pollutant with the moist air additional aerosol formation may occur.

This chapter discusses the standard HGSYSTEM two-phase thermodynamics model, new in HGSYSTEM version 3.0 as compared with version 1.0 (NOV90), that allows for a multi-compound pollutant and takes into account effects of possible aerosol formation. This chapter also discusses the implementation of this thermodynamic model into the HGSYSTEM dispersion models.

Thermodynamic Model

Following mixing of the pollutant with the moist air, the mixture is assumed to be in thermodynamic equilibrium, and the compounds contained in the mixture are assumed not to react with each other or to (de)polymerise.

Non-ideal liquid solutions (see below for details) and reactions with water (for example needed for ammonia and SO_3) are not taken into account. Concerning the mathematical description of aerosols the following possibilities for a pollutant compound are considered.

1. The compound has a *very low boiling point*. In this case the compound is always in the vapour phase and does not form part of an aerosol. Examples: oxygen, nitrogen, etc.

2. The compound has a *very high boiling point*. In this case the compound is always in the liquid phase and does not evaporate. Example: H_2SO_4 aerosol upon release of pollutant consisting of propane and H_2SO_4.

3. The compound may be present in both vapour and liquid phase. The following types of aerosols can be distinguished (see for example [1] for details).

   a. The compound forms a single, separate aerosol (individual droplets), which does not interact with possible aerosols for other pollutant compounds. For this case the amount of aerosol formation can be calculated using *Dalton's law*. This law states that in the presence of an aerosol, the mole fraction of the compound in the vapour equals the ratio of the partial vapour pressure for the compound and the total vapour pressure. Example: separate propane and water aerosols upon release of (cold) propane in humid air.

b. The compound forms a so-called *ideal liquid solution* with a number of other compounds. The vapour and liquid mole fractions for each compound in the aerosol can be derived via *Raoult's law*. This law states that in the presence of an aerosol, the ratio of the mole fraction of the compound in the vapour and the mole fraction of the compound in the aerosol equals the ratio of the partial vapour pressure for the compound and the total vapour pressure. Ideal solutions will usually be formed for compounds which have a similar chemical structure. Example: single propane/butane aerosol upon release of a pollutant consisting of propane and butane

c. The compound forms a *non-ideal liquid solution* with a number of other compounds. In this case Raoult's law as stated above is not applicable.

While the aerosol formation for an ideal solution can be determined via Raoult's law from individual saturated vapour-pressure functions for each individual compound, the determination of the aerosol formation for an non-ideal solution involves much more empiricism. In literature this is usually determined by means of one of the following two methods:

- By means of *generalisation of Dalton's law* by adding an empirical parameter called the 'convergence pressure'. The value of this convergence pressure is purely empirically determined and depends on the precise composition of the mixture, i.e. the amount of each compound present in the mixture.
- By means of a *Peng-Robinson equation of state* of the mixture, which involves empirical binary interaction coefficients between the compounds.

The reader is referred to [1] for further details.

It is clear from the above that the determination of the aerosol formation for a non-ideal liquid solution requires a massive amount of empiricism, and is therefore not practical for implementation into HGSYSTEM.

However, it is believed that for most practical release scenarios either one of the above cases a and b should enable sufficient accurate dispersion predictions.
Therefore non-ideal liquid solutions will not be taken into account, and *ideal liquid* solutions are assumed in HGSYSTEM.

Implementation of thermodynamic model in HGSYSTEM

The above thermodynamic model is complex and requires a large number of physical properties for each of the compounds. Thus the development of the HGSYSTEM property database program DATAPROP is required, which generates the required pollutant properties to each of the HGSYSTEM models.

See the HGSYSTEM User's Manual chapter on DATAPROP for use of the database program. Technical details of DATAPROP (only useful for expert users) can be found in [2]. In [2] it is also discussed how new compounds can be added to DATAPROP. Users are advised not to change the DATAPROP database without first consulting the HGSYSTEM developers.

Outside the thermodynamic routines within the HGSYSTEM dispersion models, averaged properties are adopted for the pollutant, whereas within the thermodynamic routines properties for each of the individual pollutant compounds are required (specific heats, heat of vaporisation, saturated vapour pressure, etc.).

Outline of this chapter

The outline for the rest of this chapter is as follows.

Paragraph 2.A.2 describes the new theoretical thermodynamics model. A set of thermodynamic equations for the unknown thermodynamic quantities is derived, and the criteria for aerosol formation is defined.

Paragraph 2.A.3 discusses the algorithm for solving these equations for both the general case. the specific case of a series of one-compound aerosols and the specific case of a single two-compound aerosol. It also discusses the implementation of the thermodynamic model into the HGSYSTEM dispersion models.

2.A.2. Thermodynamics model

This paragraph describes the two-phase thermodynamics model for mixing of moist air with a pollutant consisting of a number of ideal non-reactive fluids and water. In case of ground-level dispersion (HEGADAS and HEGABOX but not AEROPLUME)), the model may take into account water-vapour transfer and heat transfer from the substrate to the cloud.

The mixture is assumed to consist of dry air and a number of non-reactive compounds. Each of the compounds may occur both in liquid and vapour phase. Water may consist of liquid water and/or ice.

It is assumed that the liquid in the mixture is composed of a number of non-interacting aerosols and that each compound forms part of not more than one of these aerosols. If an aerosol consists of more than one compound, the aerosol is assumed to be an ideal liquid solution of its constituent compounds.

Paragraph 2.A.2.1 describes the model parameters that are required as input to the thermodynamics model.

Paragraph 2.A.2.2 lists the basic unknown thermodynamic variables in the model and derives the thermodynamic equations for these variables.

In paragraph 2.A.2.3 the criterion is determined for aerosol formation.

2.A.2.1. Model parameters

The model parameters are as follows:

1. Pollutant (original release) data:
   - Mole fraction of pollutant in mixture, y_{pol}.

   - Mole fraction of each compound in the pollutant, η_α ($\alpha = 0,...,N$).
     In addition to possibly dry air and water it is assumed that the pollutant consists of N - 1 compounds ($N > 2$); α = 0, 1 are taken to correspond to dry air and water, respectively.

   - Pollutant enthalpy, H_{pol} (J/kmole).
     Enthalpies are taken to be zero at 0 °C, with unmixed gaseous compounds.
     The pollutant enthalpy H_{pol} can be calculated from the pollutant temperature and the pollutant composition by imposing thermodynamic equilibrium to the initial pollutant state.
     See the end of paragraph 2.A.3.2 and Chapter 7.A, Appendix 7.A.D. for details (HEGADAS and HEGABOX).

The above data uniquely define the amount of pollutant in the mixture, the pollutant composition and the pollutant enthalpy.

2. Ambient data:
   - humidity r_H (-).

- ambient temperature T_a (°C).

The above data uniquely define the composition of the air (mole fractions of dry air and water) and the enthalpy H_{air}^{wet} of the moist air (Joule/kmole of moist air).

3. Substrate data:
   - mole fraction y_{w3} of water vapour added from substrate (-)
   - heat added from the substrate, H_e (J/kmole)
   - substrate temperature T_s (°C)

The data y_{w3} and T_s uniquely define the amount and enthalpy of the water vapour added to the mixture. These parameters only apply to HEGADAS and HEGABOX.

4. Properties of each compound in the mixture.
   Dry air (α=0):
   - molecular weight m^a (kg/kmole)
   - specific heat C_p^a (J/kmole/K)

- Other compounds (α = 1,2,...,N; α = 1 is chosen to correspond to water)
  - molecular weight m^α (kg/kmole)
  - specific heats $C_p^{\alpha v}$, $C_p^{\alpha l}$ (J/kmole/K) for vapour and liquid
  - heat of condensation H^α_{cond} (J/kmole)
  - coefficients in the formula defining the saturated vapour pressure of the compound $P_v^\alpha(T_m)$ as function of the mixture temperature T_m. This (Wagner) equation is given in the description of the GASDATA input block, SPECIES keyword, for each model using the two-phase thermodynamical model.
  - in addition for water only (α = 1): specific heat of ice, C_p^{wi} (J/kmole/K), and heat of fusion, H_{fus}^w (J/kmole)

Furthermore compounds $\alpha = n_{\beta-1}+1, n_{\beta-1}+2, \ldots, n_\beta$ are known to potentially form aerosol β ($\beta = 1, 2, \ldots, M$; $0 = n_0 < n_1 < n_2 < \ldots < n_M = N$). Notice that aerosol $\beta = 1$ includes the liquid water (compound $\alpha = 1$).

The values of specific heats, heats of condensation and fusion are assumed to correspond with values at standard atmospheric pressure (1 atmosphere) and at an appropriately chosen reference temperature. The specific heat values for typical temperatures between -50 °C and 50 °C and pressures 'close' to 1 atmosphere are not expected to differ considerably from these values.

5. Total vapour pressure P.
   This pressure equals the ambient atmospheric pressure, which for a pressurised release equals the pressure immediately following the depressurisation of the pollutant at the point of release.

The above mentioned parameters uniquely define the composition of the mixture (mole fractions y_α ($\alpha = 0, 1, \ldots, N$) and the total enthalpy of the mixture, H_{tot} (J/kmole).

2.A.2.2. Basic thermodynamic unknowns and equations

The unknown thermodynamic variables are as follows:

1. mole fraction $y_{\alpha v}$ of *vapour* for each mixture compound ($\alpha = 1, \ldots, N$) (-)

2. mole fraction $y_{\alpha n}$ of *liquid* for each mixture compound ($\alpha = 1, \ldots, N$) (-)

3. mole fraction liquid L_β of each aerosol ($\beta = 1, \ldots, M$) (-)

4. total mole fraction of liquid, L (-)

5. mixture temperature T_m (°C)

The above unknowns must satisfy the following equations:

1. *Conservation of molar flow for each compound*

$$y_\alpha = y_{\alpha v} + y_{\alpha n} \tag{1}$$

2. *Raoult's law for each compound*

$$y_{\alpha v} = \min\left\{ y_\alpha, \left[\left(\frac{y_{\alpha n} \cdot (1-L)}{L_\beta} \right) \cdot \left(\frac{P_v^\alpha(T_m)}{P} \right) \right] \right\} \tag{2}$$

Application of the above law implies that each aerosol β (β = 1,..,M) is assumed to be an ideal liquid solution of its constituent compounds $\alpha = n_{\beta-1}+1,.., n_\beta$.

Raoult's law states that in the presence of aerosol β, the ratio of the mole fraction $y_{\alpha v}/(1\text{-}L)$ of the compound α in the vapour and the mole fraction $y_{\alpha n}/L_\beta$ of the compound α in the liquid solution β equals the ratio $P_v^\alpha(T_m)/P$ of the saturated vapour pressure of compound α in the vapour and the total vapour pressure.

For a one-compound aerosol ($y_{\alpha n} = L_\beta$; $\alpha = n_\beta = n_{\beta-1} + 1$), Raoult's law reduces to Dalton's law $y_{\alpha v}/(1\text{-}L) = P_{v\alpha}(T_m)/P$.
Thus Dalton's law states that the mole fraction of the compound in the vapour equals the ratio of the partial pressure of compound α in the vapour and the total pressure.

The reader is referred to, for example, [1] for further details of Raoult's and Dalton's laws.

3. *The amount of each aerosol is the sum of its liquid compounds:*

$$L_\beta = \sum_{\alpha=n_{\beta-1}+1}^{n_\beta} y_{\alpha n} \qquad (\beta = 1,\dots, M) \tag{3}$$

4. *The total amount of liquid is the sum of all individual aerosols:*

$$L = \sum_{\beta=1}^{M} L_\beta \tag{4}$$

5. *Conservation of energy:*

$$H_{tot} = \sum_{\alpha=0}^{N} H_\alpha = y_{pol} \cdot H_{pol} + (1 - y_{pol} - y_{w3}) \cdot H_{air}^{wet} + H_e + y_{w3} \cdot C_p^{wv} \cdot T_s \tag{5}$$

where the post-mixing enthalpy of compound α (α = 0, 1,..., N) is given by

$$H_\alpha = y_\alpha \cdot C_p^a \cdot T_m \qquad \text{(dry air, } \alpha = 0)$$

$$\begin{array}{ll} y_{\alpha v} \cdot C_p^{wv} \cdot T_m + y_{\alpha n} \cdot (C_p^{wl} \cdot T_m - H_{cond}^{w}) & \text{(water with } T_m > 0\ °\text{C}, \alpha = 1) \\ y_{\alpha v} \cdot C_p^{wv} \cdot T_m + y_{\alpha n} \cdot (C_p^{wl} \cdot T_m - H_{cond}^{w} - H_{fus}^{w}) & \text{(water with } T_m < 0\ °\text{C}. \alpha = 1) \\ y_{\alpha v} \cdot C_p^{\alpha v} \cdot T_m + y_{\alpha n} \cdot (C_p^{\alpha l} \cdot T_m - H_{cond}^{\alpha}) & (\alpha = 2,\dots,N) \end{array} \tag{6}$$

Dry air corresponds with $\alpha = 0$ and water with $\alpha = 1$.

Equation (5) expresses that the total post-mixing enthalpy H_{tot} equals the sum of the pollutant enthalpy, the enthalpy of the ambient moist air, the heat added from the substrate and the enthalpy of the water-vapour added from the substrate.

2.A.2.3. Criterion for aerosol formation

The thermodynamic equations (1), (2), (3), (4) and (5) are to be solved for the thermodynamic unknowns $y_{\alpha v}$, $y_{\alpha n}$ ($\alpha = 1,\dots, N$), L_β ($\beta=1,\dots, M$), L and T_m.
The unknowns $y_{\alpha v}$ and $y_{\alpha n}$ can be eliminated as unknowns using Equations (1) and (2),

$$y_{\alpha v} = \left\{ 1 + \frac{L_\beta}{1-L} \cdot \frac{P}{P_v^\alpha(T_m)} \right\}^{-1} \cdot y_\alpha \qquad (\alpha = n_{\beta-1}+1,\dots,n_\beta;\ \beta = 1,\dots,M) \tag{7}$$

$$y_{\alpha n} = \left\{ 1 + \frac{1-L}{L_\beta} \cdot \frac{P_v^\alpha(T_m)}{P} \right\}^{-1} \cdot y_\alpha \qquad (\alpha = n_{\beta-1}+1,\dots,n_\beta;\ \beta = 1,\dots,M) \tag{8}$$

Insertion of equation (8) into (3) leads to the equation $F_\beta(L_\beta;L,T_m) = 1$ for L_β, with the function $F_\beta(L_\beta;L,T_m)$ defined by

$$F_\beta(L_\beta;L,T_m) = \sum_{\alpha=n_{\beta-1}+1}^{n_\beta} \left[\frac{y_\alpha \cdot \left(\dfrac{P}{P_v^\alpha(T_m)} \right)}{1 - L + L_\beta \cdot \left(\dfrac{P}{P_v^\alpha(T_m)} \right)} \right] \tag{9}$$

The function $F_\beta(L_\beta;L,T_m)$ monotonously decreases with increasing values of L_β. Aerosol formation requires that the equation $F_\beta(L_\beta;L,T_m) = 1$ has a positive root L_β. Thus the criterion for formation of aerosol β is $F_\beta(0;L,T_m) > 1$, or equivalently,

$$S[\beta;T_m] \overset{\text{def}}{=} 1 - \sum_{\alpha=n_{\beta-1}+1}^{n_\beta} \left[y_\alpha \left(\frac{P}{P_v^\alpha(T_m)} \right) \right] < L \Leftrightarrow L_\beta > 0 \qquad (\beta = 1,\dots,M) \tag{10}$$

If the above condition $S[\beta;T_m] < L$ is satisfied, the equation $F_\beta(L_\beta;L,T_m) = 1$ has precisely one positive root L_β.

Note that according to formula (9), multiplication of the equation $F_\beta(L_\beta;L,T_m) = 1$ with each denominator $[1-L+L_\beta \cdot P/P_v^\alpha(T_m)]$, $\alpha = n_{\beta-1}+1,.., n_\beta$ leads to a polynomial equation for L_β of the order $(n_\beta - n_{\beta-1})$.

This equation can be solved analytically for $n_\beta - n_{\beta-1} = 1, 2$ and 3.

For higher orders equation (9) can be solved, without transformation to a polynomial, using the non-linear algebraic equations solver NAESOL [3]. This is used in the AEROPLUME and SPILL implementation of the aerosol model.

Thus the overall equation for L_β ($\beta = 1,..., M$) is given by

$$\begin{aligned} &F_\beta(L_\beta;L,T_m) = 1, \quad && \text{if } S[\beta;T_m] < L \quad && (L_\beta > 0;\ \text{aerosol formation}) \\ &L_\beta = 0 && \text{if } S[\beta;T_m] \geq L && (\text{no aerosol formation}) \end{aligned} \qquad (11)$$

The thermodynamic equations (7), (8), (11), (4) and (5) are to be solved for the thermodynamic unknowns $y_{\alpha v}$, $y_{\alpha n}$ ($\alpha = 1,..., N$), L_β ($\beta = 1,..., M$), L and T_m.

Elimination of $y_{\alpha v}$ and $y_{\alpha n}$ ($\alpha = 1,..., N$) using equations (7) and (8) leads to the reduced set of equations (11), (4)and (5) for L_β ($\beta = 1,..., M$), L and T_m.

2.A.3. Solution algorithm

This paragraph describes the solution algorithm with which the thermodynamic equations described in paragraph 2.A.2 are solved.

Paragraph 2.A.3.1 contains the solution algorithm for the general problem, paragraph 2.A.3.2 discusses the solution algorithm for the specific case of separate one-compound aerosols (absence of multi-compound aerosols), whereas paragraph 2.A.3.3 discusses the solution algorithm for the specific case of a single two-compound aerosol. Paragraph 2.A.3.4 discusses the implementation of the thermodynamics solution algorithm into the dispersion model.

2.A.3.1. General problem

This paragraph describes the algorithm for solving the equations (7), (8), (11), (4) and (5) for the thermodynamic unknowns $y_{\alpha v}$, $y_{\alpha n}$ ($\alpha = 1,..., N$), L_β ($\beta = 1,..., M$), L and T_m.

It is this *general algorithm* which is used in AEROPLUME and SPILL. Note that HEGADAS and HEGABOX use less general algorithms as discussed below (paragraphs 2.A.3.2 and 2.A.3.3).

For details on how AEROPLUME uses the thermodynamical model, see Chapter 5.A., paragraphs 5.A.3 and 5.A.7. The SPILL implementation of the aerosol model is identical to the AEROPLUME one (only slightly more dry air is added for numerical reasons).

The algorithm below is formulated in terms of four convergence control parameters, these are

- the absolute convergence tolerance ε_T for the mixture temperature T_m,
- the absolute convergence tolerance ε_L for the liquid fraction L,
- the maximum number i_{max} of outer iteration steps for T_m,
- the maximum number k_{max} of inner-most iteration steps for L.

The subsequent steps in the thermodynamic routine are as follows:

1. Assume that no fog forms: set $y_{\alpha n} = 0$, $y_{\alpha v} = y_\alpha$ ($\alpha = 1,\dots, N$), $L_\beta = 0$ ($\beta = 1,\dots,M$), $L = 0$ and determine T_m from equation (5).

2. Initialise the outer iteration loop for evaluation of T_m (i is number of iterations, T_m^i is estimate of T_m after i iterations): $i = 0$, $T_m^i = T_m$.

3. Carry out the next outer iteration step i+1 for the temperature T_m:

   a) Order $S[\beta;T_m^i]$ in ascending order ($\beta = 1,\dots,M$): $S[\beta_1;T_m^i] < S[\beta_2;T_m^i] < \dots < S[\beta_M;T_m^i]$. According to equation (11) aerosol β_j can only be present if the aerosols $\beta_1,\dots, \beta_{j-1}$ are also present ($j = 1,\dots,M$). Thus aerosol β_1 forms 'first' and aerosol β_M forms 'last'.

   b) Initialise inner iteration loop for evaluation of L [aerosols β_1, β_2, .., β_j have been established to be present at temperature T_m^i, and L_j is the value for L assuming the presence of aerosols $\beta_1,\dots, \beta_j$ only]: $j = 0$, $L_j = 0$.

   c) Establish if aerosol β_{j+1} is present by carrying out the next inner iteration j+1 for the liquid fraction L:

      1. If $S[\beta_{j+1};T_m^i] > L_j$, than according to equation (11) aerosols $\beta_{j+1},\dots, \beta_M$ do *not* form at temperature T_m^i ($L_\beta = 0$ for $\beta = \beta_{j+1},\dots, \beta_M$): set $L = L_j$ and go to Step d)

2. If $S[\beta_{j-1};T_m']$ < L_j, than according to equation (11) aerosol β_{j+1} *does* form at temperature T_m'; calculate the aerosol formation (L_{j+1}, β_1,..., β_{j-1}) assuming the presence of aerosols β_1,..., β_{j+1} only:

   (a) Initialise the inner-most iteration loop: $k = 0, L^k = L_j, L = L^k$.

   (b) $k = k+1$; set L_β for $\beta = \beta_1,..., \beta_{j+1}$ from $F_\beta(L_\beta;L,T_m')=1$, which using equation (9) can be transformed into a polynomial equation in L_β of order (n_β-$n_{\beta-1}$).
   In the general case this equation need not be transformed, but can be solved directly using the NAESOL solver [3]. This method is followed in SPILL and AEROPLUME.

   (c) Set L from L_β ($\beta = \beta_1,..,\beta_{j+1}$) using equation (4), $L^k = L$.

   (d) Check for convergence (three cases):

   - If $k < k_{max}$ and $|L^k - L^{k-1}| > \varepsilon_L$ (no convergence): go to (b) (carry out next inner-most iteration for L).

   - If $k = k_{max}$ and $|L^k - L^{k-1}| > \varepsilon_L$ (no convergence within maximum number of inner-most iterations): stop thermodynamic calculations and produce error message.

   - If $|L^k - L^{k-1}| < \varepsilon_L$ (convergence): $j = j+1, L_j = L^k, L = L_j$.

   (e) If $j < M$ establish if aerosol β_{j+1} is present: go to start of Step c).

d) Set $y_{\alpha v}$, $y_{\alpha n}$ from L_β ($\beta = 1,..,M$), L, T_m^i using Equations (7) and (8).

e) Set T_m from $y_{\alpha v}$, $y_{\alpha n}$ using equation (5); $i = i+1$; $T_m^i = T_m$.

f) Check for convergence of temperature T_m (three cases):

- If $i < i_{max}$ and $|T_m^i - T_m^{i-1}| > \varepsilon_T$ (no convergence): go to Step a) (carry out next iteration for temperature).

- If $|T_m^i - T_m^{i-1}| < \varepsilon_T$ (convergence): *end of thermodynamic calculations.*

- If $i = i_{max}$ and $|T_m{}' - T_m{}^{i-1}| > \varepsilon_T$ (no convergence within i_{max} iterations), and if assuming $T_m < 0$ °C, equation (5) leads to $T_m > 0$ °C and if assuming $T_m > 0$ °C, equation (5) leads to $T_m < 0$ °C, than ice is partially melted. Set for this case $T_m = 0$ °C and set L, $y_{\alpha v}$, $y_{\alpha n}$ ($\alpha = 1,\ldots, N$) as described in Steps a), b), c) and d): *end of thermodynamic calculations*.

2.A.3.2. Case of separate one-compound aerosols

In this paragraph the special case is considered for the mixture consisting of *non-interacting one-compound aerosols* (individual droplets).

This case is available in HEGADAS and HEGABOX. AEROPLUME and SPILL use the general case as described in paragraph 2.A.3.1.

Following the notation of paragraph 2.A.2, $M = N$, $L_\alpha = y_{\alpha n}$ ($\alpha = 1,\ldots, N$), $n_\beta = \beta$ ($\beta = 1,\ldots, N$). Furthermore Raoult's law given by equation (2) reduces to Dalton's law,

$$y_{\alpha v} = \min\left\{ y_\alpha, (1-L)\cdot\frac{P_v^\alpha(T_m)}{P} \right\} \qquad (\alpha = 1,\ldots,N) \qquad (12)$$

and it follows from Equations (1), (12) and (4) that the total mole fraction of aerosol can be expressed by

$$L = 1 - \frac{A}{(1-B)} \qquad (13)$$

where A is the total mole fraction in the *mixture* of those compounds for which an aerosol does not form ($y_{\alpha n} = 0$), and where B is total mole fraction in the *vapour* of those compounds for which an aerosol does form ($y_{\alpha n} > 0$),

$$A = y_0 + \sum_{\alpha=1,\ldots,N;\, y_{\alpha n}=0} y_\alpha$$

$$B = \sum_{\alpha=1,\ldots,N;\, y_{\alpha n}>0} \frac{P_v^\alpha(T_m)}{P} \qquad (14)$$

Solution to Thermodynamic Equations

The equations (1), (12), (13) and (5) for $y_{\alpha v}$, $y_{\alpha n}$ ($\alpha = 1,\ldots, N$), L, T_m are solved by means of the following algorithmic steps in the thermodynamic routine (ε_T = convergence tolerance for mixture temperature T_m, i_{max} = maximum number of iterations for T_m):

1. Assume that no fog forms: set $y_{\alpha n} = 0$, $y_{\alpha v} = y_\alpha$ ($\alpha = 1,\dots, N$), $L = 0$ and determine T_m from equation (5).

2. Initialise the outer iteration loop for evaluation of T_m (i is number of iterations, T_m^i is estimate of T_m after i iterations): $i = 0$, $T_m^i = T_m$.

3. Carry out the next outer iteration i+1 for the temperature T_m:

   a) Order $S[\alpha;T_m^i] = 1 - y_\alpha \cdot P/P_v^\alpha(T_m^i)$ in ascending order ($\alpha = 1,\dots,N$): $S[\alpha_1;T_m^i] < S[\alpha_2;T_m^i] < \dots < S[\alpha_N;T_m^i]$.
   Note from equation (10) that aerosols 'first' form for compound α_1 and 'last' form for compound α_N.

   b) Initialise the inner iteration loop for evaluation of L [aerosols for compounds $\alpha_1,\dots,\alpha_j$ do form at temperature T_m^i.
   L_j, A and B are the values for L, A and B from Equations (13) and (14) assuming the presence of aerosols for compounds $\alpha_1,\dots,\alpha_j$ only]: $j = 0$, $L_j = 0$, $A = 1$, $B = 0$.

   c) Establish if aerosol α_{j+1} is present at temperature T_m^i by carrying out the next inner iteration j+1 for the liquid fraction L:

      1. If $S[\alpha_{j+1};T_m^i] > L_j$ than aerosols for compounds $\alpha_{j+1},\dots,\alpha_N$ do *not* form ($y_{\alpha n} = 0$ for $\alpha = \alpha_{j+1},\dots, \alpha_N$): set $L = L$ and go to Step d).

      2. If $S[\alpha_{j+1};T_m^i] < L_j$, than aerosol for compound α_{j+1} *does* form:

         - increment j: $j = j+1$, $A = A - y_{\alpha j}$, $B = B + P_v^{\alpha j}(T_m^i)/P$, $L_j = 1 - A/(1 - B)$, $L = L_j$

         - if $j < N$ carry out next iteration: go to Step c).

   d) Set $y_{\alpha v}$, $y_{\alpha n}$ ($\alpha = 1,\dots,N$) from L and T_m^i using Equations (1) and (12)

   e) Set T_m from $y_{\alpha v}$, $y_{\alpha n}$, L using equation (5); $i = i+1$; $T_m^i = T_m$

   f) Check for convergence of temperature T_m (three cases):

   - If $i < i_{max}$ and $|T_m^i - T_m^{i-1}| > \varepsilon_T$ (no convergence): go to Step a) (carry out next iteration for temperature).

- If $|T_m^{i} - T_m^{i-1}| < \varepsilon_T$ (convergence): *end of thermodynamic calculations.*

- If $i = i_{max}$ and $|T_m^{i} - T_m^{i-1}| > \varepsilon_T$ (no convergence within i_{max} iterations), and if assuming $T_m < 0$ °C equation (5) leads to $T_m > 0$ °C and if assuming $T_m > 0$ °C equation (5) leads to $T_m < 0$ °C , than ice is partially melted. Set for this case $T_m = 0$ °C and set L, $y_{\alpha v}$, $y_{\alpha n}$ ($\alpha = 1,\ldots,N$) as described in Steps a), b), c), and d): *end of thermodynamic calculations.*

Order of Aerosol Formation During Mixture Cooling

Assume that during temperature cooling of a mixture with given constant composition y_0, $y_1,\ldots, y_N$ ($\alpha = 0$ corresponds to dry air) aerosols for compounds $\alpha = 1,.., N$ form successively at the temperatures $T_1, T_2,.., T_N$ (with $T_1 > T_2 > .. > T_N$).
Thus compound 1 condenses first and compound N condenses last.

Consider a temperature T with $T_{j-1} > T > T_j$ ($j = 2,..,N$), i.e. aerosols $\alpha = 1,..,j-1$ are present and compounds $\alpha = j,..,N$ occur in vapour phase only. Following Equations (13) and (14), L is given by

$$L = 1 - \frac{\left\{1 - \sum_{\alpha=1}^{j-1} y_\alpha\right\}}{\left\{1 - \sum_{\alpha=1}^{j-1} \frac{P_v^\alpha(T)}{P}\right\}} \qquad T_{j-1} > T > T_j \qquad (15)$$

At the temperature T_j onset of formation of aerosol j starts.

Thus following equation (10), $S[j;T_j] = 1 - y_j \cdot P/P_v^j(T_j) = L$, or equivalently, using the above equation (15),

$$y_j \cdot \left\{1 - \sum_{\alpha=1}^{j-1} \frac{P_v^\alpha(T)}{P}\right\} = \left(\frac{P_v^j(T)}{P}\right) \cdot \left\{1 - \sum_{\alpha=1}^{j-1} y_\alpha\right\} \qquad (16)$$

Above equation (16) defines the temperature T_j at which aerosol j forms.

Note that for j=1, this equation reduces to Dalton's law $y_1 = P_v^1(T_1)/P$, defining the onset of condensation of the first compound within the mixture (formation of first aerosol).

For j = N with absence of air ($y_0 = 0$), equation (16) reduces to

$$\sum_{\alpha=1}^{N} \frac{P_v^{\alpha}(T)}{P} = 1 \qquad \text{(for } y_0 = 0\text{, no dry air)} \qquad (17)$$

defining the onset of condensation of the last compound within the mixture.

The temperature T will stay equal to the temperature T_N until all vapour has been condensed (L = 1). For temperature $T < T_N$, the mixture will be pure liquid.

Initial Pollutant State

Applying the above discussion to the initial pollutant (prior to mixing), it follows from equation (17) and (14) that B = 1 in the expression (13) for the liquid fraction L at the temperature T_N.

Thus the thermodynamic problem is ill conditioned if all compounds do occur in two phases. To avoid associated numerical problems 0.01% of dry air is added to the initial pollutant in order to force the presence of at least one compound in the pure vapour phase.
This holds for the general version of the algorithm (paragraph 2.A.3.1) as well. Dry air is added in all HGSYSTEM modules using the aerosol thermodynamical model. In SPILL 0.1% dry air is added for numerical reasons.

For HEGADAS and HEGABOX, input to the thermodynamic model is either the temperature T_{pol} or the enthalpy H_{pol} of the pollutant prior to mixing with the air. If $T_{pol} \approx T_N$ the user is advised not to prescribe T_{pol} but H_{pol}.
The calculation of H_{pol} should be based on equation (6) using the known value of T_{pol} and the amount of liquid present for each pollutant compound.
The latter liquid fractions could be derived either from flash calculations or by imposing thermodynamic equilibrium to the initial pollutant state (i.e. by imposing equations (1-5), with $y_{pol} = 1$, $H_e = 0$, $y_{w3} = 0$).

Note that for AEROPLUME and SPILL, the user does not have to give this input to the thermodynamical model as the data is calculated by the model from reservoir (or stack) conditions as given by the user.

For a pollutant consisting of a single compound (N = 1) the above situation arises if the temperature of the pollutant equals the boiling temperature of the pollutant. Thus in this case the user needs to know the amount of liquid fraction in the pollutant, in order to evaluate the pollutant enthalpy.

2.A.3.3. Case of single two-compound aerosol

In this paragraph the special case is considered of the mixture consisting of *one two-compound aerosol* (ideal solution; compounds $\alpha = 1, 2$). All other compounds occur in vapour phase only (compounds $\alpha = 3,..,N$).
Thus following the notation of paragraph 2.A.3.2.: $M = 1$, $L_1 = L$, $n_1 = 2$, $y_{\alpha n}=0$ ($\alpha=3,..,N$), $y_{\alpha v}=y_\alpha$ ($\alpha = 3,..,N$).

This case is available in HEGADAS and HEGABOX. Note that SPILL and AEROPLUME have the general case available as discussed in paragraph 2.A.3.1.

The 6 remaining unknowns to be evaluated are $y_{\alpha v}$, $y_{\alpha n}$ ($\alpha = 1,2$), L and T_m.

The 6 governing equations for these unknowns are equations (7), (8), (11) and (5). Using formula (9), equation (11) can be rewritten as a square equation for L,

$$q_1 q_2 L^2 - (r_1 q_2 + r_2 q_1)L - (1 + r_1 + r_2) = 0 \tag{18}$$

where the auxiliary parameters q_α, r_α ($\alpha = 1,2$) are given by

$$q_\alpha(T_m) = \left(\frac{P}{P_v^\alpha(T_m)}\right) - 1$$

(19)

$$r_\alpha(T_m) = y_\alpha \cdot \left(\frac{P}{P_v^\alpha(T_m)}\right) - 1$$

where $-1 < r_\alpha \le q_\alpha$.

The root to equation (18) satisfying $L \rightarrow y_1+y_2$ for $P_v^\alpha(T_m) \rightarrow 0$ (i.e. compounds $\alpha = 1,2$ are 100% liquid for very low temperatures), equals

$$L = \frac{\left([r_1 q_2 + r_2 q_1] + \{[r_1 q_2 + r_2 q_1]^2 + 4[q_1 q_2][1 + r_1 + r_2]\}^{1/2}\right)}{[2 q_1 q_2]}$$

or, written alternatively (20)

$$L = \frac{2[1 + r_1 + r_2]}{\left(-[r_1 q_2 + r_2 q_1] + \{[r_1 q_2 + r_2 q_1]^2 + 4[q_1 q_2][1 + r_1 + r_2]\}^{1/2}\right)}$$

Solution to Thermodynamic Equations

The equations (7), (8), (20) and (5) for $y_{\alpha v}$, $y_{\alpha n}$ ($\alpha = 1,2,\ldots,N$), L, T_m are solved by means of the following algorithmic steps in the thermodynamic routine (ε_T = convergence tolerance for mixture temperature T_m, i_{max} is maximum number of iterations for T_m):

1. Assume that no fog forms: set $y_{\alpha n} = 0$, $y_{\alpha v} = y_\alpha$ ($\alpha = 1,\ldots,N$), $L = 0$ and determine T_m from equation (5).
   If $[1+r_1+r_2] < 0$ (aerosol does not form): *end of thermodynamic calculations.*

2. Initialise the iteration loop for the evaluation of T_m (i is number of iterations, T_m^i is estimate of T_m after i iterations): $i = 0$, $T_m^i = T_m$.

3. Carry out the iteration loop for the temperature T_m:

   a. Set $L = L(T_m^i)$ from equation (20). Set $y_{\alpha v}$, $y_{\alpha n}$ ($\alpha = 1,2$) from Equations (7) and (8).

   b. Set T_m from $y_{\alpha v}$, $y_{\alpha n}$, L using equation (5); $i = i+1$; $T_m^i = T_m$.

   c. Check for convergence of temperature T_m (three cases):

      - If $i < i_{max}$ and $|T_m^i - T_m^{i-1}| > \varepsilon_T$ (no convergence): go to Step a. (carry out next iteration for temperature).

      - If $|T_m^i - T_m^{i-1}| < \varepsilon_T$ (convergence): *end of thermodynamic calculations.*

      - If $i = i_{max}$ and $|T_m^i - T_m^{i-1}| > \varepsilon_T$ (no convergence within i_{max} iterations), and if assuming $T_m < 0$ °C, equation (5) leads to $T_m > 0$ °C and if assuming $T_m > 0$ °C, equation (5) leads to $T_m < 0$ °C, than ice is partially melted. Set for this case $T_m = 0$ °C and set L, $y_{\alpha v}$, $y_{\alpha n}$ ($\alpha = 1,\ldots,N$) as described in Step a.

2.A.3.4. Implementation of thermodynamics into dispersion model

This paragraph discusses the implementation of the thermodynamics solution algorithm into the HGSYSTEM dispersion models.

Paragraph 2.A.2.1 outlined the parameters required as input to the thermodynamic model. These input parameters are obtained as follows:

1. User-specified parameters.

The user is required to input to the dispersion model:

- the pollutant composition (mole fractions η_α, $\alpha = 1,\ldots,N$)
- pollutant temperature T_{pol} or alternatively, pollutant enthalpy H_{pol} *(only for HEGADAS and HEGABOX)*
- ambient humidity r_H, ambient temperature T_a, ambient pressure P
- ground temperature T_s *(only for HEGADAS and HEGABOX)*.

For model-specific information on input parameters, see the relevant chapter in the HGSYSTEM User's Manual.

2. Properties generated by the property database program DATAPROP.

Based on the user-specified pollutant composition, the physical property database program DATAPROP is used to calculate the required pollutant properties. See DATAPROP chapter in the HGSYSTEM User's Manual for more information on how to use DATAPROP.

3. Solution parameters generated by dispersion program.

The pollutant molar fraction y_{pol}, the heat H_c and the water vapour y_{w3} added from the substrate are a function of downwind distance and are generated by the dispersion model as input to the thermodynamic routine. The latter two apply only to HEGADAS and HEGABOX.

These variables are calculated internally by the dispersion model by solving ordinary differential equations in the downwind direction, i.e. by solving empirical entrainment, heat-transfer and water-vapour transfer equations.

For details on how AEROPLUME uses the thermodynamical model, see Chapter 5.A., paragraphs 5.A.3 and 5.A.7.

In the HEGADAS and HEGABOX dispersion model the thermodynamics model is required to evaluate from the above input parameters the mixture temperature T_m (°C), the mixture volume V_m (m^3/kmole) and the mixture density ρ_m (kg/m^3). V_m and ρ_m are set as follows

$$V_m = \left(R \cdot \frac{(T_m + 273.15)}{P}\right) \cdot (1 - L)$$

$$\rho_m = \frac{1}{V_m} \cdot \sum_{\alpha=0}^{N} (m^\alpha \cdot y_\alpha) \qquad (21)$$

where R is the universal gas constant.

2.A.4. References

1. McCain, W.D., '*The properties of petroleum fluids*', 2nd Edition, Penwell Publishing Company, Tulsa, Oklahoma, 1990.

2. Witlox, H.W.M., '*Two-phase thermodynamic model for mixing of a non-reactive multi-component pollutant with moist air*', Shell Research Limited, Thornton Research Centre, TNER.93.022, 1993.

3. Scales, L.E., '*NAESOL - A Software toolkit for the solution of nonlinear algebraic equation systems; User Guide - Version 1.5*', Shell Research Limited, Thornton Research Centre, TRCP.3661R, 1994.

2.A.5. Notation

C_p^α	specific heat at constant pressure of compound α (J/kmole/K)
	- compound a = 0 (dry air): C_p^a
	- compound a = 1 (water): liquid, C_p^{wl}, vapour, C_p^{wv}
	- compounds a = 2,..,N: liquid, $C_p^{\alpha l}$, vapour $C_p^{\alpha v}$
$F_\beta(L_\beta;L,T_m)$	function defined by equation (9)
H^w_{cond}	heat of condensation of water (J/kmole)
H^α_{cond}	heat of condensation of compound (J/kmole)
H_e	heat added from the substrate (J/kmole)
H^w_{fus}	heat of fusion of water (J/kmole)
H_{pol}	pollutant enthalpy (J/kmole)
H_{tot}	total mixture enthalpy (J/kmole)
H^{wet}_{air}	enthalpy of moist air (J/kmole)
H_α	enthalpy of compound α after mixing of pollutant/moist air (J/kmole)
L	mole fraction of liquid in mixture (-)
L_β	mole fraction of liquid compound β in mixture (-)
P	total pressure (atm)
$P_v^\alpha(T_m)$	saturated vapour pressure of compound α at temperature T_m (°C) (atm)
R	universal gas constant (= 0.082057 atm·m^3/kmole/K)
r_H	relative humidity of the ambient air (-)
$S(\beta;T_m)$	function defined by equation (10)
T	temperature (K)
T_a	ambient temperature (°C)
T_m	mixture temperature (°C)
T_{pol}	pollutant temperature (°C)

y_{pol}	mole fraction of pollutant in mixture (-)
y_{α}	mole fraction of compound α in mixture (-)
$y_{\alpha n}$	mole fraction of liquid (non-vapour) phase of compound α in mixture (-)
$y_{\alpha v}$	mole fraction of vapour phase of compound α in mixture (-)
η_{α}	mole fraction of compound α in (released, original) pollutant (-)

2.B. THE HYDROGEN FLUORIDE MODEL

2.B.1. Introduction

The HGSYSTEM software package consists of a number of programs capable of modelling the release and dispersion of hydrogen fluoride (HF). The thermodynamics and chemistry adopted in these programs to describe the mixing of air with HF is based on a model developed by Schotte [1,2]. This Schotte model assumes the pollutant to be 100% HF.
The thermodynamics and chemistry for HF is complex because of formation of HF polymers, de-polymerisation of the gas to the monomer state HF (endothermic reaction), and exothermic reaction of HF with water vapour.

In accidental HF releases, the released pollutant is often *not* 100% pure HF, but may also consist of water and/or a mixture of hydrocarbons.

This chapter 2.B describes a thermodynamics and chemistry model for mixing of moist air with a pollutant consisting not only of HF, but also possibly water and possibly an additional mixture of non-reactive chemicals. This additional inert mixture will be indicated by 'N-gas'. N-gas is assumed to be in a pure vapour phase and is considered to be an ideal gas with known specific heat and molecular weight; it may be, for example, nitrogen, air, hydrocarbon or a mixture of ideal gases.

Following *mixing* of the *pollutant* with *moist air* a mixture forms at any downwind cross-section, consisting of the following mixture components:

- A vapour mixture, consisting of HF monomer (HF), HF dimer $(HF)_2$, HF hexamer $(HF)_6$, HF octamer $(HF)_8$, $HF{\bullet}H_2O$ complex, water, N-gas and air.

- An aqueous HF fog, that is, a liquid fog consisting of water and HF monomer.

Although the model described in this chapter was formulated for a pollutant containing HF, it can also be used to simulate the thermodynamics of a mixture of wet gas (ideal gas, water) and moist air (water, dry air).

The thermodynamical model does not include the effects of ambient fog, rain or snow. Neither does it take deposition of liquid fog from the cloud into account.

2.B.2. Thermodynamics model

This paragraph describes the thermodynamics and chemistry model for the mixing of moist air with a pollutant consisting of HF, water and N-gas. A set of thermodynamic equations for the unknown thermodynamic quantities is derived.

2.B.2.1. Model Parameters

In the thermodynamic model the following data are assumed to be known quantities (input):

1. The mixture composition defined by

   - Pollutant mole fraction, y_{pol} (mole/mole of mixture)
   - Water in pollutant, η_w (mole/mole of pollutant)
   - N-gas in pollutant, η_N (mole/mole of pollutant)
   - Relative ambient humidity, r_H (fraction; $0 \leq r_H \leq 1$)
   - Ambient temperature, T_a (°C)

   The mole fractions y_{pol}, η_w, η_N are defined to be *equivalent* mole fractions based on *all* HF being in the monomer state.
   The ambient data r_H, T_a are needed to determine the enthalpy of the air and the mole fraction of water in the air.
   The parameters y_{pol}, η_w, η_N, r_H, T_a uniquely define the equivalent *molar flows* M_{HF}, M_w, M_N, M_a of HF, water, N-gas and dry air respectively.
   Without loss of generality, M_{tot} ($M_{tot} = M_{HF} + M_w + M_N + M_a$) is taken to be equal to 1.

2. Pollutant enthalpy, H_{pol} (Joule/kmole of pollutant)

3. Heat added from the substrate, H_e (Joule/kmole of mixture)
   Heat transfer from the substrate to the dispersing cloud can be caused by both natural convection and forced convection.

4. Specific heat C_p^N (J/kmole/K) of N-gas

2.B.2.2. Thermodynamic unknowns and equations

The thermodynamic state after the mixing of pollutant with moist air is defined by the following unknown quantities (output):

- Molar fractions of HF-monomer, HF-dimer, HF-hexamer, HF-octamer, HF-complex, water, N-gas, air in vapour mixture (y_{11}, y_{12}, y_{16}, y_{18}, y_c, y_w, y_N, y_a) and molar flow of vapour (M_{vap}; kmole/s): 9 unknowns
- Molar fraction HF in liquid H_2O/HF fog (denoted by x, dimensionless) and molar flow of fog (denoted by L; kmole/s): 2 unknowns (unknowns in presence of fog only)
- Mixture temperature T_m (°C)

The above unknowns must satisfy the following equations:

1. *Conservation of equivalent molar flow* for HF, water, N-gas and dry air (equivalent molar flow before mixing = equivalent molar flow after mixing):

$$M_{HF} = (y_{11} + 2y_{12} + 6y_{16} + 8y_{18} + y_c)\cdot M_{vap} + x\cdot L \quad (1)$$

$$M_w = (y_w + y_c)\cdot M_{vap} + (1 - x)\cdot L \quad (2)$$

$$M_N = y_N\cdot M_{vap} \quad (3)$$

$$M_a = y_a\cdot M_{vap} \quad (4)$$

2. *Sum of molar fractions* of all components in vapour mixture must be 1:

$$y_{11} + y_{12} + y_{16} + y_{18} + y_c + y_w + y_N + y_a = 1 \quad (5)$$

3. *Peng-Robinson equations* of state for HF dimer, HF hexamer, HF octamer, and HF•H_2O complex (see [2])

$$y_{12}(f_1,T_m) = K_2(T_m)\cdot(f_1)^2/(\Phi_1\cdot P) \quad (6)$$

$$y_{16}(f_1,T_m) = K_6(T_m)\cdot(f_1)^6/(\Phi_1\cdot P) \quad (7)$$

$$y_{18}(f_1,T_m) = K_8(T_m)\cdot(f_1)^8/(\Phi_1\cdot P) \quad (8)$$

$$y_c(f_1,y_w,T_m) = K_c(T_m)\cdot f_1\cdot P_{wt}/(\Phi_1\cdot P) \quad (9)$$

where the fugacity $f_1 = \Phi \cdot y_{11} \cdot P$ (in atm), the (dimensionless) fugacity coefficient $\Phi_1 \approx 1$, the total (ambient) vapour pressure P is taken to be 1 atm and $P_{wt} = y_w \cdot P$ is the true partial pressure (excluding $HF \bullet H_2O$ complex) of water in the vapour.

$K_2(T_m)$, $K_6(T_m)$, $K_8(T_m)$, $K_c(T_m)$ are equilibrium constants associated with the reactions for the formation of $(HF)_2$, $(HF)_6$, $(HF)_8$, $HF \bullet H_2O$, respectively, and are defined as function of the temperature T_m by Schotte [2]. See paragraph 2.B.6 for the functional shape of these constants.

4. In the presence of liquid fog (L > 0), the partial vapour pressures of HF (including $HF \bullet H_2O$ complex) and water (including $HF \bullet H_2O$ complex) are set as a function of x and T_m from empirical expressions $p_w(x,T_m)$, $p_{HF}(x,T_m)$ given by equations (1) and (2) in Schotte [2]. These expressions consist of different formulae for x < 0.4738 and x > 0.4738. In the HEGADAS formulation these expressions are smoothed (identical to the smoothing carried out in the program HFPLUME) to arrive at functions $p_w(x,T)$, $p_{HF}(x,T)$ which are everywhere continuous and differentiable. See [3], figure 1 for these curves at 26 °C.

In the *absence* of fog and with all HF assumed to be HF monomer, the partial pressures of the water and HF are given by $(M_w/M_{tot}) \cdot P$ and $(M_{HF}/M_{tot}) \cdot P$, respectively.

In the *presence* of fog, the amounts of HF and water in the vapour are smaller than in the absence of fog, and the partial vapour pressures must also be correspondingly smaller. Thus the following equations apply in the presence of liquid fog (L > 0):

$$y_w + y_c = P_w/P = \min\left\{\frac{p_w(x,T_m)}{P}, \frac{M_w}{M_{tot}}\right\} \tag{10}$$

$$y_{11} + y_{12} + y_{16} + y_{18} + y_c = P_{HF}/P = \min\left\{\frac{p_{HF}(x,T_m)}{P}, \frac{M_{HF}}{M_{tot}}\right\} \tag{11}$$

5. *Conservation of energy*: the total enthalpy H_{tot} following mixing of the pollutant with the moist ambient air, equals the sum of the enthalpy of the pollutant, the enthalpy of the moist air and the heat H_e added from the substrate

$$H_{tot} = H_{HF} + H_w + H_N + H_a = y_{pol} \cdot H_{pol} + (1 - y_{pol}) \cdot H_{air}^{wet} + H_e \tag{12}$$

where the post-mixing enthalpies of HF (including water in fog and HF in $HF \bullet H_2O$), water (excluding fog; including water in $HF \bullet H_2O$), N-gas, and air are given by

$$H_{HF} = \text{TERM1} - \text{TERM2}$$

with

$$\text{TERM1} = [M_{HF} - x \cdot L] \cdot \{H^{\Delta HF} + C_p^{HFV} \cdot (T_m - T^*)\} - x \cdot L \cdot \{H^{HF}_{cond} + H_{mix}\} \qquad (13a)$$

$$\text{TERM2} = (1 - x) \cdot L \cdot H^{w}_{cond} - L \cdot C_p^{fog}(x, T_m) \cdot (T_m - T^*)$$

$$H_w = [M_w - (1 - x) \cdot L]\, C_p^{wv}\, (T_m - T^*) \qquad (13b)$$

$$H_N = M_N \cdot C_p^N \cdot (T_m - T^*) \qquad (13c)$$

$$H_a = M_a \cdot C_p^a \cdot (T_m - T^*) \qquad (13d)$$

with H^{HF}_{cond}, H^{w}_{cond} the heats of condensation of HF and water, H_{mix} the heat of mixing liquid HF with liquid water, $C_p^{HFV}, C_p^{fog}, C_p^{wv}, C_p^N, C_p^a$ the specific heats of HF-vapour, fog, water-vapour, N-gas and air, respectively.

In the equations above, it is assumed that the enthalpy is zero at the reference temperature T^* with unmixed gaseous components (HF, water, N-gas, air) and all HF in the monomer state; H^{HF}_{cond}, H^{w}_{cond} and H_{mix} are taken at T^*. Following Schotte [2], $T^* = 25$ °C is taken.

In equation (13a), the enthalpy departure $H^{\Delta HF}$ of the HF vapour from the ideal monomeric gas at the final temperature T_m, is given by

$$H^{\Delta HF} = \frac{y_{12} \cdot \Delta H_2 + y_{16} \cdot \Delta H_6 + y_{18} \cdot \Delta H_8 + y_c \cdot \Delta H_c}{y_{11} + 2y_{12} + 6y_{16} + 8y_{18} + y_c} \qquad (14)$$

where ΔH_2, ΔH_6, ΔH_8 and ΔH_c are the enthalpies of association of HF-dimer, hexamer, octamer and complex, respectively (Joule/kmole) at the reference temperature T^*.

2.B.2.3. Enthalpy of Air

In equation (12), the enthalpy H^{wet}_{air} of the moist air (Joule/kmole of moist air) is given by

$$H^{wet}_{air} = [1 - P^{amb}_w/P] \cdot C_p^a \cdot (T_a - T^*) + [P^{amb}_w/P] \cdot C_p^{wv} \cdot (T_a - T^*) \qquad (15)$$

with P^{amb}_w the partial vapour pressure of water in the air and with P the total atmospheric pressure (P is always 1 atm in HEGADAS, but can be user-specified in HFPLUME. For consistency of the thermodynamical description, P should be taken (almost equal to) 1 atm).

$P^{amb}_w = r_H \cdot P_V^w(T_a)$, with r_H the relative ambient humidity and with $P_V^w(T_a)$ the saturated vapour pressure of water (atm) at temperature T_a.

Note that the ratio P^{amb}_w/P equals the mole fraction of water in the moist air.

2.B.2.4. Pollutant Enthalpy

For an evaporating liquid pool (unpressurised release), the pollutant enthalpy H_{pol} in equation (12) corresponds to 100% liquid with the pool temperature T_{liq}. Assuming the liquid to consist of 100% HF, this implies that $H_{pol} = C_p^{HFL} \cdot (T_{liq} - T^*) - H_{cond}^{HF}$ with $T^* = 25$ °C and C_p^{HFL} the specific heat of HF liquid.

For pressurised releases of pollutant containing HF, a flash occurs immediately upon release. The following two cases are distinguished.

1. The pollutant *contains no water*. For this case the model requires as input the pollutant temperature, T_{pol}, and the equivalent mole fraction of liquid HF in the pollutant, η_{HFL}. This data should correspond to the post-flash state and are in HGSYSTEM derived from flash calculations in either the HFPLUME model or the HFFLASH model. The composition of the pollutant vapour is evaluated from equations (1) to (9).

2. The pollutant *contains water*. For this case the model adopts $\eta_{HFL} = 0$ and the model requires as input the pollutant temperature T_{pol} only. The pollutant is assumed to be in thermodynamic equilibrium, and consists of a vapour mixture (HF with enthalpy departure $H_{pol}^{\Delta HF}$ from monomer, N-gas, water) and an aqueous liquid fog (equivalent mole fraction L_{pol} of fog in pollutant; mole fraction x_{pol} of HF in fog). The pollutant composition is evaluated from equations (1) to (11).

For pressurised releases the enthalpy H_{pol} must include the kinetic energy E_{pol}^{kin} (Joule/kmole of pollutant) of the post-flash pollutant; E_{pol}^{kin} given by

$$E_{pol}^{kin} = ½ \cdot m_{pol} \cdot V_{fl}^2 \qquad \text{with } m_{pol} = g_{HF} \cdot m_{HF} + g_w \cdot m_w + g_N \cdot m_N \qquad (16)$$

with m_{pol} the mean molecular weight (kg/kmole) of the pollutant, m_α the molecular weight of species α (α can be: HF, w, N for HF, water and N-gas, respectively) and V_{fl} the post-flash velocity (m/s). The pollutant enthalpy is now given by the following formula (compare with equations (12) and (13)),

$$\begin{aligned} H_{pol} = \; & E_{pol}^{kin} + \\ & + \eta_{HFL} \cdot \{C_p^{HFL} \cdot (T_{pol} - T^*) - H_{cond}^{HF}\} + \\ & + \{\eta_N \cdot \{C_p^N \cdot (T_{pol} - T^*)\} + \\ & + [\eta_w - (1 - x_{pol}) \cdot L_{pol}] \, C_p^{wv} \cdot (T_{pol} - T^*) + \\ & + [\eta_{HF} - \eta_{HFL} - x_{pol} \cdot L_{pol}] \cdot \{H_{pol}^{\Delta HF} + C_p^{HFV} \cdot (T_{pol} - T^*)\} + \qquad (17) \end{aligned}$$

$$
\begin{aligned}
&- x_{pol}\cdot L_{pol}\cdot\{H^{HF}_{cond} + H_{mix}\} + \\
&- (1 - x_{pol})\cdot L_{pol}\cdot H^{w}_{cond} + \\
&+ L_{pol}\cdot\{C^{fog}_{p}(x_{pol},T_{pol})\cdot(T_{pol} - T^{*})\}
\end{aligned}
$$

2.B.3. Solution algorithm

In the previous paragraph the set of thermodynamic equations governing the thermodynamics model has been derived, that is, the twelve equations (1-12) in the presence of a liquid fog and the ten equations (1-9), (12) in the absence of a fog.

This paragraph describes the algorithm for solving these equations as it is used in HEGADAS and HEGABOX. The algorithm used in HFPLUME is somewhat different but has been checked to give identical results.

The HEGADAS/HEGABOX algorithm is used to determine the ten unknowns in the absence of a fog (y_{11}, y_{12}, y_{16}, y_{18}, y_c/y_w, y_w, y_N, y_a, M_{vap}, T_m) and twelve unknowns in the presence of a fog (additional unknowns x, L).

The calculations described below are carried out using the model parameters described in paragraph 2.B.2 (y_{pol}, η_w, η_N, r_H, T_a, H_{pol}, H_e, C_p^N).

Without loss of generality the total molar flow M_{tot} is taken equal to unity. The molar flows before mixing of HF, water, N-gas and air (M_{HF}, M_w, M_N, M_a; $M_{tot} = M_w+M_{HF}+M_N+M_a = 1$) can be expressed in terms of the input parameters as follows:

$$
\begin{aligned}
M_{HF} &= (1 - \eta_w - \eta_N)\cdot y_{pol}\cdot M_{tot} \\
M_w &= \eta_w\cdot y_{pol}\cdot M_{tot} + [P^{amb}_w/P]\cdot(1 - y_{pol})\cdot M_{tot} \\
M_N &= \eta_N\cdot y_{pol}\cdot M_{tot} \qquad\qquad (18) \\
M_a &= [(P - P^{amb}_w)/P]\cdot(1 - y_{pol})\cdot M_{tot}
\end{aligned}
$$

with $P^{amb}_w/P = r_H\cdot P_V{}^w(T_a)/P$ and P the total atmospheric pressure.

2.B.2.1. Solving the equations

The set of equations is reduced to a set of two (in the absence of liquid fog) or three (with fog) equations for two or three basic unknowns. These unknowns are the molar fraction y_{11} of the HF monomer, the mixture temperature T_m, and (in case of fog) the molar fraction x of HF in the fog. The algorithm for the derivation of the reduced set of equations is as follows.

1. Set y_{12}, y_{16}, y_{18}, y_c/y_w as function of y_{11} and T_m from the Peng-Robinson equations of state (6), (7), (8) and (9).

2. Set M_{vap}, y_w and L.

a In the presence of a liquid fog (L > 0), M_{vap}, y_w, L are set as functions of y_{11}, T_m, x by imposing conservation of the sum of molar flow of air and N-gas (see equations (10), (11), (3-5)), the water vapour pressure relation (equation (10)) and conservation of energy (equation (12)).

$$M_{vap} = [M_a + M_N]/[1 - P_{HF}/P - P_w/P + y_c] \tag{19}$$

$$y_w = [1 + y_c/y_w]^{-1} \cdot \min\left\{\frac{p_{HF}(x,T_m)}{P}, \frac{M_{HF}}{M_{tot}}\right\} \tag{20}$$

$$L = \frac{TERM1}{TERM2 + TERM3} \tag{21}$$

with

$$TERM1 = H_a + H_N - H_{tot} + M_w \cdot C_p^{wv} \cdot (T_m - T^*) + M_{HF} \cdot \left\{H^{\Delta HF} + C_p^{HFV} \cdot (T_m - T^*)\right\}$$

$$TERM2 = (1-x) \cdot \left\{C_p^{wv} \cdot (T_m - T^*) + H_{cond}^{w}\right\} - C_p^{fog}(x, T_m) \cdot (T_m - T^*)$$

$$TERM3 = x \cdot \left\{H^{\Delta HF} + C_p^{HFV} \cdot (T_m - T^*) + H_{cond}^{HF} + H_{mix}\right\}$$

b In the absence of a liquid fog (L = 0), M_{vap}, y_w are set as functions of y_{11}, T_m.
For $M_{HF} > 0.5$ conservation of HF molar flow (equation (1)) and conservation of water molar flow (equation (2)) is imposed, while for $M_{HF} < 0.5$ conservation of the sum of air, N-gas and water molar flow (see equations (2-5)) and conservation of water molar flow (equation (2)) is imposed:

$$M_{vap} = \begin{cases} M_{HF} / [y_c + y_{11} + 2y_{12} + 6y_{16} + 8y_{18}] & (M_{HF} > 0.5) \\ \\ [M_a + M_N + M_w] / [1 - y_{11} - y_{12} - y_{16} - y_{18}] & (M_{HF} < 0.5) \end{cases} \tag{19*}$$

$$y_w = \begin{cases} \left[1 + \left(1 - \frac{M_w}{M_{HF}}\right) \cdot \frac{y_c}{y_w}\right]^{-1} \cdot [y_{11} + 2y_{12} + 6y_{16} + 8y_{18}] \cdot \frac{M_w}{M_{HF}} & (M_{HF} > 0.5) \\ \\ \left[1 + \frac{y_c}{y_w}\right]^{-1} \cdot \frac{M_w}{M_{vap}} & (M_{HF} < 0.5) \end{cases} \tag{20*}$$

$$L = 0 \tag{21*}$$

3. Set y_a and y_N from conservation of air and N-gas moles (equations (3-4)):

$$y_a = M_a/M_{vap}$$

$$y_N = M_N/M_{vap} \qquad (22)$$

4. Formulate basic set of equations for basic unknowns: HF-monomer molar fraction y_{11}, the final temperature T_m and (in the presence of fog) the molar fraction x of HF in the fog.

   a In the presence of a liquid fog (L > 0) the equations represent conservation of HF molar flow (equation (1)), conservation of water molar flow (equation (2)), and the HF-vapour pressure relation (equation (11)):

$$M_{HF} = (y_c + y_{11} + 2y_{12} + 6y_{16} + 8y_{18})\cdot M_{vap} + x\cdot L \qquad (I)$$

$$M_w = (y_w + y_c)\cdot M_{vap} + (1 - x)\cdot L \qquad (II)$$

$$y_{11} + y_{12} + y_{16} + y_{18} + y_c = \min\left\{\frac{p_{HF}(x,T_m)}{P}, \frac{M_{HF}}{M_{tot}}\right\} \qquad (III)$$

   The above set of equations is solved iteratively for y_{11}, T and x.

   b In the absence of a liquid fog (L = 0) the equations represent conservation of energy (equation (12)), and the consistency equation of all components in vapour mixture (equation (5); for $M_{HF} > 0.5$) or conservation of HF molar flow (equation (1); for $M_{HF} < 0.5$),

$$H_{tot} = H_{HF} + H_w + H_N + H_a = y_{pol}\cdot H^0_{pol} + (1 - y_{pol})\cdot H^{wet,0}_{air} + H_e \qquad (I^*)$$

$$M_{HF} = (y_c + y_{11} + 2y_{12} + 6y_{16} + 8y_{18})\cdot M_{vap} \qquad M_{HF} < 0.5$$

$$y_{11} + y_{12} + y_{16} + y_{18} + y_c + y_w + y_N + y_a = 1 \qquad M_{HF} > 0.5 \qquad (II^*)$$

   The above set of equations is solved iteratively for y_{11} and T_m.

2.B.2.2. Evaluation of pollutant enthalpy

For given pollutant temperature T_{pol}, one can evaluate the pollutant enthalpy H_{pol} from equation (17), if one knows $H^{\Delta HF}_{pol}$, x_{pol}, L_{pol}. To this purpose the previous equations are considered for the special case of $y_{pol} = 1$ ($y_a = 0$) and the temperature $T_m = T_{pol}$ ($H^{\Delta HF} = H^{\Delta HF}_{pol}$, $x = x_{pol}$, $L = L_{pol}$).

In the presence of fog ($L > 0$) the equations are solved as follows:

- The unknowns y_{12}, y_{16}, y_{18} and y_c/y_w are set as a function of y_{11} from equations (6), (7), (8) and (9)
- The unknown y_w is determined as function of y_{11} and x from equation (20)
- The unknowns M_{vap} and L are set from equations (1) and (2)
- The unknown y_N is set from equation (3)
- The remaining two unknowns y_{11} and x are set by iteratively solving the equations (5) and (11)

In the absence of fog ($L = 0$) the equations are solved as follows:

- The unknowns y_{12}, y_{16}, y_{18} and y_c/y_w are set as a function of y_{11} from equations (6), (7), (8) and (9)
- The unknowns M_{vap}, y_w are determined from equations (19*) and (20*)
- The unknown y_N is set from equation (3)
- The remaining unknown y_{11} is set by iteratively solving equation (5) for $M_{HF} > 0.5$ and equation (1) for $M_{HF} < 0.5$.

2.B.2.3. Evaluation of molar mixture volume and mixture density

The algorithm described above has been implemented into the heavy gas dispersion program HEGADAS and in the instantaneous heavy gas release model HEGABOX, to calculate thermodynamic data for given pollutant molar fraction y_{pol} and added heat from the surface H_e. These calculations are carried out by the routine THRMHF, which outputs data required for further HEGADAS dispersion calculations, i.e. the mixture temperature T_m, the molar mixture volume V_m and the molar mixture density ρ_m. The temperature T_m follows from the iterative solution of the HF thermodynamic equations described above. The molar mixture volume V_m and the molar mixture density ρ_m are set as follows.

1. The molar mixture volume V_m, m^3/kmole of mixture, is the ratio of the total volume flow (m^3/s; volume of liquid fog can be neglected) and the total molar flow (kmole/s; vapour and fog). Thus it is seen that

$$V_m = \frac{[R\cdot(T_m + 273.15)/P]\cdot M_{vap}}{M_{vap} + L} \qquad (23)$$

with R = 0.082 atm·m^3/K/kmole being the universal gas constant.

Note that the term between square brackets in the numerator of equation (23) signifies the molar volume (m^3/kmole) of an ideal gas at temperature T_m and pressure P.

2. The mixture density is the ratio of the total mass flow (kg/s: vapour and fog) and total volume flow (m^3/s). Thus it is seen that

$$\rho_m = \frac{m_a \cdot M_a + m_N \cdot M_N + m_w \cdot M_w + m_{HF} \cdot M_{HF}}{[R \cdot (T_m + 273.15)/P] \cdot M_{vap} + [m_w \cdot (1-x) + m_{HF} \cdot x] \cdot L/\rho_{fog}} \tag{24}$$

with $m_a = 28.95$, m_N, $m_{HF} = 20.01$, $m_w = 18.02$ the molecular weights of dry air, N-gas, HF-monomer and water, respectively and $\rho_{fog} = 1200$ kg/m^3 the density of the fog.

3. The ratio ρ_m/ρ_{amb} of the mixture density ρ_m and the density of the ambient humid air ρ_{amb} is output by the HEGADAS HF-thermodynamics routine. It is set from equation (24) and

$$\rho_{amb} = P \cdot m_{amb}/[R \cdot (T_a + 273.15)] \tag{25}$$

with m_{amb}, the molecular weight of the humid air (kg/kmole), given by

$$m_{amb} = m_a \cdot [1 - P_w^{amb}/P] + m_w \cdot [P_w^{amb}/P] \tag{26}$$

2.B.4. General trends of HF thermodynamics model

Following implementation of the algorithm as described in paragraph 2.B.2 into the heavy gas dispersion program HEGADAS, a sensitivity analysis has been carried out for a pollutant consisting of HF (liquid or vapour), propane and water. In this limited exercise, fully described in [3], the following results were obtained. These results are given here to give the HGSYSTEM user some feeling for the thermodynamic and chemistry model described in this chapter.

1. Upon mixing of dry HF vapour with moist air, initial cooling resulting from de-polymerisation of HF is diminished because of formation of an aqueous fog and because of heat convection from the ground. For increasing humidity, the fog formation and mixture temperature increase, and the mixture density, molar entrainment and cloud width increase. Dependence of peak concentration on humidity is complex. See [3] for more details.

2. If a part of the HF in the pre-mixed pollutant is liquid, less additional liquid fog forms, the mixture temperature decreases and the mixture density increases. For less than 5% initial liquid, cloud widths and concentrations do not significantly depend on the amount of initial liquid HF.

3. If the pollutant contains an ideal gas in addition to HF, the pollutant will be less polymerised, less additional de-polymerisation occurs upon mixing and the mixture temperature increases. The precise effect of the presence of ideal gas in the pollutant on mixture density depends both on the molecular weight of the ideal gas and the increase in mixture density because of previous cooling. See [3] for more details.

4. If the pollutant contains water in addition to HF, the pollutant contains an initial aqueous fog, less additional fog forms, the mixture temperature decreases and the mixture density increases. For less than 4% initial water, cloud widths and concentrations do not significantly depend on the amount of initial water.

2.B.5. References

1. Schotte, W., '*Fog formation of hydrogen fluoride in air*', Ind. Eng. Chem. Res. vol 26, 300-306, 1987.

2. Schotte, W., '*Thermodynamic model for HF fog formation*', Letter from Schotte to Soczek, E. I. Du Pont de Nemours & Company, Du Pont Experimental Station, Engineering Department, Wilmington, Delawere 19898, 31 August 1988.

3. Witlox, H.W.M., '*Thermodynamics model for mixing of moist air with pollutant consisting of HF, ideal gas and water*, Shell Research Limited, Thornton Research Centre, TNER.93.021, 1993.

2.B.6. Notation

C_p^α specific heat at constant pressure of species α, J/kmole/K

α = HFL: liquid HF

$$C_p^{HFL} = C_p^{HFL}(T^0) = 50260 + 68.6T^0$$

HFV: gaseous HF, $C_p^{HFV} = 29120$

fog: aqueous fog, C_p^{fog} is as a function of x and T (°C) (equation (24) in [2]),

$$C_p^{fog}(x,T) = 75519 + 1.661\cdot T - (58475 - 63.6\cdot T)\cdot x + (35686 + 7.83\cdot T)\cdot x^2$$

wl: water liquid, $C_p^{wl} = 75700$

wv: water vapour, $C_p^{wv} = 33690$

N: N-gas,

a: dry air, $C_p^a = 29120$

f_1	fugacity of HF-monomer (after mixing; $f_1 = \Phi \cdot y_{11} \cdot P$) (atm)
H_e	heat added from the substrate to the pollutant/air mixture (Joule/equivalent kmole of mixture)
H_{air}^{wet}	enthalpy of moist air (Joule/kmole of moist air)
H_{cond}^{HF}	heat of condensation of HF monomer at 25 °C (J/kmole) $H_{cond}^{HF} = 30258000$
H_{mix}	heat of mixing of liquid HF and H_2O at 25 °C (J/kmole of HF) $H_{mix} = H_{mix}(x) = 18831000 \cdot (1 - x^2)$
H_{pol}	enthalpy of pollutant (Joule/equivalent kmole of pollutant)
H_{cond}^{w}	heat of condensation of water at 25 °C (J/kmole) $H_{cond}^{w} = 44017000$
H_α	enthalpy (J/kmole) of species α after mixing of pollutant and moist air α can be: tot (total enthalpy), HF (HF; including water in fog and HF in $HF \bullet H_2O$), w (water; excluding fog and including water in $HF \bullet H_2O$), N (N-gas) or a (dry air)
$H^{\Delta HF}$	enthalpy departure (J/equivalent kmole of HF vapour) of HF vapour in pollutant/air mixture from the ideal monomeric gas
$H_{pol}^{\Delta HF}$	enthalpy departure (Joule/equivalent kmole of HF vapour) of HF vapour in the pre-mixed pollutant from the ideal monomeric gas
$K_i(T)$	$K_1(T) = 1$ For i > 1, $K_i(T)$ is chemical equilibrium constant at temperature T (Kelvin) for the dimer (i = 2), hexamer (i = 6), octamer (i = 8) formation at temperature T, (atm^{-i+1}). $K_i(T)$ (i > 1) is given by equation (5) in [2]: $\ln(K_2) = [53458.697/T - 200.76387]/R$ $\ln(K_6) = [175448.07/T - 579.77837]/R$ $\ln(K_8) = [209734.20/T - 694.02013]/R$

with the universal gas constant R given by R = 8.3143 J/K/mole

$K_c(T)$ chemical equilibrium constant at temperature T (Kelvin) for the formation of the HF•H_2O complex at temperature T, (atm^{-1})
$K_c(T)$ is given by equation (5) in [2]:

$$\ln(K_c) = [26220.445/T - 94.989486]/R$$

L total molar flow of aqueous fog (after mixing) (kmole/s)

M_{vap} total molar flow of vapour (after mixing) (kmole/s)
the number of moles after mixing must be equal to the number of moles prior to mixing, if *all* HF is based on HF-monomer:

$$(y_{11} + 2y_{12} + 6y_{16} + 8y_{18} + 2y_c + y_w + y_N + y_a)\cdot M_{vap} + L = M_{tot}$$

M_α equivalent molar flow of species α after mixing of pollutant and moist air (with *all* HF based on HF monomer) (kmole/s)
α can be: tot (total molar flow), HF (HF), w (water), N (N-gas), a (dry air)

$$M_{tot} = M_{HF} + M_w + M_N + M_a$$

P total (ambient or atmospheric) pressure (atm)

P_{HF} partial vapour pressure of HF (including HF•H_2O) (atm)

$P_V^w(T)$ vapour pressure of water in air at temperature T (atm)

P_w partial vapour pressure of water (including HF•H_2O) (atm)

P_w^{amb} partial vapour pressure of water in the ambient wet air (before mixing) (atm)

$$P_w^{amb} = r_H \cdot P_V^w(T_a)$$

r_H relative humidity of the ambient air (-)

T_a ambient temperature (°C)

T_m mixture temperature (°C)

T_{pol} (post-flash) temperature of pre-mixed pollutant (°C)

x	molar fraction of HF (monomer) in aqueous fog (after mixing) (-)
x_{pol}	molar fraction of HF (monomer) in aqueous fog in pre-mixed pollutant (-)
y_{pol}	equivalent molar fraction of pollutant (HF, water, N-gas) in final mixture; *equivalent* fraction means that the fraction is calculated with *all* HF based on HF monomer (-)
y_α	molar fraction of species α in vapour (after mixing) (-) α 11, 12, 16, 18, c, w, N or a (dry air) the sum of these fractions must be 1: $y_{11} + y_{12} + y_{16} + y_{18} + y_c + y_w + y_N + y_a = 1$
ΔH_α	enthalpy of association of HF species α (J/kmole) α can be: 2 (dimer, $\Delta H_2 = -53458000$), 6 (hexamer, $\Delta H_6 = -175448000$), 8 (octamer, $\Delta H_8 = -209734000$) or c ($HF{\bullet}H_2O$, $\Delta H_c = -26220000$)
η_α	equivalent molar fraction of species α in pre-mixed pollutant (-) α can be: HF (total HF), w (water), N (N-gas), HFL (HF liquid; excluding HF in fog), HFV (HF vapour; including HF in fog and in $HF{\bullet}H_2O$), N (N-gas) $\eta_{HF} + \eta_w + \eta_N = 1$, $\eta_{HF} = \eta_{HFL} + \eta_{HFV}$
Φ_1	fugacity coefficient of HF in vapour phase; approximated by $\Phi_1 = 1$ (-)

3. THE SPILL MODEL

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3. THE SPILL MODEL

3.1. Introduction

HGSYSTEM version 1.0 (or NOV90 version) already contained a module HFSPILL to simulate the transient release of liquid hydrogen fluoride (HF) from a pressurised reservoir. This chapter describes the implementation of a new HGSYSTEM module, SPILL, a general transient release model for two-phase multi-compound mixtures in a pressurised reservoir. SPILL is available in HGSYSTEM version 3.0. HFSPILL is the HF-specific version of SPILL and uses similar correlations to calculate discharge rates. HFSPILL is therefore not discussed in the Technical Reference Manual.

Although SPILL's main use will be the simulation of pure *liquid* phase releases, it can also deal with releases that are pure vapour phase initially and SPILL will also simulate the vapour-only discharge after liquid exhaustion has occurred in a reservoir that initially contained a two-phase fluid.

A complication in describing a multi-compound release from a two-phase reservoir mixture, is that as long as there is a multi-compound liquid in the reservoir, *the composition of the liquid and vapour phase changes with time*. With decreasing reservoir pressure, the more volatile components in the liquid will vaporise more easily than less volatile compounds. Once the liquid is exhausted the reservoir mixture is vapour-only and the composition will no longer change with time. The SPILL program takes these effects into account, but to be able to do so it has to calculate the *number of kilomoles of each compound* in the reservoir as a function of time, which adds to the complexity of the model. Increasing the number of compounds in the reservoir mixture will increase the model run-time accordingly.

SPILL uses the standard HGSYSTEM non-reactive, multi-compound, two-phase thermodynamical model (AEROPLUME version) as described in Chapter 2.A. It is therefore intended to be run in combination with the physical properties database program DATAPROP, which will prepare a link file for SPILL containing all physical compound properties.

SPILL can be used as a front-end to the HGSYSTEM model AEROPLUME and it will generate the necessary link file.

The liquid discharge rates used in SPILL are based on literature correlations [2] and they are completely identical to the one used in AEROPLUME.

In this chapter, a detailed discussion of the SPILL model equations will be given. A detailed discussion of SPILL input parameters is given in the SPILL chapter in the User's Manual. A sensitivity analysis for the SPILL model is described in [4].

3.2. The model equations

The basic *time-dependent* variables that are used in the SPILL algorithm are: **P(t)** (in Pa), the (absolute) pressure in the reservoir, **M(t)** (in kg), the total mass contained in the reservoir, **E(t)** (in J), the (internal) energy of the reservoir mixture, **h(t)** (in J/kg), the enthalpy of the reservoir mixture and $\mathbf{N_\alpha(t)}$ (-), the number of kmoles of chemical compound α present in the reservoir multi-compound mixture, $\alpha = 1, 2, ..., N$, where N is the total number of compounds in the mixture.

Thus there are N+4 variables which are all functions of time t (s) and N+4 equations are needed to define the problem completely.

For given values of the mixture enthalpy h and the reservoir pressure P, the *thermodynamical* state is fixed and using the thermodynamical model equations, values for the density $\rho(t)$ (kg/m^3) and the temperature T(t) (K) of the reservoir mixture can be calculated for every time t. Thus ρ and T are not basic variables but they can be calculated from these at every moment in time.

The thermodynamical model used in SPILL is the HGSYSTEM two-phase non-reactive multi-compound model as described in Chapter 2.A.

The set of N+4 equations consists of 2 algebraic equations and N+2 first order ordinary differential equations. These equations are solved as one set using the same numerical solver, SPRINT [1], as employed in AEROPLUME and HFPLUME.

3.2.1. Algebraic equations

The two algebraic equations are given by:

$$V\cdot\rho(t) = M(t) \qquad (1)$$

and

$$E(t) = \left(h(t) - \frac{P(t)}{\rho(t)}\right)\cdot M(t) \qquad (2)$$

where V is the (constant) user-specified reservoir volume (m^3).

These two relations ensure *physical consistency* between the several model variables.

Please note that h, P and ρ also must satisfy the *thermodynamical equations* as dictated by the thermodynamical model being used.

3.2.2. Conservation of total reservoir mass

The first differential equation expresses *conservation of mass* and it governs the rate of change of the total reservoir mass content M:

$$\frac{dM(t)}{dt} = \dot{m}(t) \tag{3}$$

where $\dot{m}(t)$ (kg/s) is the (instantaneous) mass flow rate leaving the reservoir at time t, the value of $\dot{m}(t)$ is taken negative here as it is an *outflowing* rate.

The value of $\dot{m}(t)$ is given by correlations from literature [2].

For a *vapour-only* release, the discharge rate used is simply the well-known (maximum) discharge rate found for an ideal gas release, either *choked* or *unchoked.* For a choked vapour-only release the result is

$$\dot{m} = -C_D^g \cdot A \cdot \left(\frac{2}{1+\gamma}\right)^{1/(\gamma-1)} \cdot \left(\frac{\gamma}{1+\gamma}\right) \cdot \sqrt{2\cdot\rho(t)\cdot P(t)} \tag{4}$$

and for unchoked vapour-only flow the result is

$$\dot{m}(t) = -C_D^g \cdot A \cdot \sqrt{\frac{\gamma}{\gamma-1}} \cdot \sqrt{2\cdot\rho(t)\cdot P(t)\cdot\left\{\left(\frac{P_{atm}}{P(t)}\right)^{\frac{2}{\gamma}} - \left(\frac{P_{atm}}{P(t)}\right)^{\frac{\gamma+1}{\gamma}}\right\}} \tag{5}$$

where P_{atm} (Pa) is the atmospheric pressure, A (m^2) is the area of the discharge opening, γ (-) is the ratio of specific heats (c_p/c_v) and C_D^g (-) is the vapour discharge coefficient. C_D^g has a default value of 1.0, but the user of SPILL can override this value if necessary.

For a *liquid* release, first the mixture saturation pressure P_{sat} is calculated as

$$P_{sat} = \frac{\sum_{\alpha=1}^{N} y_{\alpha\ell} \cdot P_{sat,\alpha}(T)}{\sum_{\alpha=1}^{N} y_{\alpha\ell}} \tag{6}$$

where $y_{\alpha\ell}$ is the molar fraction *within the total mixture* of liquid compound α and $P_{sat,\alpha}(t)$ is the saturation pressure of compound α at temperature T. Note that this definition of P_{sat} is inspired by Raoult's law as discussed in Chapter 2.A.

If P_{sat} is less than P_{atm} then the liquid mixture is *subcooled* even at atmospheric conditions and no flashing will occur at the exit. In SPILL the flow regime is then called *unchoked liquid flow*. From Fauske and Epstein [2] a Bernoulli-like expression for the discharge rate is found

$$\dot{m}(t) = -C_D^\ell \cdot A \cdot \sqrt{2 \cdot \rho_\ell(t) \cdot (P(t) - P_{atm})} \tag{7}$$

where ρ_ℓ is the density of the *liquid* in the reservoir. The liquid discharge coefficient C_D^ℓ has a default value of 0.61 [2], but again the user can override this value by setting the relevant SPILL input parameter (see the SPILL chapter in the User's Manual).

When P_{sat} exceeds P_{atm}, the flow regime is called *choked liquid flow* in SPILL. If this occurs, i.e. the liquid mixture in the reservoir, which is subcooled at reservoir conditions, is *not* subcooled at atmospheric conditions, then a distinction must be made between reservoir conditions that are *near the saturation point* and those that are not.

If $|P(t) - P_{sat}| > 10 \cdot P_{sat}$ (reservoir conditions far from the saturation point) then following [2]

$$\dot{m}(t) = -C_D^\ell \cdot A \cdot \sqrt{2 \cdot \rho_\ell \cdot |P(t) - P_{sat}|} \tag{8}$$

If $|P(t) - P_{sat}| < 0.1 \cdot P_{sat}$ (reservoir conditions near the saturation point), [2] gives

$$\dot{m}(t) = -C_D^\ell \cdot A \cdot \sqrt{\left|\frac{1}{dv/dP}\right|} \tag{9}$$

where v = 1/ρ (m³/kg) is the specific volume of the mixture. The term $\left|\frac{1}{dv/dP}\right|$ is estimated, following [2], by

$$\left|\frac{1}{dv/dP}\right| = \left(\frac{h_{vap}}{\Delta v_{vap}}\right)^2 / (T \cdot C_{p,\ell}) \tag{10}$$

where h_{vap} (J/kg) is the heat of vaporisation, Δv_{vap} (m^3/kg) the change in specific volume going from the liquid to the vapour state, $C_{p,\ell}$ (J/(kg·K)) is the specific heat of the liquid mixture and T (K) is the reservoir temperature.

For the intermediate stage, $0.1 \cdot P_{sat} \le |P(t) - P_{sat}| \le 10 \cdot P_{sat}$, *linear interpolation* between the two previous cases is used. Let FACTOR, TERM1 and TERM2 be defined by

$$\mathrm{FACTOR} = \frac{|P(t) - P_{sat}|}{P_{sat}} \tag{11}$$

$$\mathrm{TERM1} = 2 \cdot \rho_\ell \cdot |P(t) - P_{sat}| \tag{12}$$

$$\mathrm{TERM2} = \left| \frac{1}{dv / dP} \right| \tag{13}$$

Define the variable TERM3 by using linear interpolation between TERM1 and TERM2 using FACTOR, that is

$$\mathrm{TERM3} = \mathrm{TERM2} + (\mathrm{FACTOR} - 0.1) \cdot \frac{\mathrm{TERM1} - \mathrm{TERM2}}{10.0 - 0.1} \tag{14}$$

and the reservoir mass discharge rate when $0.1 \cdot P_{sat} \le |P(t) - P_{sat}| \le 10 \cdot P_{sat}$, is given by

$$\dot{m}(t) = -C_D^\ell \cdot A \cdot \sqrt{\mathrm{TERM3}} \tag{15}$$

This linear interpolation procedure for the case where $0.1 \cdot P_{sat} \le |P(t) - P_{sat}| \le 10 \cdot P_{sat}$ is found to give more satisfactory results than the recommendation in [2] , the latter being equivalent to taking TERM3 = TERM1 + TERM2.

Please note that the mass discharge literature correlations and the definition of P_{sat} used in SPILL and AEROPLUME (HGSYSTEM version 3.0) are completely identical.

3.2.3. Conservation of energy

The second differential equation expresses *conservation of energy*

$$\frac{dE(t)}{dt} = h_{exit}(t) \cdot \dot{m}(t) + Q_{atm}(t) \tag{16}$$

where h_{exit} (J/kg) is the enthalpy of the discharged fluid and Q_{atm} (W) is the total heat exchange with the atmosphere surrounding the reservoir. For a pure liquid release h_{exit} is equal to the enthalpy of the liquid phase in the reservoir which is *not* equal to the mixture enthalpy h. For vapour-only situations this difference does not occur.

Q_{atm} can be calculated as

$$Q_{atm} = A_{heat} \cdot (\Phi_{rad} + \Phi_{conv} + \Phi_{solar}) \tag{17}$$

where A_{heat} (m^2) is the user-specified total reservoir area over which heat transfer with the surrounding atmosphere takes place, Φ_{rad} (W/m^2) is the radiative heat flux given by

$$\Phi_{rad} = \sigma \cdot \varepsilon \cdot (T_{atm}^4 - T^4) \tag{18}$$

where σ is the Stefan-Boltzmann constant ($5.67 \cdot 10^{-8}$ $W/(m^2 \cdot K)$), ε (-) the user-specified emissivity of the reservoir outside wall material and T_{atm} (K) the user-specified temperature of the surrounding air.

Φ_{conv} (W/m^2) is the convective heat flux, given by [3]

$$\Phi_{conv} = 1.97 \cdot (T_{atm} - T) \cdot |T_{atm} - T|^{0.25} \tag{19}$$

Φ_{solar} (W/m^2) is a user-specified direct solar heat flux on the reservoir.

Note that a user-specified value for A_{heat} of 0.0, effectively sets the heat transfer between the reservoir and the ambient atmosphere to 0.0.

3.2.4 Conservation of mixture compound α

The final N differential equations express *conservation of each compound* α in the mixture.

For a *vapour-only release* (after liquid exhaustion or for a vapour-filled reservoir), the *total* number of kmoles leaving the reservoir is equal to $\dot{m}/M$, where M (kg/kmole) is the molar mass of the reservoir vapour, which is constant once the release is vapour-only. The number of kmoles of compound α leaving the reservoir per second is then simply $y_\alpha \cdot \dot{m}(t)/M$ (kmole/s), where y_α is the molar fraction of compound α in the mixture. Again, y_α does not change with time for vapour-only releases. So in this case for all compounds α the following equation holds

$$\frac{dN_\alpha(t)}{dt} = y_\alpha \cdot \dot{m}(t) / M \qquad \alpha = 1, 2, \ldots, N \tag{20}$$

For a *multi-compound liquid-only release*, where the reservoir contains a real two-phase multi-compound mixture, the situation is more complicated, as the mixture composition both in the vapour and the liquid phase changes with time.

For a liquid-only release, the change per second in the number of kmoles of compound α, $\frac{dN_\alpha}{dt}$, is given by

$$\frac{dN_\alpha}{dt} = \frac{N_{\alpha,\ell}}{N_\ell} \cdot \frac{dN_\ell}{dt} \qquad \alpha = 1, 2, \ldots, N \tag{21}$$

where N_ℓ is the total number of kmoles of liquid in the reservoir. In this expression $\frac{dN_\ell}{dt}$ is equal to $\frac{\dot{m}}{M_\ell}$, where M_ℓ is the (now time-dependent) molar mass (kg/kmole) of the total liquid phase fluid.

The term $\frac{N_{\alpha,\ell}}{N_\ell}$ in (21) can be interpreted as the mole fraction of liquid compound α in the total liquid phase of the reservoir mixture. The thermodynamic model uses as a basic variable $y_{\alpha,\ell}$, which is the molar fraction of compound α within the *total mixture*. Let L denote the total liquid mole fraction within the reservoir, then $\frac{N_{\alpha,\ell}}{N_\ell} = \frac{y_{\alpha,\ell}}{L}$.

Thus for a *liquid-only release* the equation expressing conservation of compound α will be

$$\frac{dN_\alpha(t)}{dt} = \frac{y_{\alpha,\ell}(t)}{L(t)} \cdot \frac{\dot{m}(t)}{M_\ell(t)} \qquad \alpha = 1, 2, \ldots, N \tag{22}$$

3.2.5. Initial conditions

Initial conditions for the N+2 first order differential equations are needed. The initial values for the reservoir pressure P and temperature T are user-specified. The initial value for the reservoir mass contents M is either user-specified or calculated by SPILL as the maximum reservoir contents for given P and T.

Based on the initial P and T and the initial mixture composition, all user-specified, SPILL calculates the initial value for h, the reservoir enthalpy, ρ, the mixture density and the initial values of N_α for all compounds α. This is done using the thermodynamic model.

There is a slight complication when the user has specified an initial reservoir mass contents, M, lower than the maximum for the given initial P and T. In this case the value of ρ given by relation (1) on one hand and the value of ρ following from the thermodynamical relations will not be consistent. In other words, the correct value for P for the given mass M at the given temperature would be lower than specified by the user. In this case SPILL changes the initial mixture composition by adding *dry air* to the mixture. The needed amount is calculated using the solver NAESOL in such a way that finally all relevant relations (relation (1) plus thermodynamical relations) are satisfied. SPILL is actually pressurising the given amount of material to the required pressured using dry air.

If the user specifies a value of M larger than the maximum possible for the given P and T, SPILL simply resets M to the maximum value.

The input option of specifying the initial value of M is only effective if the SPECIES keyword in the GASDATA input block is being used *and* if the initial reservoir mixture is more dense than dry air. In all other cases, the initial value of M is calculated by the program based on mixture composition and reservoir pressure, temperature and volume.

The initial value for the total energy E is simply calculated by using relation (2) in which all other (initial) values are now known.

This completes the description of the N+4 equations of the SPILL mathematical model.

3.3. Notation

A	surface area of release opening (m^2)
C_D	discharge coefficient (-)
C_p	specific heat (J/(kg·K))
E	reservoir mixture (internal) energy (J)
h	reservoir mixture enthalpy (J/kg)
$\dot{m}$	mass flow rate out of reservoir (kg/s)
M	reservoir total mass content (kg)
$\mathcal{M}$	molar mass (kg/kmole)
N	total number of chemical compounds in reservoir mixture
N_α	number of kmoles of compound α in reservoir (-)
P	reservoir pressure (Pa)
Q	total heat transfer reservoir-ambient atmosphere (W)
T	reservoir temperature (K)

t	time (s)
V	reservoir volume (m^3)
v	fluid specific volume (m^3/kg)
y_α	molar fraction of compound α (-)
α	chemical compound indicator
Δv	change in specific volume liquid-vapour (m^3/kg)
γ	ratio of specific heats (c_p/c_v) for ideal gas (-)
ρ	reservoir mixture density (kg/m^3)
Φ	heat flux (W/m^2)

Subscripts and superscripts

atm	ambient atmosphere
α	chemical compound indicator
conv	convective heat transfer
g	vapour (gas) phase
ℓ	liquid phase
rad	radiative heat transfer
sat	saturation
vap	vaporisation
solar	solar heat

3.4. References

1. Berzins, M., Furzeland, R.M., '*A user's manual for SPRINT - a versatile software package for solving systems of algebraic, ordinary and partial differential equations: Part 1 - Algebraic and ordinary differential equations*', Shell Research Limited, Thornton Research Centre, TNER.85.058 (non-confidential), 1985.
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4. THE LPOOL MODEL

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4. THE LPOOL MODEL

4.1. Introduction

The EVAP model describing the evaporation of liquid pools, as available in HGSYSTEM version 1.0 (or NOV90), has been replaced by a completely new pool model called LPOOL. LPOOL is based on the LSM90 model developed by Exxon Research and Engineering Company (USA). Technical information on the LSM90 model is given in references [1,2].

LPOOL can calculate transient (time-dependent) evaporative fluxes coming from a multi-compound liquid pool on ground or water. LPOOL can treat boiling and non-boiling pools. It allows for the specification of a circular dike (dam or bund).
LPOOL allows the user to specify liquid spill rates, but it can also *calculate* spill rates from a (pressurised) cylindrical vessel using either choked flow or liquid Bernoulli relations.

All basic technical information concerning the LPOOL/LSM90 model can be found in [1]. Here only the specific LPOOL features will be discussed.

4.2. Differences between LPOOL and LSM90

The LPOOL model is basically the same as the LSM90 model of the Exxon Research and Engineering Company. However, it was necessary to modify some aspects of the LSM90 model. These differences are listed here.

4.2.1. Physical properties database

The LSM90 uses the proprietary *physical properties database* DIPPR. DIPPR is sponsored by the American Institute of Chemical Engineers (AIChE).
To enable unrestricted public release of HGSYSTEM, the use of DIPPR had to be replaced by the use of the HGSYSTEM database program DATAPROP.
DIPPR is used as an on-line database, however, DATAPROP can only be used as a separate model prior to an LPOOL model run.

4.2.2. Updating physical properties

In the original LSM90 code, all compound properties were fully updated as a function of temperature. In LPOOL, properties as generated by DATAPROP at a representative temperature are used. The saturated pressures of all compounds are still evaluated as full functions of fluid temperature.

Two properties, not available in DATAPROP, were given a constant value for all compounds which is a good approximation as these properties are not very important in the simulation.

These properties are: liquid surface tension (used value is 0.02 N/m^2 = 0.02 kg/s^2) and liquid thermal conductivity (used value is 0.15 W/(m·K)). *These two properties are only used in the (optional) auto-aerosol calculation and then only for single-compound mixtures.*

Tests have shown that the differences caused by using DATAPROP rather than DIPPR are smaller than 10 % in calculated average evaporative fluxes and pool properties.

4.2.3. Input parameters

The structure of the input file for LPOOL is the same as that of other HGSYSTEM modules and quite different from the LSM90 input file format. However, almost all LSM90 input parameters are still available to LPOOL users. The LSM90 parameters that are used in the auto-aerosol algorithm (Weber number, N density etc.) are used with their default values and cannot be changed by setting LPOOL input parameters.

Some LPOOL input parameters are not used by LSM90 directly, but are only relevant for the specific HGSYSTEM implementation. For example DTLINK in the CONTROL input block, which is used to write the HEGADAS-T file.

Using the LPOOL input data, a standard LSM90 input file (LSM90.IN) is written and then the LSM90 model is invoked.

File names associated with an LPOOL run are completely in line with the HGSYSTEM file naming conventions as explained in Chapter 3, paragraph 5 of the HGSYSTEM User's Manual.

4.3. References

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5. PLUME OR JET MODELS IN HGSYSTEM

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5. PLUME OR JET MODELS IN HGSYSTEM

The HGSYSTEM package contains two models to describe the dispersion of a jet release from a pressurised vessel. AEROPLUME can be applied to non-reactive, multi-compound two-phase jets and HFPLUME describes jet dispersion using the full hydrogen fluoride (HF) chemistry and thermodynamics. The two thermodynamical models used, are discussed in detail in Chapter 2. Chapter 2.A. describes the thermodynamics as used in AEROPLUME and Chapter 2.B. describes the hydrogen fluoride thermodynamical model as used in HFPLUME.

AEROPLUME and HFPLUME both have a similar discharge model to estimate release (discharge) rates from a given pressurised vessel.

In the new HGSYSTEM version 3.0, AEROPLUME replaces the PLUME model which was available in the first plublic domain release, HGSYSTEM version 1.0 (also called NOV90 version). PLUME could only deal with ideal gas releases.

In Chapter 5.A, the *AEROPLUME implementation* in HGSYSTEM version 3.0 is discussed in considerable detail.

AEROPLUME, HFPLUME and the old PLUME model, all share the same basic *plume development description*. This basic plume model is discussed in Chapter 5.B. In this chapter also validation studies for the HGSYSTEM plume models are discussed.

The main difference between AEROPLUME and HFPLUME (and PLUME) is the thermodynamical description of the released fluid. Also the way in which the thermodynamical relations are solved is different in AEROPLUME and HFPLUME. This is discussed in Chapter 5.A., paragraph 5.A.7.

As HFPLUME is very similar to AEROPLUME, apart from the thermodynamics, there is no separate discussion of HFPLUME in this Technical Reference Manual.

5.A. THE AEROPLUME MODEL

5.A.1. Introduction

The module in HGSYSTEM version 1.0 (or NOV90 version) describing steady-state pressurised releases of a non-reactive pollutant, PLUME, has been updated considerably for use in HGSYSTEM version 3.0, resulting in the newly named AEROPLUME model.

This chapter provides details about the implementation of the AEROPLUME (version 1.4) module of HGSYSTEM version 3.0. AEROPLUME can be used to simulate the jet (plume) development of a release, from a pressurised vessel or from a stack, of a mixture of several non-reacting compounds, which can form one or more single or multi-compound aerosols.

AEROPLUME is in fact the result of combining the multi-compound, two-phase thermodynamical model as described in Chapter 2.A. with a PLUME (HFPLUME) jet description.

After a general introduction into the AEROPLUME code, the aerosol algorithms will be summarised, then the reservoir and the post-flash calculations will be reviewed and finally a summary of the equations describing the jet development will be given.

In Chapter 5.B, the general plume or jet description developed for the old PLUME model, is given. This chapter gives more details on the plume relations as discussed in paragraph 5.A.7 of the current Chapter 5.A.

Detailed information on AEROPLUME input parameters can be found in the AEROPLUME chapter of the HGSYSTEM 3.0 User's Manual.

Please note that the HFPLUME model in HGSYSTEM is simply an HF-specific version of the AEROPLUME model. The basic discharge model and jet description are very similar to the one described in the current chapter. For this reason, HFPLUME will not be described separately in this Technical Reference Manual. HFPLUME input parameters are described in the HGSYSTEM 3.0 User's Manual.

5.A.2. The AEROPLUME code

Within the AEROPLUME code several main program blocks can be distinguished.

First there are the *specific thermodynamic routines* which contain the multi-compound aerosol model. These routines calculate the plume thermodynamic variables, the reservoir state and the post-flash or stack conditions. The structure is completely modular in the sense that the thermodynamic routines are completely separated from the routines calculating the plume development. The only communication is via the parameter lists.

The second main block consists of the routines to calculate the *jet (plume) development*. These are basically the same routines as used in the old PLUME model (HGSYSTEM version 1.0) and in HFPLUME. They contain, among other things, the entrainment models, the geometry model and the plume integration routines which describe the position and composition (air and pollutant) of the plume as it travels onward from its release point.
The original jet development description as used for the old PLUME model can be found in Chapter 5.B.
In the current chapter the specific AEROPLUME implementation is discussed.

Two of the solved variables are the plume enthalpy H and the total mass flow rate (pollutant plus mixed-in air) $\dot{m}$ (see paragraph 5.A.7). Together with the pollutant mass flow rate (or discharge rate), which is a constant, these variables are communicated to the thermodynamic routine in which the complete thermodynamic state of the plume at the current position is then calculated. The plume density and temperature and the pollutant concentration are output from the thermodynamic routine. Only the plume density is actually being used by the plume integration routines as will be discussed in more detail in paragraph 5.A.7.

A third main block contains the routines describing the *thermodynamic state of the ambient atmosphere* as a function of height, given the stability class and a set of reference values.

A last block that can be distinguished contains the *input and output* routines.

Because the thermodynamics is now built in a systematic, modular way, it should be a straightforward task to replace the current thermodynamics model by another one if required.

Finally it should be noted that it is still possible to run AEROPLUME in the vapour-only mode (i.e. the old PLUME model), but condensation of ambient water is now fully taken into account.

5.A.3. Summary of the aerosol algorithm

A more detailed exposure of the HGSYSTEM multi-compound, two-phase aerosol model can be found in Chapter 2. The formulation as given in this chapter is as used in HEGADAS and HEGABOX. AEROPLUME uses a slightly different formulation as will be discussed below.

onsider a mixture of *N* chemical compounds which in principle can form *M* aerosols. Aerosol β ($\beta = 1, 2, \ldots, M$), when actually formed, will contain the compounds α where $\alpha = n^{\beta-1}+1, \ldots, n^{\beta}$ ($0 = n^0 < n^1 < \ldots < n^M = N$). See Chapter 2 for more details.

Thus any combination of single compound and multi-compound aerosols is possible.

A slightly modified version of the *general* solution algorithm for the aerosol equations as given in Chapter 2.A.

The set of equations, occurring in the innermost iteration loop of the aerosol algorithm, from which the mole fraction liquid L^{β} of each aerosol β that forms is calculated, is solved using the non-linear algebraic equation solver NAESOL [1]. The solver proves to be very robust: the solutions for the L^{β}'s are found without any convergence problems.

The modification made to the algorithm as proposed in Chapter 2, concerns the handling of the singular point at T = 0° C (273.15 K) where a phase change of liquid water to ice takes place, if any water is present in the mixture.
To prevent a discontinuity occurring in the enthalpy H at 0° C, because of the ice formation term, a *melting range* $[T_1,T_2]$ has been introduced, where $T_1 < 0°$ C and $T_2 > 0°$ C. Within this melting range the enthalpy changes *linearly* from its value at T_1 to its value at T_2 and thus effectively the sharp jump has been removed. This was necessary because during the jet development calculations the former discontinuity gave rise to convergence problems of the solver of the differential equations involved. In the present implementation $T_1 = -0.15°$ C and $T_2 = +0.15°$ C .

When calculating the overall aerosol mixture density, in the original formulation (Chapter 2.A.), the volume of the liquid phase is neglected. Within a pressurised release context however, this is no longer a valid simplification as liquid mole fractions can be high. Therefore the overall mixture density ρ in AEROPLUME is calculated as follows:

$$\rho = \frac{M}{\left\{ \sum_{\alpha=1}^{N} \frac{M_{\alpha} \cdot y_{\alpha\ell}}{\rho_{\alpha\ell}} + (1-L) \cdot \frac{R_0 \cdot T}{P} \right\}} \tag{1}$$

where M is the mixture molar mass, M_{α} the molar mass of compound α, $y_{\alpha\ell}$ the molar fraction within the mixture of the liquid phase of compound α, $\rho_{\alpha\ell}$ is the liquid density of compound α, L is the overall liquid mole fraction of the mixture, R_0 the universal gas constant, T the mixture temperature and P the mixture (vapour phase) pressure.

Of course the first term within the curly brackets is associated with the *liquid volume* and the second term with the *vapour volume*, assuming ideal gas behaviour.
The mixture molar mass M is found from

$$M = \sum_{\alpha=1}^{N} y_\alpha \cdot M_\alpha \tag{2}$$

where y_α is the mixture mole fraction of compound α.

5.A.4. The reservoir state calculation

Within the context of two-phase fluid storage and discharge, it is important to emphasise that the reservoir conditions being used should be representative of the fluid conditions in the immediate neighbourhood of the discharge orifice. The aerosol model in fact uses a *pseudo-one-phase* approach: liquid and vapour are assumed to be *homogeneously* distributed in terms of the vapour-liquid ratios. Single liquid droplets can *not* be distinguished and a droplet size distribution is *not* being used.

For a given situation the user should realise that the location of the orifice can strongly influence the liquid-vapour ratio of the discharged fluid. E.g. if in a reservoir filled with propane half of the volume is occupied by liquid propane and the other half by propane vapour, depending on the location of the discharge orifice either a pure liquid release or a pure vapour release would occur. It is the user's responsibility to supply the correct reservoir conditions. The code will give details on the reservoir state and on the post-flash state to enable the user to check if the correct case is being simulated.

From the user-supplied reservoir conditions (temperature and pressure) and from the user-supplied mixture composition (compound names and mole fractions) the equilibrium reservoir state can be calculated using a simplified version of the aerosol algorithm as mentioned above. The simplification lies in the fact that the temperature T is now given. Instead of a double iteration loop to calculate T and the L^β's, a single loop for the L^β's only, is being used.
Again, the algorithm proves to be very robust.

When using the aerosol thermodynamics model, the user has the option *not* to specify the reservoir pressure. In this case the AEROPLUME program will calculate the reservoir mixture *saturation pressure* at the (user-supplied) reservoir temperature T_{res} using Raoult's law as follows

$$P_{sat,mix} = \sum_{\alpha=1}^{N} y_\alpha \cdot P_{sat,\alpha}(T_{res}) \tag{3}$$

where y_α is the mixture mole fraction of compound α and $P_{sat.\alpha}(T)$ is the saturated vapour pressure of compound α. It is assumed in (3) that the sum of the molar fractions y_α is 1.

The reservoir pressure is then set to this saturation pressure.

It is thus assumed that all compounds α are in the *liquid-only* state. If this assumption is reasonable, then relation (3) will give a reasonable reservoir pressure.

5.A.5. Calculation of post-flash conditions

To initiate the actual jet development calculations, the initial post-flash jet properties are calculated from the reservoir state and the user-supplied orifice diameter and discharge mass flow rate. These properties are: U_{flash}, H_{flash} and D_{flash}, which are velocity, enthalpy and diameter of the jet respectively.

From these the thermodynamic (aerosol) model gives values for the temperature T_{flash} and density ρ_{flash}.

The pollutant concentration is taken to be 100 % as air entrainment is assumed to be negligible during this initial flashing process.

The calculation consists of two parts. First an adiabatic and frictionless acceleration of the (stagnant) reservoir fluid to a point just outside the orifice is assumed. Vapour and liquid velocities are assumed equal. There is no inter-phase heat exchange.

The maximum possible mass flow rate is calculated using choked flow relations and some vapour is assumed to be present in all cases, because for a liquid only mixture ($L = 1$) there is no limitation to the mass flow rate (frictionless flow). The vapour phase is assumed to behave as an ideal gas.

It is also assumed that the mixture liquid-vapour composition does not change during this (rapid) acceleration phase (frozen equilibrium). The fluid velocity and enthalpy just outside the orifice or *stack* are denoted by U_{stk} and H_{stk} respectively and the local fluid pressure there is P_{stk}.

The second part of the calculation is called the 'flashing' of the mixture: the new thermodynamic state of the mixture is calculated using the full aerosol algorithm, assuming that the pressure decreases from P_{stk} to the ambient atmospheric pressure P_{atm}. At this stage the liquid-vapour composition does change and the post-flash fluid properties as mentioned above are then calculated.

More details about the actual relations being used will now be given below.
To describe the adiabatic and frictionless acceleration from the reservoir to the stack two basic equations are used. Momentum conservation gives

$$dP/\rho + d(U^2/2) = 0 \tag{4}$$

and energy conservation gives

$$H_{res} = H + U^2/2 \tag{5}$$

These relations are valid at every point between the reservoir and the orifice.

During the acceleration process the vapour phase of the mixture, assumed to be an ideal gas, will experience adiabatic expansion and thus

$$P \cdot \rho_g^{-\gamma} = Cst \tag{6}$$

where γ is the ratio of the specific heats of the vapour, i.e. $\gamma = c_p/c_v$ and ρ_g is the vapour density.

The liquid density is *not* affected by the change in pressure.

Integrating (4) and using (1) and (6), $U^2/2$ at any point between reservoir and stack is found to be equal to

$$\frac{U^2}{2} = \frac{\sum_{\alpha=1}^{N} \frac{M_\alpha \cdot y_{\alpha\ell}}{\rho_{\alpha\ell}}}{M} \cdot (P_{res} - P) + \frac{1-L}{1-1/\gamma} \cdot \left(\frac{1}{a_{g,res}} - \frac{1}{a_g} \right) \tag{7}$$

where the auxiliary variables a_g and $a_{g,res}$ are given by

$$a_g = \frac{M}{R_0 \cdot T} \tag{8a}$$

$$a_{g,res} = \frac{M}{R_0 \cdot T_{res}} \tag{8b}$$

To find the maximum mass discharge rate, it can be seen that this is equivalent to finding the maximum of $\rho \cdot u$ (discharge area is constant) or (equivalently) the maximum of $\rho^2 \cdot u^2$, all as function of ρ. Thus the equation to be solved is

$$\frac{d}{d\rho}\left(\rho^2 \cdot U^2\right) = 0 \tag{9}$$

When working out this constraint by using (7), it is found that for the maximum discharge rate occurring at the choke pressure P and choke velocity U the condition

$$\frac{(1-L) \cdot R_0 \cdot T}{M} \cdot \frac{1}{\gamma} \cdot \left(\frac{\rho \cdot U}{P}\right)^2 = 1 \tag{10}$$

holds, which is valid together with relation (7).

Note that for L = 1 (liquid-only mixture) this relation (10) *no longer* holds: for a frictionless flow the liquid-only mass flow rate is *not* limited.

Using the NAESOL package[1], the set of equations (7) and (10) can be solved for P and U when using the adiabatic expansion relation for an ideal gas to calculate T

$$\frac{T}{T_{res}} = \left(\frac{P}{P_{res}}\right)^{1-1/\gamma} \tag{11}$$

It is the vapour phase of the mixture which can limit the mass flow rate to the choked flow value, and equation (11) is used to take a temperature drop during expansion of *the vapour* into account because this will significantly influence the value of the maximum (choked) mass flow rate. Using (11), the heat *exchange* between the two phases (liquid and vapour) in the mixture is being neglected.

Once U is found, the maximum mass flow (discharge) rate, $\dot{m}_{max}$, dictated by choked flow, is equal to $\dot{m}_{max} = A_{stk} \cdot U \cdot \rho$, where A_{stk} is the orifice surface area ($= \pi \cdot D_{stk}^2/4$).

It is interesting to consider the alternative approach which *replaces* the condition of maximum mass flow rate (9) by the condition that the maximum mass flow rate occurs when

$$U = C \tag{12}$$

where C is the local speed of sound in the two-phase mixture. An expression for C given by Wallis ([2], equation 2.51) is used

$$\frac{1}{C^2} = \left(v \cdot \rho_g + (1-v) \cdot \rho_\ell\right) \cdot \left(\frac{v}{\rho_g \cdot C_g^2} + \frac{1-v}{\rho_\ell \cdot C_\ell^2}\right) \qquad (13)$$

where v is the volumetric void fraction (volume fraction vapour in the mixture) and C_g and C_ℓ the speeds of sound in the gas and liquid phase respectively and ρ_g and ρ_ℓ the respective densities.

Now substitute for the speed of sound in the vapour phase, C_g, the well-known expression valid for ideal gases

$$C_g^2 = \gamma \cdot \frac{P}{\rho_g} \qquad (14)$$

To express v in mass fractions some auxiliary relations are needed, it can be seen after some manipulation that

$$v = \frac{\rho_\ell \cdot (1-X)}{\rho_\ell \cdot (1-X) + \rho_g \cdot X} \qquad (15a)$$

where X is the *mass* fraction liquid in the mixture.
X can be expressed in terms of L by the relations

$$\frac{X}{\rho_\ell} = \frac{\sum_{\alpha=1}^{N} \frac{M_\alpha \cdot y_{\alpha\ell}}{\rho_{\alpha\ell}}}{M} \qquad (15b)$$

and

$$\frac{1-X}{\rho_g} = (1-L) \cdot \frac{R_0 \cdot T}{M \cdot P} \qquad (15c)$$

At this point (and not earlier!) the limit for C_ℓ going to infinity is

$$U^2 = C^2 = \frac{\gamma \cdot P^2 \cdot M}{(1-L) \cdot R_0 \cdot T \cdot \rho^2} \qquad (16)$$

which is identical to (10).

Thus the *maximum mass flow rate constriction is equivalent to the constriction* $U = C$, which is a well-known result for ideal gases but is shown here to hold for two-phase flow also.

However, given the fact that the whole concept of *speed of sound* for two-phase fluids is unclear, this result should be considered to be merely a (nice) coincidence. The only correct, unambiguous, way to derive equation (10) is to use the maximum mass flow rate argument, i.e. start from equation (9).

For the special case of a vapour only mixture ($L = 0$, $X = 0$ and $\nu = 1$) the following relations are valid

$$P = P_{res} \cdot \left(\frac{2}{1+\gamma} \right)^{\gamma/_{\gamma-1}} \qquad (17a)$$

and

$$\frac{U^2}{2} = \frac{\gamma}{1+\gamma} \cdot \frac{P_{res}}{\rho_{res}} \qquad (17b)$$

Thus for this case an *analytical solution* for the set of equations (7) and (10) is available and the numerical code NAESOL is not needed to find U and P.

If the choke pressure turns out to be less than the ambient pressure P_{atm}, then the maximum mass flow rate is calculated based on the assumption that $P = P_{atm}$. In fact *unchoked flow* occurs in this case.

The AEROPLUME code checks if the user-specified mass flow rate is admissible (i.e. less than the maximum mass flow rate as calculated above) and if it is, then the *stack conditions* U_{stk}, P_{stk}, ρ_{stk} and D_{stk} are calculated by solving the mass conservation equation

$$A_{stk} \cdot \rho_{stk} \cdot U_{stk} = \dot{m} \qquad (18)$$

and equation (7) simultaneously.

In general $\dot{m}$ is the plume mass flow rate, but before the actual plume calculations have started $\dot{m}$ is equal to the pollutant release rate (in kg/s) because no ambient air has been entrained into the plume yet.

If P_{stk} is less than the ambient pressure then the AEROPLUME code halts with an error message and the user should modify either $\dot{m}$ or the reservoir conditions.

The enthalpy H_{stk} is calculated using (5)

$$H_{stk} = H_{res} - \frac{U_{stk}^2}{2} \tag{19}$$

From (19) it can be seen that for high orifice velocities H_{stk} can become large negative. It even can occur that H_{stk} falls below a physically acceptable minimum value (dictated by $T > 0$ K). The code calculates the minimum value of H for the current mixture composition and halts execution if H_{stk} is less than this minimum value.

If H_{stk} is acceptable then the actual flash calculation is started: the new thermodynamic state of the mixture, when the pressure has dropped from P_{stk} (always $\geq P_{atm}$) to P_{atm}, is calculated. In general, the liquid-vapour ratio will change during flashing.

The velocity after depressurisation is calculated to be

$$U_{flash} = U_{stk} + \frac{P_{stk} - P_{atm}}{\rho_{stk} \cdot U_{stk}} \tag{20}$$

which follows from a control volume analysis, valid for (assumed) one-dimensional flow and considering momentum-*flux*. It is *not* assumed that the cross-sectional area remains constant during depressurisation.

The enthalpy of the post-flash mixture is then simply

$$H_{flash} = H_{res} - \frac{U_{flash}^2}{2} \tag{21}$$

Again the code checks whether H_{flash} exceeds the minimum value.

The value of the enthalpy H_{flash} together with the fact that the jet is assumed to be pure pollutant (no entrained air yet) completely determine the thermodynamic state of the post-flash jet and this state is calculated using the standard aerosol thermodynamic routines. Density, temperature and liquid mole fraction are thus calculated.

The diameter of the post-flash jet is calculated by

$$D^2_{flash} = \frac{4 \cdot \dot{m}}{\pi \cdot \rho_{flash} \cdot U_{flash}} \qquad (22a)$$

This completes the post-flash jet state calculation.

Please note that instead of the release from a reservoir scenario, the user has the option of simulating a *vent stack* problem using AEROPLUME (see information on input parameters in Appendix A). In this case the reservoir and post-flash calculations, as discussed in paragraph 5.A.4 and 5.A.5, are skipped and the post-flash velocity U_{flash} is calculated directly from the pollutant mass flow rate $\dot{m}$, stack release temperature T_{stk} and the stack diameter D_{stk} (all three user-specified), by simply using

$$U_{flash} = \frac{4 \cdot \dot{m}}{\pi \cdot \rho_{stk} \cdot D^2_{stk}} \qquad (22b)$$

The density of the stack release, ρ_{stk}, is calculated by AEROPLUME using the full thermodynamic model and assuming that the stack release mixture has the user-specified temperature T_{stk} and is at the ambient atmospheric pressure P_{atm}. This also gives the value of the pollutant stagnation enthalpy at the stack and H_{flash} is found from relation (21) with H_{res} being replaced by the stack stagnation enthalpy.

This option was introduced to simplify the use of AEROPLUME for stack simulations where the concept of a reservoir is not applicable (i.e. the old PLUME scenario).

5.A.6. Discharge rate specification

From the discussion above (paragraph 5.A.5), it follows that the user can specify any pollutant discharge rate (mass flow rate) that does not exceed the maximum possible discharge rate as dictated by the AEROPLUME discharge model.

However, it is not always easy to predict the discharge rate for given reservoir conditions and orifice dimensions. Therefore the user of AEROPLUME has the option *not* to specify the pollutant mass flow rate and in this case the code will use a literature correlation to fix its value. Again it is noted that at the start of the plume calculation, the plume mass flow rate $\dot{m}$ is equal to the pollutant mass flow rate, as no ambient air has been entrained yet.

A value of $\dot{m}$ that follows from AEROPLUME's own discharge model is also printed out to give the user more information on the possible range of values and enable him to make a reasonable choice for the actual value of $\dot{m}$ to be used in the simulations.

For a *gas-only* release the discharge rate used by the program is simply the (maximum) discharge rate found for an ideal gas (either choked or unchoked) which the AEROPLUME discharge model will calculate.

For choked vapour only flow, using relations given above, the discharge rate is

$$\dot{m} = C_D^g \cdot A_{stk} \cdot \left(\frac{2}{1+\gamma}\right)^{1/(\gamma-1)} \cdot \left(\frac{\gamma}{1+\gamma}\right) \cdot \sqrt{2 \cdot \rho_{res} \cdot P_{res}} \qquad (23a)$$

and for unchoked vapour only flow, using ideal gas relations

$$\dot{m} = C_D^g \cdot A_{stk} \cdot \sqrt{\frac{\gamma}{\gamma-1}} \cdot \sqrt{2 \cdot \rho_{res} \cdot P_{res} \cdot \left\{ \left(\frac{P_{atm}}{P_{res}}\right)^{\frac{2}{\gamma}} - \left(\frac{P_{atm}}{P_{res}}\right)^{\frac{\gamma+1}{\gamma}} \right\}} \qquad (23b)$$

The vapour discharge coefficient C_D^g has a default value of 1.0, but the user of the AEROPLUME model can override this value if necessary.

For a *two-phase* release, first the mixture saturation pressure P_{sat} is calculated as

$$P_{sat} = \frac{\sum_{\alpha=1}^{N} y_{\alpha\ell} \cdot P_{sat,\alpha}(T)}{\sum_{\alpha=1}^{N} y_{\alpha\ell}} \qquad (24)$$

where $y_{\alpha\ell}$ is the molar fraction within the total mixture of liquid compound α and $P_{sat,\alpha}(t)$ is the saturation pressure of compound α at temperature T.

This relation is based on Raoult's law and should be compared with relation (3). Note that in (3) the sum of the molar fractions is always 1, but in (24) the sum of the $y_{\alpha\ell}$ is not necessarily equal to 1.

If P_{sat} is less than P_{atm} then the liquid mixture is *subcooled* even at atmospheric conditions and no flashing will occur at the exit.

From Fauske and Epstein [3] a Bernoulli-like expression for the discharge rate is found

$$\dot{m}(t) = -C'_D \cdot A \cdot \sqrt{2 \cdot \rho_\ell(t) \cdot (P(t) - P_{atm})} \tag{25}$$

where ρ_ℓ is the density of the *liquid* in the reservoir. The liquid discharge coefficient C'_D has a default value of 0.61 [3], but again the user can override this value by setting a SPILL input parameter.

When P_{sat} exceeds P_{atm}, i.e. the liquid mixture in the reservoir, which is subcooled at reservoir conditions, is *not* subcooled at atmospheric conditions, then a distinction must be made between reservoir conditions that are *near the saturation point* and those that are not.

If $|P(t) - P_{sat}| > 10 \cdot P_{sat}$ (reservoir conditions far from the saturation point) then following [3]

$$\dot{m}(t) = -C'_D \cdot A \cdot \sqrt{2 \cdot \rho_\ell \cdot |P(t) - P_{sat}|} \tag{26}$$

If $|P(t) - P_{sat}| < 0.1 \cdot P_{sat}$ (reservoir conditions near the saturation point), [3] gives

$$\dot{m}(t) = -C'_D \cdot A \cdot \sqrt{\left|\frac{1}{dv/dP}\right|} \tag{27}$$

where $v = 1/\rho$ (m^3/kg) is the specific volume of the mixture. The term $\left|\frac{1}{dv/dP}\right|$ is estimated, following [3], by

$$\left|\frac{1}{dv/dP}\right| = \left(\frac{h_{vap}}{\Delta v_{vap}}\right)^2 / (T \cdot C_{p,\ell}) \tag{28}$$

where h_{vap} (J/kg) is the heat of vaporisation, Δv_{vap} (m^3/kg) the change in specific volume going from the liquid to the vapour state, $C_{p,\ell}$ (J/(kg·K)) is the specific heat of the liquid mixture and T (K) is the reservoir temperature.

For the intermediate stage, $0.1 \cdot P_{sat} \le |P(t) - P_{sat}| \le 10 \cdot P_{sat}$, *linear interpolation* between the two previous cases is used. Let FACTOR, TERM1 and TERM2 be defined by

$$\text{FACTOR} = \frac{|P(t) - P_{sat}|}{P_{sat}} \tag{29}$$

$$\text{TERM1} = 2 \cdot \rho_\ell \cdot |P(t) - P_{sat}| \tag{30}$$

$$\text{TERM2} = \left| \frac{1}{dv/dP} \right| \tag{31}$$

Define the variable TERM3 by using linear interpolation between TERM1 and TERM2 using FACTOR, that is

$$\text{TERM3} = \text{TERM2} + (\text{FACTOR} - 0.1) \cdot \frac{\text{TERM1} - \text{TERM2}}{10.0 - 0.1} \tag{32}$$

and the reservoir mass discharge rate when $0.1 \cdot P_{sat} \leq |P(t) - P_{sat}| \leq 10 \cdot P_{sat}$, is given by

$$\dot{m}(t) = -C_D^f \cdot A \cdot \sqrt{\text{TERM3}} \tag{33}$$

This linear interpolation procedure for the case where $0.1 \cdot P_{sat} \leq |P(t) - P_{sat}| \leq 10 \cdot P_{sat}$ is found to give more satisfactory results than the recommendation in [3] , the latter being equivalent to taking TERM3 = TERM1 + TERM2.

Please note that the mass discharge literature correlations and the definition of P_{sat} used in SPILL and AEROPLUME are completely identical. The SPILL model is discussed in Chapter 3.

The AEROPLUME code will use the appropriate correlation to specify $\dot{m}$ if the user does not specify $\dot{m}$ himself. However if the discharge rate given by the correlations exceeds the maximum mass flow rate as calculated by the AEROPLUME discharge model, then $\dot{m}$ will be set to the value of this maximum mass flow rate. All relevant calculated mass flow rates are given in the AEROPLUME output messages.

Also note that when following the vent stack scenario (no specification of reservoir conditions but specification of the stack release temperature instead) the user *must* specify a positive value for the mass flow rate to completely prescribe the release conditions. In this case (no reservoir and discharge calculations) *any* mass flow rate is acceptable as there is no choked-flow mass flow rate restriction.

5.A.7. Plume development model

The development of the plume as it travels from its release point through the ambient atmosphere, including touchdown with the ground surface, is described by a mathematical model as given in Chapter 5.B.

In the current AEROPLUME code, a set of 4 algebraic and 10 first order ordinary differential equations is used to describe the plume development. This set of equations is different from the one used in the old PLUME model or in HFPLUME, because the thermodynamic equations are no longer solved *coupled* with the plume integration ones, but they have been *separated out* into the specific thermodynamic routines as discussed earlier. See Chapter 5.B. for more details on the general PLUME and HFPLUME jet formulation. Furthermore, the temperature T is no longer being used as a basic variable, but the enthalpy H instead. And finally, as the thermodynamic routine calculates the pollutant concentration, using the total mass flow rate and the pollutant mass flow rate, it is no longer needed to have the pollutant concentration as an explicit variable in the plume integration system, as was the case in PLUME and HFPLUME.

For completeness sake the complete set of equations governing the plume development is given below.

The fourteen basic plume variables used are: enthalpy H, velocity U, diameter D, inclination with respect to the horizontal φ, ambient velocity U_{atm}, ambient pressure P_{atm}, ambient temperature T_{atm}, total mass flowrate $\dot{m}$, excess energy flux $\dot{E}$, excess horizontal momentum flux $\dot{P}x$, excess vertical momentum flux $\dot{P}z$, horizontal displacement X, plume centroid height Z and finally time t.

All variables are plume-diameter-averaged. This is the 'top-hat' approach as mentioned in Chapter 5.B.

The time t is not needed for the actual AEROPLUME calculations, but the total elapsed time (release duration) is communicated to HEGADAS if a link between the two programs is being made.

The fourteen equations are now given; first the four *algebraic constraints*, then the ten *ordinary differential equations*.

Conservation of mass

$$\dot{m} = A(D,Z,\varphi)\cdot\rho\cdot U \qquad \text{(I)}$$

where the plume surface area A(D,Z,φ) depends on the plume state (airborne, touchdown or slumped) as discussed in Chapter 5.B.

Note that the plume density ρ is *not* one of the solved variables, but is calculated within the thermodynamic routine which is called every time the thermodynamic state needs to be updated.

Conservation of excess horizontal momentum

$$\dot{P}x = \dot{m} \cdot (U \cdot \cos(\varphi) - U_{atm}) \qquad \text{(II)}$$

Conservation of excess vertical momentum

$$\dot{P}z = \dot{m} \cdot U \cdot \sin(\varphi) \qquad \text{(III)}$$

Conservation of excess energy

$$\dot{E} = \dot{m} \cdot \left(H + \frac{U^2}{2} - H_{atm} - \frac{U^2_{atm}}{2} \right) \qquad \text{(IV)}$$

where H_{atm} is given by a standard atmospheric correlation.

Next, three differential equations describe the change in atmospheric state variables as the plume travels along.

$$\frac{dU_{atm}}{ds} = \frac{dU_{atm}}{dZ} \cdot \sin(\varphi) \qquad \text{(V)}$$

$$\frac{dP_{atm}}{ds} = -\rho_{atm} \cdot g \cdot \sin(\varphi) \qquad \text{(VI)}$$

$$\frac{dT_{atm}}{ds} = \frac{dT_{atm}}{dZ} \cdot \sin(\varphi) \qquad \text{(VII)}$$

where $\frac{dU_{atm}}{dZ}$, ρ_{atm} and $\frac{dT_{atm}}{dZ}$ are given by standard atmospheric correlations. The parameter s is the integration parameter along the plume axis. Finally, g is the acceleration of gravity.

Next, the differential equations describing the change of the four conserved physical quantities (mass, horizontal and vertical momentum and energy) are given.

$$\frac{d\dot{m}}{ds} = \text{Entr}^{A(s)}_{Amb} \qquad \text{(VIII)}$$

where $\mathrm{Entr}_{\mathrm{Amb}}^{\mathrm{A(s)}}$ is the amount of ambient air entrained by the jet as given by the entrainment model as described in Chapter 5.B.

$$\frac{d\dot{E}}{ds} = -\dot{m} \cdot \left(\frac{dH_{atm}}{dZ} + U_{atm} \cdot \frac{dU_{atm}}{dZ} + g \right) \cdot \sin(\varphi) \qquad \text{(IX)}$$

where $\frac{dH_{atm}}{dZ}$ is again given by a correlation.

$$\frac{d\dot{P}x}{ds} = -\mathrm{Shear} - \mathrm{Drag}_x - \mathrm{Impact}_x \qquad \text{(X)}$$

Shear, Drag and Impact are the forces working on the plume. For details see Chapter 5.B.

$$\frac{d\dot{P}x}{ds} = -\mathrm{Buoy} - \mathrm{Foot} - \mathrm{Drag}_z - \mathrm{Impact}_z \qquad \text{(XI)}$$

where again expressions for Buoy and Foot are given in Chapter 5.B.

Finally there are three simple differential equations describing displacement, height and time development.

$$\frac{dX}{ds} = \cos(\varphi) \qquad \text{(XII)}$$

$$\frac{dZ}{ds} = \sin(\varphi) \qquad \text{(XIII)}$$

$$\frac{dt}{ds} = \frac{1}{U} \qquad \text{(XIV)}$$

This complete set of fourteen equations is solved using the SPRINT package [4] in the same way as in PLUME and HFPLUME.

5.A.8. References

1. Scales, L.E., '*NAESOL - A Software toolkit for the solution of nonlinear algebraic equation systems; User Guide - Version 1.5*', Shell Research Limited, Thornton Research Centre, TRCP.3661R, 1994.

2. Wallis, G.B., '*One-dimensional two-phase flow*', McGraw-Hill, New York, 1969.

3. Fauske, H.K., Epstein, M., '*Source term considerations in connection with chemical accidents and vapour cloud modelling*', J. Loss Prev. Process Ind., vol 1, April 1988.

4. Berzins, M., Furzeland, R.M., '*A user's manual for SPRINT - a versatile software package for solving systems of algebraic, ordinary and partial differential equations: Part 1 - Algebraic and ordinary differential equations*', Shell Research Limited, Thornton Research Centre, TNER.85.058, 1985.

5.A.9. Notation

A	surface area (m^2)
C	speed of sound (m/s)
C_D	discharge coefficient (-)
D	diameter (m)
$\dot{E}$	excess energy flux (J/s)
g	acceleration of gravity (m/s^2)
H	enthalpy (J/kg)
L	mole fraction liquid in aerosol mixture (-)
M	molar mass of mixture (kg/mole)
M	number of aerosols in mixture
$\dot{m}$	mass flow rate or discharge rate (kg/s)
N	total number of compounds
P	pressure (Pa)
$\dot{P}x$	excess horizontal momentum flux ($kg \cdot m/s^2$)
$\dot{P}z$	excess vertical momentum flux ($kg \cdot m/s^2$)
R_0	universal gas constant (8314 J/(kmole·K))
s	distance along plume axis (m)
T	temperature (K or °C)
t	time (s)
U	plume velocity in direction of plume axis (m/s)
v	specific volume (m^3/kg)
X	mass fraction liquid (-)
X	horizontal plume displacement (m)
y	molar fraction (-)
Z	plume centroid height (m)
γ	ratio of specific heats (c_p/c_v) for ideal gas (-)
φ	plume inclination with respect to horizontal (°)
ρ	plume density (kg/m^3)

ν	volumetric void fraction (-)

Subscripts and superscripts

atm	ambient atmosphere
α	compound indicator
flash	post-flash
g	vapour (gas) phase of a two-phase mixture
ℓ	liquid phase of a two-phase mixture
res	reservoir
sat	saturation
stk	stack, orifice

5.B. DEVELOPMENT OF PLUME AND JET RELEASE MODELS

5.B.1. Introduction

This chapter sets out the basic formulation and structure of the plume models PLUME, AEROPLUME and HFPLUME. The model describes initial jet flow, elevated plume, plume touchdown, and gravity-slumping following a pressurised release of an ideal gas (PLUME) or a two-phase multi-compound mixture (AEROPLUME) or an anhydrous hydrogen fluoride (HFPLUME).

PLUME and HFPLUME are available in version 1.0 of HGSYSTEM (NOV90 version). In version 3.0 of HGSYSTEM, PLUME has been replaced by AEROPLUME.

The HGSYSTEM plume models are comprehensive models of dispersion in the near-field. Prediction of far-field dispersion requires that these plume models be 'matched' (linked) either to a heavy gas dispersion model, such as HEGADAS-S, or else, for neutral or buoyant releases, to a passive dispersion model PGPLUME. See relevant Chapters on these far-field models in the HGSYSTEM documentation.

Previous work (Ooms 1972; Wheatley 1987a, 1987b); Forney and Droescher 1985; Birch and Brown 1988; McFarlane 1988; Raj and Morris 1987) on dense and buoyant plumes, two-phase and pressurised gas jets, reactive and ground-affected jets, supported the view that predictions accurate in context could be obtained by means of an essentially simple, one-dimensional, integral-averaged model.

The plume models have been validated against thermodynamic data for HF/moist-air systems (Schotte 1987, 1988); their entrainment formulations have been checked against observed dispersion of buoyant (Peterson 1987) and dense (Hoot, Meroney and Peterka 1973) (ideal) gases, and against (atmospheric) releases of liquid propane gas (Cowley and Tam 1988, McFarlane 1988).

The two-phase model AEROPLUME has been validated using data of liquid propane releases (Post 1994).

In addition the model combination HFPLUME/HEGADAS-S has been used (Chapter 7.A.) to simulate large-scale experimental releases of anhydrous hydrogen fluoride (Blewitt, Yohn, Koopman and Brown 1987; Blewitt, Yohn and Ermak 1987; Blewitt 1988).

The indications are that the plume models are satisfactory predictors of the early dispersion (plume rise, fall, touchdown, and early slumping) of a dense, neutral, or buoyant release.

5.B.2. The Stages of Plume Development

Prior to the development of the HGSYSTEM plume models, specifically for the HFPLUME model, we conducted a literature review in order to determine whether any existing model could be adapted to simulate a jet of anhydrous hydrogen fluoride (HF). The following sub-sections describe the results of that review for a number of models. The discussion is presented for the various zones of importance: external flashing, flow establishment, airborne plume, touchdown plume, slumped plume, and the far field.

From point of release to the far-field a dense plume passes through a series of (phenomenological) stages. These stages form the basis of the computer based models AEROPLUME, PLUME and HFPLUME: the identification, sequence, and characteristics of these stages is therefore of considerable importance. This section should make clear the need for a careful selection of literature available models, and for their extension to cover regions not previously considered.

External Flashing

Consider a pressurised release of an evaporating liquid (say HF). Such a release forms at the orifice a narrow zone in which take place pressure relaxation and violent 'flashing'. 'Flashing' is the sudden and disruptive evaporation of superheated liquid in response to a sharp fall in fluid pressure. This results in prompt atomisation of any residual liquid and in the development of a two-phase flow. This stage of plume development is extremely complex.

Fortunately details of 'flashing' flow are not needed: it is sufficient to 'bridge' this zone by means of integral conservation laws and by assuming that air entrainment during flashing is negligible (Wheatley 1987a, Raj and Morris 1987). The flashing zone ends when approximate thermal equilibrium, ambient pressure, and negligible inter-phase slip between vapour and liquid (droplet) phases are established. The velocity profile is roughly uniform; the cross-section may be assumed circular; deflection due to ambient pressure in cross-flow is typically negligible (Figure 5.1).

Flow Establishment

Immediately beyond the flashing zone there exists a second zone 'of flow establishment': air entrainment as the result of shear-induced turbulence results in the progressive dilution of the evaporating liquid jet, and in the radial diffusion of air towards the plume centre-line.

The flow is described by an unperturbed 'core' region, which diffusion of air has not reached, and by an axi-symmetric 'outer' region, in which turbulent diffusion has resulted in a near Gaussian distribution of entrained air. This zone ends with the complete 'erosion' of the core region and with the establishment of approximately self-similar conditions within the flow. The cross-section may be assumed circular (Figure 5.2).

Generally this region is either neglected (Raj and Morris 1987; Hoot, Meroney and Peterka 1973; Forney and Droescher 1985), or else considered in conjunction with such effects as stack 'downwash' (Hanna 1982; Ooms 1972; Havens 1987) and represented by an empirically derived correlation (Keffer and Baines 1963, Kanatani and Greber 1972). The discussion follows an analysis of Albertson Dai, Jensen and Hunter Rouse (1948), and of Abramovich (1963).

Airborne Plume

Following flow establishment, plume development is described by the interaction of plume, ambient wind, and buoyancy effects: the influence of the ground, except as a generator of ambient turbulence and of wind-shear is negligible.

This is the simplest of all the stages of plume development: nonetheless it is not without controversy. Arguments exists over the level of description necessary: whether *Gaussian* (Ooms 1972; Ooms and Duijm 1983; Petersen 1986; Schatzmann 1979) or '*top-hat*' (Hoot, Meroney and Peterka 1973; Forney and Droescher 1985; Davidson 1986) models are preferable; whether the effects of gradients within the atmosphere need be considered (Schatzmann and Policastro 1984); and whether or not significant 'drag' forces act upon a plume in cross-wind (Briggs 1984; Ooms 1972; Schatzmann 1979, Hoult, Fay and Forney 1969; Coelho and Hunt 1989).

Several different formulations for the crosswind entrainment have been proposed and checked against experimental data (Peterson 1978, 1987; Schatzmann 1978, Spillane 1983).

Even the basic formulation of the equations of motion has resulted in discussion (Schatzmann 1978, 1979; McFarlane 1988), and in the use of special devices, such as plume 'truncation' and dilute gas thermodynamics (Ooms 1972, Petersen 1978).

The cross-section is generally assumed to be circular; the flow axi-symmetric. However the presence of trailing vortices in cross-flow, and the cumulative effect of differences in vertical and horizontal diffusivity in the undisturbed atmosphere, will result in asymmetry and ultimately in an elliptic cross-section (Bloom 1980; Li, Leijdens and Ooms 1986). The role of dilute plume asymptotics in allowing estimation of certain entrainment coefficients from plume-rise and other data should be emphasised. Such early work as that of Briggs (1975) in the development of semi-empirical plume-rise correlations based on such analyses should not be neglected. (Figure 5.3).

Touchdown Plume

Dense plumes must ultimately drift to ground or at any rate expand as the result of entrainment so as to intersect the ground surface.

The ground interacts with a descending plume in several ways. First it acts as a geometrical constraint resulting in the redistribution of plume material. Second the ground allows the development of pressure forces as the result of pre-existing vertical momentum within the plume. These are impact forces resulting in the conversion of vertical to horizontal momentum. Third the ground permits the development of internal pressure within the plume as the result of gravity-slumping, in which the transverse motion of a gravity current is driven by an internally generated pressure acting at the ground surface. Finally drag forces must act at the ground as the result of differences in horizontal speed between plume and ambient wind.

In this region a transition must be made between a circular cross-section appropriate to an airborne plume, and a semi-elliptical (say) cross-section appropriate to an advected heavy-gas plume resting upon the ground (Figure 5.4). The touchdown region is described by a cross-section in the form of a circular segment. The region ends when a semi-circular cross-section first develops.

This transition region is neglected by Havens (1987, 1988a) following Ooms (1972) and Ooms and Duijm (1984), as well as (inter alia) by Bloom (1980), by Schatzmann (1979) and by Raj and Morris (1987).
No previous model exists which attempts to make a smooth transition from airborne dense to advected slumped plume. Limited experimental evidence does exist in the form of an unpublished study of dense salt water plumes (Karman 1986). In addition photographic evidence collected but not published by Hoot, Meroney and Peterka (1973) may form a useful data set for model validation.

Slumped Plume

Following touchdown the plume cross-section may be assumed semi-elliptic. Changes in plume eccentricity (aspect ratio) accommodate gravity slumping and the influence of residual ground-drag and impact pressure-forces. Vertical motions will be small compared to horizontal (Figure 5.5). An asymptotic approach, based on assumed horizontal flow, prescribed air entrainment, and a representation of gravity-spreading, is therefore possible.

Such a model is that proposed by Raj and Morris (1988) for dense plumes released horizontally at or near ground-level. The model incorporates jet entrainment, ground drag, and a formula for dense-gas gravity spreading. This model is (however) not valid for buoyant slumped plumes; neither is an interface for initially vertical releases provided.

Havens (1988) does not attempt to deal rigorously with the transition zone, for which horizontal momentum may be significant, but rather makes a simple transition from first plume/ground contact to heavy-gas advection. It may be questioned whether such a transition is physically appropriate.

The Far-Field

Ultimately differences in velocity between (heavy-gas) plume and ambient atmosphere must become negligible, so that the representation of the HGSYSTEM plume models or that of Raj and Morris (1988) must merge into a heavy gas dispersion model such as HEGADAS. This is accomplished (Chapter 7.A, section 7.A.4.2.) by means of *asymptotic matching*.

Alternatively for asymptotically buoyant plumes a transition may be made directly to a passive advection (Gaussian) model such as PGPLUME (Chapter 6, Hanna 1982). It is also possible to incorporate the observed horizontal and vertical diffusion for a passive plume into the near-field formalism (Bloom 1980, Disselhorst 1984). This procedure is computationally costly; its advantage over simple matching unclear.

Curiously for horizontal slumped releases Raj and Morris (1988) are content to use their grounded jet model throughout the heavy-gas advection region, matching ultimately with a passive advection model (Figures 5.6, 5.7). This procedure fails to make use of well-validated models for heavy-gas dispersion.

To summarise: a review of the literature revealed clear gaps in existing models of early plume dispersion. These relate particularly to complex thermodynamics, to plume touchdown, and to the dispersion on the ground of possibly buoyant possibly dense clouds, such as arise for example from the interaction of HF and moist air. There was need of a *consistent* fundamentally-based model capable of describing all of the stages of plume development. No such formalism existed prior to the development of HFPLUME. It is to the development and validation of such a comprehensive model that this Chapter is addressed.

5.B.3. Control Volume Analysis: Basic equations of Motion

Consider a steady plume or jet issuing from a pipe break at pressure and at an angle to the horizontal. The atmosphere into which a release takes place is in a state of steady turbulent flow and has a mean wind-speed which is both horizontal and aligned with the horizontal component of the released jet. This last assumption is inessential, and is introduced to simplify the equations of plume motion.

We shall regard the jet and ambient atmosphere as a single fluid (of variable composition due to entrainment of ambient air) occupying the upper half-plane above a horizontal ground-surface. The jet and ambient atmosphere merge infinitesimally so that no jet 'boundary' exists at finite distance from the jet-axis; entrainment occurs therefore 'at infinity'. No slip occurs amongst the constituent phases of the developing jet; mean-flow within both ambient atmosphere and jet/plume is everywhere steady.

We begin by introducing a set of control-volumes $\tau(s)$, $s > 0$, an analysis of which results in an integral-averaged description of jet development independent of detailed assumptions regarding induced and ambient turbulence.

> *The Control-Volume* $\tau(s)$: First construct a vertical surface at such distance upwind of the release-point that ambient flow is negligibly perturbed. Second, at arbitrary distance $s > 0$ downwind of the release-point, construct a 'cross-section' $A(s)$ through the developing jet. Third link these (semi-infinite) surfaces by skirting the ground and pipe-work surfaces and passing through the jet at the plane of release. Finally construct a fourth bounding surface A_∞ at great (notionally infinite) distance from the jet-axis such as to enclose the (infinite) volume $\tau(s)$. [See Figure 5.1-5.3; Figure 5.8]

By a 'cross-section' $A(s)$ we intend a curved surface locally perpendicular to the (turbulent mean) flow-velocity u. We shall assume that these surfaces form a family parameterized by a distance $s > 0$ measured along a (mean flow) stream-line (the plume-axis) originating at the point of release. Such a cross-section is orthogonal to the plume centre-line and asymptotically vertical at great off-axis distance. It reflects the progressive rotation of the mean plume velocity from centre-line to undisturbed atmospheric values.

We shall assume that the characteristic length-scales for plume development parallel and perpendicular to the mean-flow are asymptotically ordered, at any rate in those regions of the flow for which departures between the plume and undisturbed ambient flows are significant. Specifically we shall take the parallel length-scale to be much greater than the perpendicular: it is in this sense that the jet/plume may be described, following Hinze (1959), as 'thin'. Finally we shall have regard to that part of the ground surface over which there exist significant departures from the undisturbed ambient either in pollutant concentration, in pressure, or in ground-shear. This area, the intersection of plume and ground, we term the plume 'footprint' $F(s)$.

Integration of the basic equations of motion over such a control-volume results, given an assumed 'thin' jet, in the integral forms (Hinze 1959):

Pollutant mass-flux

$$\iint_{A(s)} c\mathbf{u}\cdot d\mathbf{A} = (c_0/\rho_0)\, dm/dt_0 \tag{1}$$

Entrained mass-flux

$$\iint_{A(S)} (\rho\mathbf{u} - \rho_\infty\mathbf{u}_\infty)\cdot d\mathbf{A} = \mathbf{A}_0\cdot(\rho_0\mathbf{u}_0 - \rho_\infty\mathbf{u}_\infty) - \iint_{A_\infty(s)} \rho\mathbf{u}\cdot d\mathbf{A} \tag{2}$$

Horizontal excess-momentum flux

$$\begin{aligned}\iint_{A(s)} [\rho\mathbf{u}(u_x - u_\infty) + (p - p_\infty)\mathbf{e}_x]\cdot d\mathbf{A} &= (u_{x,0} - u_\infty) dm/dt_0 + A_0\cos\phi_0(p_0 - p_\infty) + \\ -\iiint_{\tau(s)} \rho\mathbf{u}\cdot\nabla u_\infty d\tau - \iint_{F(s)} (\Sigma_{xz} - \Sigma_{xz}^{\infty}) dA\end{aligned} \tag{3}$$

Vertical momentum flux

$$\begin{aligned}\iint_{A(s)} [\rho\mathbf{u}u_z + (p - p_\infty)\mathbf{e}_z]\cdot d\mathbf{A} &= u_{z,0}\, dm/dt_0 + A_0\sin\phi_0(p_0 - p_\infty) \\ -\iiint_{\tau(s)} (\rho - \rho_\infty) g\, d\tau + \iint_{F(s)} (p - p_\infty)\, dA\end{aligned} \tag{4}$$

Total energy flux

$$\begin{aligned}\iint_{A(s)} [\rho\mathbf{u}(h + \tfrac{1}{2}\mathbf{u}^2 - h_\infty - \tfrac{1}{2}\mathbf{u}_\infty^2)]\cdot d\mathbf{A} &= \iint_{F(s)} (\Phi - \Phi_a) dA + \\ +(h_0 + \tfrac{1}{2}u_0^2 - h_{\infty,0} - \tfrac{1}{2}u_{\infty,0}^2)\, dm/dt_0 - \iiint_{\tau(s)} \rho\mathbf{u}\cdot\nabla(h_\infty + \tfrac{1}{2}u_\infty^2 + gz)\, d\tau\end{aligned} \tag{5}$$

Notation: vectors are given in bold type and the '·' denotes a vector product, dm/dt_0, mass flow-rate issuing from the release-point; (ρ,c,**u**,p,h), density, pollutant mass-concentration, velocity, absolute pressure, and specific enthalpy of the ensemble-averaged flow. ϕ angle to the horizontal of the plume-axis (co-ordinate stream-line). Φ the surface to air heat-flux. Σ_{xz} the Reynolds stress as the result (ultimately) of viscous drag at the ground. $\mathbf{e}_x$ and $\mathbf{e}_y$ denote unit vectors in the horizontal (wind aligned) and vertical (upward) directions. The affix '0' identifies conditions at the release-plane; the suffix '∞' conditions within the unperturbed atmosphere.

These equations express in integral form conservation of pollutant (e.g. HF) mass-flux, air entrainment, conservation of the excess above ambient of momentum (both horizontal and vertical), and conservation of energy.

The pollutant continuity equation (**Pollutant mass-flux**) expresses that the released pollutant (for example HF), is merely transported and diluted by the atmosphere.

Total mass continuity (**Entrained mass-flux**) allows the identification of the entrained air mass-flux with the integrated sum of mass-flows induced 'at infinity', that is at great distance from the plume centre-line. The equation is formulated as a difference in mass-flux between the undisturbed atmosphere and the system that exists following a sustained release of a pollutant. This has advantages over conventional (total mass-flux) formulations (Ooms 1972, Petersen 1987) in that it is not necessary to introduce a 'cut-off' point in a Gaussian plume model beyond which conditions revert (discontinuously) to atmosphere values (Schatzmann 1978). This permits *true* Gaussian profiles to be introduced in estimating concentrations and temperatures within the developing plume or jet, with a consequent improvement in the accuracy of predicted centre-line concentrations (Davidson 1986, McFarlane 1988).

The horizontal momentum equation (**Horizontal excess-momentum flux**) states that (in the absence of ground drag and significant vertical wind-shear) the excess-flux of horizontal momentum is conserved. Horizontal momentum excess is therefore a natural variable of the jet/plume system (Hinze 1959, McFarlane 1988). Conventional plume models neglect 'ground-effects' (have zero 'footprint' area) and consider only the weak effect of vertical wind-shear upon horizontal momentum flux. The present model, in dealing consistently with 'jet', buoyant plume, and 'slumped' plume, necessarily incorporates a ground-drag force, acting over the plume 'footprint', the effect of which is (substantially) to decelerate an 'airborne' plume at first ground 'impact'. Note that the drag force is expressed over the 'footprint' area F(s), and in terms of the *difference* between the ground-level stresses Σ_{xz} and Σ_{xz}^{∞} in the presence or absence of released material. Clearly drag forces exist even in the undisturbed atmosphere: these, however, are balanced in steady atmosphere flow by (weak) horizontal gradients in the ambient pressure field, and are therefore absent from the difference formulation adopted here.

The vertical momentum equation (**Vertical momentum-flux**) expresses the variation in the flux of vertical momentum in terms of forces arising from either buoyancy or pressures developed at the ground surface at 'touchdown' and beyond. Conventional descriptions model either buoyancy forces alone, or else buoyancy together with 'airborne' plume drag, that is the pressure force that arises over the cross-section A(s) as the result of small local differences between undisturbed ambient and plume pressure (Frick 1984).

'Airborne' drag is a controversial element (Briggs 1984), being found necessary by some (Ooms 1972, Petersen 1978, Schatzmann 1979) but not by others (Petersen 1987; Forney and Droescher 1985; Hoot, Meroney and Peterka 1973). The present model necessarily includes pressure forces developed over the plume 'footprint' in response to velocity changes implied by air entrainment, buoyancy, ground-drag, and the geometrical constraint of an impermeable (level) ground. Pressure forces at the ground develop in response to the interaction of 'top' entrainment and 'gravity slumping', and hence are plausibly expressed in terms of the spreading velocity and buoyancy force in a manner consistent with the gravity current spreading (van Ulden 1984, Raj and Morris 1987).

Finally consider the energy equation (**Total energy flux**), which expresses the near constancy of the excess flux above ambient values of the plume total energy (essentially enthalpy). This flux is altered by small vertical gradients in atmospheric enthalpy and wind-speed, and by the potential energy changes associated with vertical motion under terrestrial gravity The 'airborne' plume is assumed to exert negligible influence on the heat transfer from ground to atmosphere. In addition for a touchdown plume whose temperature differs substantially from that of the ground the heat flux at the ground surface may become important. The heat-flux from the ground is mediated via a heat transfer coefficient the magnitude of which is related to the vertical turbulent transport of heat from ground surface into the overlying plume. For the unperturbed atmosphere such fluxes are also present but are balanced by vertical temperature gradients and by (typically small) systematic variation in temperature downwind. This unperturbed heat flux is therefore absent from the difference model here developed, except inasmuch as it determines the Monin-Obukhov length, wind-speed and temperature profiles within the undisturbed atmosphere (Plate 1982, Colenbrander 1985). No provision has been made for this enhanced ground/plume heat transfer in the current model formulation. Such provision is however encoded within the heavy-gas advection module HEGADAS.

Inasmuch as the HGSYSTEM plume models are intended as a 'front-end' to a heavy-gas advection model such as HEGADAS, the neglect of heat transfer from the ground at touchdown and beyond was judged insignificant.

5.B.4. External flashing; Flow Establishment; Gaussian profiles

This section 'bridges' the external flash (depressurisation) and flow-establishment zones prior to the development within a released plume/jet of (approximately) self-similar conditions. The discussion of flow establishment relates particularly to the prediction of *point-local* from *sectionally averaged* concentrations within the early jet, and to the prediction of the zone length. This analysis is *not* incorporated within the (integral averaged) HGSYSTEM plume models. Such detailed formulation (as it affects air entrainment) requires careful experimental validation and exerts a modest influence upon predictions in the range of greatest interest, perhaps 10 to 500 m downwind of release; it has, however, clear implications for a purely Gaussian plume model.

External Flashing

Having set up the basic equations of motion in integral form, we specialise in order to 'bridge' the external flashing zone, or for a gas-jet the depressurisation zone, that occurs immediately beyond the breakpoint in choked flow. In the absence of choked flow this transitional region may still be present. For example, for a purely liquid release, pressure at the orifice may be an appreciable fraction of the storage (reservoir) pressure; this pressure, however, rapidly relaxes within the vena contracta to an essentially ambient value. During flashing radial and axial velocities within the developing jet are of co-magnitude so that the 'thin jet' approximation is invalid. In addition interphase slip and thermal disequilibrium are likely to occur.

Nonetheless depressurisation occurs so quickly, within a few (perhaps 5) diameters of the release plane, that 'thin jet', equilibrated conditions may be presumed to exist everywhere except within a narrow transition zone adjacent to the release point. We shall assume further, in view of the strongly expanding flow of a flashing jet, or the very large density differences between jet and ambient of a liquid jet, that negligible air entrainment occurs within this depressurisation zone. The length of the zone will in the context of evaporating liquid jets or plumes ordinarily be negligible and will hereafter be ignored: the models have initial conditions defined 'immediately post flash' at (axial) displacement zero.

Neglecting further the influence of gravity and of wind-shear upon the integral conservation laws, we deduce, for the conditions 'immediately post flash', the elementary forms (Figure 5.1)

$$u = u_0 + \frac{A_0(p_0 - p_\infty)}{dm/dt_0}$$

$$c = \rho$$

$$\phi = \phi_0 \qquad (6)$$

$$A\,c\,u = dm/dt_0$$

$$\left[h + \tfrac{1}{2}u^2 - h_\infty^0 - \tfrac{1}{2}u_{\infty,0}^2\right] = \left[h_0 + \tfrac{1}{2}u_0^2 - h_\infty^0 - \tfrac{1}{2}u_{\infty,0}^2\right]$$

The notation is that ϕ is the angle of inclination to the horizontal, and that A_0 is the (true) area of the release orifice. The values of velocity u, density ρ, and area A are averaged values, that is they assume an essentially uniform velocity or density within the jet as it emerges from the depressurisation zone.

This is approximately valid for a liquid jet, (Albertson, Dai, Jensen, and Hunter Rouse 1948) and is at any rate plausible for a gaseous or two-phase jet. Certainly drag forces at the jet edge and the momentum redistribution associated with the entrainment of air are for consistency necessarily small.

Flow Establishment

Beyond the zone of depressurisation there exists a second transitional zone, a zone of 'flow establishment', in which the interaction of jet and ambient result in the progressive turbulent diffusion of air towards, and of jet momentum away from, the jet centre-line. This zone is characterised by a progressive change from a 'top-hat' velocity profile to an essentially Gaussian profile (Hinze 1959, Abramovich 1963) in the asymptotic far-field. Within this zone, neither 'top-hat' nor Gaussian profiles properly describe the cross-sectional variation in jet velocity and pollutant concentration (Figure 5.2).

What is needed is a transitional profile (Albertson, Dai, Jensen, and Hunter Rouse 1948) in which an inner 'core' jet (of uniform velocity and pollutant concentration of 100 %) is 'eroded' by a spreading Gaussian profile coupling inner 'core' and outer ambient flows. An order of magnitude analysis yield that this zone is of typical length $\ell/D = 1/e_{jet}$, in which D is a representative diameter 'immediately post flash', and in which e_{jet} is a (dimensionless) coefficient whose magnitude measures the effectiveness of jet/ambient shear in causing air entrainment.

For gas jets this magnitude is most probably comparable to that seen following the establishment of self-similar flow (Ricou and Spalding 1961), which for a 'top-hat' model yields a value $e_{jet} = 0.08$. This is certainly reduced for a two-phase system (McFarlane 1988), and may be much smaller for a liquid jet for which dynamical break-up, rather than flashing 'atomisation', may dictate the entrainment rate (Wheatley 1987a, Ohnesorge 1936, van de Sande and Smith 1976, McCarthy and Molloy 1973).

We shall assume that all modelled releases result in prompt atomisation rather than gradual break-up, as is consistent with the earlier assumptions of negligible interphase slip and thermodynamic equilibrium. This results in a zone of flow establishment whose length is perhaps 20 orifice diameters. This zone is therefore also of a negligible length compared with downwind displacements of orders ten or hundred metres.
More complex models are possible and have been suggested (Jones 1988, Ianello and Rothe 1988): they require further and uncertain details regarding jet and droplet break-up and evaporation.

This zone ends with the diffusion of air to the jet centre-line, the elimination o the undisturbed 'core' zone, and the establishment of simple Gaussian profiles for jet velocity and pollutant concentration. Given estimates of the fluxes of mass, momentum, and energy, we may locate the zone boundary at least to moderate precision simply by requiring that these principal fluxes be invariable whatever self-similar 'profiles' are assumed to describe the cross-sectional variation in velocity and pollutant concentration.

The zone boundary is then located at that displacement s > 0 for which the centre-line concentration first differs from 100 % pollutant. Let therefore the profiles of jet velocity and pollutant mass concentration be described by the Gaussian forms:

$$
\begin{aligned}
& c/c_* = \phi_c(r/D_*;\gamma^2) \\
& \frac{u-u_\infty}{u_*-u_\infty} = \phi_u(r/D_*) \\
& \phi_u(r/D_*) = \exp\left(-\frac{4r^2}{D_*^2}\right) \\
& \phi_c(r/D_*;\gamma^2) = \exp\left(-\frac{4r^2}{\gamma^2 D_*^2}\right)
\end{aligned}
\qquad (7)
$$

where r is the off-axis displacement, γ^2 the turbulent Schmidt number (Hinze 1959), $u_*(s)$ the centre-line velocity and $c_*(s)$ the centre-line concentration. $D_*(t)$ is an effective jet 'diameter'. Invariance of the principal fluxes results in a set of (non-linear) integral equations for the parameters u_*, c_* and D_*, namely (Figure 5.2),

$$\iint_{A(s)} cu\,dA = dm/dt_0$$

$$\iint_{A(s)} (\rho u - \rho_\infty u_\infty)\, dA = dm/dt$$

$$\iint_{A(s)} \rho u(u - u_\infty)\, dA = dP_x/dt - u_\infty dm/dt$$

where dm/dt_0 is the pollutant mass flux coming from the orifice and dm/dt is the total plume mass flux at any location (pollutant plus entrained air).

The above non-linear system has a solution space which properly contains the set of physically admissible 'self-similar' profiles. Additionally *a-physical* solutions exist for which $c_* > \rho_*$, that is for which the pollutant mass-concentration exceeds the total mixture density; for which $u_* > u_{post\ flash}$, that is for which the centre-line velocity is greater than the velocity immediately post flash; and finally for which $c_* > c_{post\ flash}$, that is for which the centre-line concentration, consistent with an assumed Gaussian profile, actually exceeds that found at the jet-axis immediately following jet depressurisation.

The correct diagnosis from these symptoms is that the set of principal fluxes (dm/dt_0, dm/dt, dP_x/dt) and the atmosphere properties (ρ_∞, u_∞) correspond not to Gaussian self-similarity, but rather to a cross-section located within the zone of flow development. The zone boundary is therefore defined by the simultaneous solution of the above integral equations, together with the 'boundary equation', $c_* = c_{post\ flash}$

5.B.5. The Airborne Plume: geometry and shear entrainment

We consider in this section the representation of the 'airborne' plume, that is the plume from a point 'immediately post flashing' to the point of first plume 'touchdown'. We have chosen to represent the plume development in terms of a simple, integral-averaged, or 'top-hat' model in which is tracked the plume 'centre-line'. The plume consists of a set of circular cross-sections, each of defined diameter, mean density, temperature, and mass concentration of pollutant. Within each cross-section the velocity is assumed uniform; outside conditions are those of the undisturbed atmosphere.

We seek to introduce a (global) co-ordinate system the level surfaces of which are everywhere orthogonal to the turbulent-mean flow. Such co-ordinates, however, cannot be found without detailed knowledge of the turbulent flow in the presence of a dense-gas plume. In the circumstances we must be content with an approximate co-ordinate description valid in the neighbourhood of the plume-axis. We begin by introducing a local ('canonical') co-ordinate system (s,r,θ) defined in the neighbourhood of the plume centre-line (Figures 5.8. 5.9. Schatzmann 1978):

$$\mathbf{r} = (x,y,z) = \mathbf{r}_0 + \left(\int_0^s \cos\phi \, ds, 0, \int_0^s \sin\phi \, ds\right) + r(-\sin\phi\sin\theta, \cos\theta, \cos\phi\sin\theta) \tag{8}$$

with $\quad \mathbf{r}_0 = (x_0, y_0, z_0); \quad (s,r,\theta): 0 \le s \le \infty, 0 \le r \le \infty, -\frac{\pi}{2} \le \phi \le \frac{3\pi}{2}, 0 \le \theta \le 2\pi$

The co-ordinate s marks the distance along the plume centre-line from release point to a general plume cross-section A(s). The co-ordinate pair (r,θ) defines a set of plane polar co-ordinates in the cross-section A(s). The angle φ(s) is the inclination of the plume centre-line at displacement s from the release point (Figure 5.3).

Such co-ordinates are not and cannot be globally defined. Neither do the level surfaces ds = 0 coincide precisely with the surface A(s) in the sense of the original control-volumes τ(s) of section 5.B.3. In particular the level surface ds = 0 are not asymptotically vertical as are the original surfaces A(s). They do nonetheless approximate such cross-sections A(s) in the vicinity of the plume centre-line, that is in that region of the plume for which the differences between plume and ambient are most pronounced. This certainly suggests, though it cannot confirm that it is legitimate to cast the equations of plume motion in terms of a 'top-hat' model and its associated, 'canonical', co-ordinate system.

Differentiation of the integral equations of section 5.B.3. then yields, for the canonical co-ordinates (s,r,θ), the basic differential equations;

$$\begin{aligned}
&d/ds(dm/dt) = \mathrm{Entr}^{A(s)}_{Amb};\\
&d/ds(dP_x/dt) = -\mathbf{Drag}^{A(s)}_{Amb}.\mathbf{e}_x - \mathrm{Shear}^{A(s)}_{Amb}\\
&d/ds(dP_z/dt) = -\mathbf{Drag}^{A(s)}_{Amb}.\mathbf{e}_z - \mathrm{Buoy}^{A(s)}_{Amb};\\
&d/ds(dE/dt) = -\mathrm{Ener}^{A(s)}_{Amb}\\
&dx/ds = \cos\phi\\
&dz/ds = \sin\phi
\end{aligned} \tag{9}$$

together with the algebraic constraints

$$A = (\pi/4)\, D^2$$

$$dm/dt = A\, \rho\, u$$

$$dm/dt_0 = A\, c\, u$$

$$dP_z/dt = dm/dt\; u \sin\phi \qquad (10)$$

$$dP_x/dt = dm/dt\, (u \cos\phi - u_\infty)$$

$$dE/dt = dm/dt\, (h + \tfrac{1}{2}u^2 - h_\infty - \tfrac{1}{2}u_\infty^2)$$

Notation: A cross-section area, D plume diameter (circle), x horizontal axis-displacement, z axis height above level ground, dm/dt released and entrained mass-flux, (dP_x/dt, dP_z/dt) excess (horizontal, vertical) momentum flux, dE/dt excess energy flux, dm/dt_0 pollutant mass-flux; u mean flow-speed, ϕ axis inclination, ρ mean plume-density, c mean pollutant mass-concentration, $h(\rho,c,P_\infty)$ specific enthalpy the suffix '∞' denotes ambient conditions at the *centroid* height $z > 0$.

The quantities **Drag,** Shear, Entr, Buoy, and Ener have the formal definitions,

$$\mathbf{Drag}^{A(s)}_{Amb} = (d/ds) \iint_{A(s)} (p - p_\infty)d\mathbf{A} \qquad (11)$$

$$\mathrm{Shear}^{A(s)}_{Amb} = \iint_{A(s)} \rho \sin\phi\, (du_\infty/dz)\, |\mathbf{J}|/r\, dA \qquad (12)$$

$$\mathrm{Entr}^{A(s)}_{Amb} = \iint_{A_\infty} \rho\, \mathbf{u.dA} \qquad (13)$$

$$\mathrm{Buoy}^{A(s)}_{Amb} = \iint_{A(s)} (\rho - \rho_\infty)\, g\, |\mathbf{J}|/r\, dA \qquad (14)$$

$$\mathrm{Ener}^{A(s)}_{Amb} = \iint_{A(s)} \rho\, u \sin\phi\, (d/dz)\, (h_\infty + \tfrac{1}{2}u_\infty^2 + gz)\, |\mathbf{J}|/r\, dA \qquad (15)$$

Notation: s displacement along plume centre-line, z height above ground, ϕ plume centre-line inclination, ρ local (turbulent averaged) density, u flow-speed, p (absolute) pressure, h specific enthalpy, $|\mathbf{J}| = r - r^2 \sin\theta\, d\phi/ds$ Jacobian determinant, g acceleration due to gravity, $dA = r dr d\theta$ (scalar) area element.

They represent (respectively) the 'drag' force $\mathbf{Drag}^{A(s)}_{Amb}$ acting on the plume in cross-flow as the result of vortex formation in the plume wake (Ooms 1972, Schatzmann 1979), the shear force $\mathrm{Shear}^{A(s)}_{Amb}$ associated with the vertical gradient of wind-speed, the total entrainment rate $\mathrm{Entr}^{A(s)}_{Amb}$ per unit axis length, the section-averaged buoyancy force $\mathrm{Buoy}^{A(s)}_{Amb}$, and the variation in plume total energy $\mathrm{Ener}^{A(s)}_{Amb}$ resulting from vertical gradients of temperature (enthalpy) and wind-speed.

The pressure is that deduced for hydrostatic equilibrium, except insofar as departures result in the (airborne) drag force.

These integrals are in actual practice replaced by empirical formulae chosen for compatibility with existing plume models and literature available data. These formulae express, for example, the contribution to air entrainment within the plume of the difference in velocity between mean cross-sectional velocity and the ambient wind-speed. Model closure is therefore in terms solely of mean cross-sectional and local atmospheric ambient parameters.

The above 'algebraic constraints' can be viewed as definitions of, for example, the total mass-flux within the plume, or the area of a circle. It is algebraically convenient to regard these as algebraic equations forming part of a differential/algebraic system. Such a system is then solved by means of the differential/algebraic package SPRINT (Berzins, Dew, and Furzeland 1983; Berzins and Furzeland 1985). Such a formulation allows the somewhat different descriptions of 'touchdown' and 'slumped' plumes to be incorporated within the same formalism.

5.B.6. The Touchdown and Slumped Plume

Consider next the representation of the plume following first 'touchdown'. Touchdown occurs at that axial displacement $s > 0$ for which an assumed circular cross-section just touches the horizontal ground surface $z = 0$.

It is also the point beyond which the plume footprint width first assumes a non-zero value.

The cross-section of a plume following touchdown is modelled not by a *circle* but rather by a *circular segment*. This centroid location will, for a dense plume, continue to fall, so that after some time a *semicircular cross section* is certain to arise. At this point the plume has passed through a transitional region between circular 'airborne' and *semi-elliptic 'slumped' cross-sections*. Further development will, at least initially, be characterised by (transverse) gravity spreading (van Ulden 1974, Raj and Morris 1987), and by air entrainment principally through the 'upper' plume surface.

These elements may be assembled within the framework of a 'top-hat' model as the differential system:

$$
\begin{aligned}
&d/ds(dm/dt) = \mathrm{Entr}^{A(s)}_{Amb} \\
&d/ds(dP_x/dt) = -\mathbf{Drag}^{A(s)}_{Amb}.\mathbf{e}_x - \mathrm{Shear}^{A(s)}_{Amb} \\
&d/ds(dP_z/dt) = -\mathbf{Drag}^{A(s)}_{Amb}.\mathbf{e}_z - \mathrm{Buoy}^{A(s)}_{Amb} + \mathrm{Foot}^{F(s)}_{Amb} \\
&d/ds(dE/dt) = \mathrm{Ener}^{A(s)}_{Amb} \\
&dx/ds = \cos\phi \\
&dz/ds = \sin\phi
\end{aligned}
\qquad (16)
$$

together with the algebraic constraints

'Touchdown' Plume

$$
\begin{aligned}
&A = \frac{D^2}{4}\left[\cos^{-1}(-\eta_c) + \sqrt{1-\eta_c^2}\right] \\
&dm/dt = A\ \rho\ u \\
&dm/dt_0 = A\ c\ u \\
&dP_z/dt = dm/dt\ u \sin\phi \\
&dP_x/dt = dm/dt\ (u\cos\phi - u_\infty) \\
&dE/dt = dm/dt\ (h + \tfrac{1}{2}u^2 - h_\infty - \tfrac{1}{2}u_\infty^2) \\
&\eta_c = \eta - \frac{2}{3}\left\{\frac{(1-\eta_c)^{3/2}}{\cos^{-1}(-\eta_c) + \eta_c\sqrt{1-\eta_c^2}}\right\} \\
&\eta = \frac{2z}{D\left|\cos\phi\right|} \\
&\eta_c = \frac{2z_c}{D\left|\cos\phi\right|}
\end{aligned}
\qquad (17)
$$

Notation: A cross-section area (circular segment), D circle diameter, x centroid horizontal displacement, z centroid height, z_C centre height; dm/dt total (released plus entrained) mass-flux, (dP_x/dt, dP_z/dt) excess (horizontal, vertical) momentum flux, dE/dt excess energy flux, dm/dt_0 pollutant mass-flux, u mean flow-speed, ϕ axis inclination, ρ mean plume density, c mean pollutant mass-concentration, h specific enthalpy; the suffix '∞' denotes ambient conditions at the centroid height. (See Figure 5.4).

Note that the *centroid* is the centre-of-mass of the plume and the *centre* is the centre of the circle of which the plume is a cut-off segment. The maximum width of the plume is D, at ground level it is $D\sqrt{1-\eta_c^2}$. The plume height is given by $D/2\,(1+\eta_c)\cos\phi$.
In the plume calculations η will be known and η_c has to be calculated using the non-linear equation for η_c as given above. This equation can be solved using a simple iterative method.

'Slumped' Plume

$$A = (e\,\pi/8)\,D^2 \quad \text{with } e = (3\pi/2)\,(z/D)\,|\cos\phi|$$

$$dm/dt = A\,\rho\,u$$

$$dm/dt_0 = A\,c\,u$$

$$dP_z/dt = dm/dt\;u\sin\phi \qquad (18)$$

$$dP_x/dt = dm/dt\,(u\cos\phi - u_\infty)$$

$$dE/dt = dm/dt\,(h + \tfrac{1}{2}u^2 - h_\infty - \tfrac{1}{2}u_\infty^2)$$

Notation: A cross-section area (semi-ellipse), D ellipse major-axis length, e ellipse eccentricity (ratio minor to major ellipse axis), x centroid horizontal displacement, z centroid height; dm/dt total (released plus entrained) mass-flux, (dP_x/dt, dP_z/dt) excess (horizontal, vertical) momentum flux, dE/dt excess energy flux, dm/dt_0 pollutant mass-flux; u mean flow-speed, ϕ axis inclination, ρ mean plume density, c mean pollutant mass-concentration, h specific enthalpy; the suffix '∞' denotes ambient conditions at the centroid height. (See Figure 5.5).

For the slumped plume the width is equal to D and the height is given by $\frac{3\pi}{4}z$.

Note that the differential system is modified in that, in addition to any 'airborne' drag forces. we have (generally significant) 'ground' drag associated with the strong shear layer at the ground-surface following plume touchdown. A further (pressure) force $\mathrm{Foot}_{\mathrm{Amb}}^{F(s)}$ is exerted at the ground surface as the result either of the destruction of vertical momentum impacting the ground, or in response to a pressure build-up associated with the limited (gravity-slumping) rate of transverse plume expansion. These additional forces exist following touchdown and in the slumped plume regime. They have the formal definitions:

$$\mathrm{Foot}_{\mathrm{Amb}}^{F(s)} = (d/ds) \iint_{F(s)} (p - p_{\infty})dA \tag{19}$$

$$\mathrm{Drag}_{\mathrm{Amb}}^{F(s)} = (d/ds) \iint_{F(s)} (\Sigma_{xz} - \Sigma_{xz}^{\infty})dA \tag{20}$$

and are replaced in the actual plume models by intuitively derived functions which reflect known spreading and impact behaviour.

For the circular cut-off segment the cross-sectional area A and centroid height z are not explicitly related but coupled via a single non-linear equation for the geometric centre z_C. In the case of the slumped plume both the area A and centroid height z are related to the eccentricity e of the semi-ellipse; however the eccentricity is given explicitly in terms of known parameters z, ϕ, and D.

5.B.7. Closure Assumptions for the 'Top-Hat' Model

In this section are considered the assumptions, arguments, and simplifications that enable closure of the 'top-hat' model: We shall ask: 'Which expressions and what coefficient values are appropriate for the formulation of impact forces, drag forces, and buoyancy in each of the three plume regions; airborne, touchdown, and slumped plume?'.

Atmosphere-Gradient Induced Forces: Plume Buoyancy:

We begin by considering the simplest of these functions, $\mathrm{Shear}_{\mathrm{Amb}}^{A(s)}$, $\mathrm{Ener}_{\mathrm{Amb}}^{A(s)}$, and $\mathrm{Buoy}_{\mathrm{Amb}}^{A(s)}$, and take first of all the buoyancy force $\mathrm{Buoy}_{\mathrm{Amb}}^{A(s)}$. This has the formal definition,

$$\mathrm{Buoy}_{\mathrm{Amb}}^{A(s)} = \iint_{A(s)} (\rho - \rho_{\infty})\, g\, |J|/r\, dA \tag{21}$$

in which the Jacobian determinant has the value

$$|J| = r - r^2 \sin\theta\, d\phi/ds, \quad |J| > 0 \tag{22}$$

The buoyancy term is well approximated by the simple expression,

$$\mathrm{Buoy}_{\mathrm{Amb}}^{A(s)} = A\,(\rho - \rho_\infty)\,g \qquad (23)$$

a result which extends for expansion about the plume *centroid* (centre-of-mass) for both touchdown and slumped plume.

Analyses and order of magnitude arguments yield analogous results for the functions $\mathrm{Shear}_{\mathrm{Amb}}^{A(s)}$, and $\mathrm{Ener}_{\mathrm{Amb}}^{A(s)}$. It follows that

$$\mathrm{Shear}_{\mathrm{Amb}}^{A(s)} = dm/dt\,\sin\phi\; du_\infty/dz \qquad (24)$$

$$\mathrm{Ener}_{\mathrm{Amb}}^{A(s)} = dm/dt\,\sin\phi\;(d/dz)[h_\infty + \tfrac{1}{2}u_\infty^2 + gz] \qquad (25)$$

Airborne Drag

Consider next the 'drag' function associated with an airborne plume in cross-flow. This function represents the force acting upon the plume as the result of pressure forces created by trailing (wake) vortices. The term 'drag' is by analogy to the drag force exerted upon a *rigid* body immersed in a uniform stream.

There are, however, major differences between the pressure field of a fluid jet and of a (geometrically similar) rigid body. Firstly there is no sharply defined boundary at which the 'no slip' condition may be applied. Secondly the external flow, and hence the boundary integral of pressure, may differ substantially between plume and body.

The analogy is therefore weak, so that not only the coefficient magnitudes but also the functional form appropriate to a rigid body may be questioned when applied to a plume in cross-flow. The form and magnitude of this airborne drag force is therefore particularly uncertain. It is found necessary by some (Ooms 1972, Petersen 1978, Schatzmann 1978), but not by others (Hoot, Meroney and Peterka 1973; Hoult, Fay and Forney 1969; Petersen 1987). A recent study (Coelho and Hunt 1989) of the near-field following release orthogonal to a steady flow found no evidence either experimental or theoretical for a significant 'drag' force. Plume deflection was satisfactorily explained by air entrainment alone.

We assume that

$$\mathbf{Drag}_{\mathrm{Amb}}^{A(s)} = 0 \qquad (26)$$

Plume impact Forces

Consider next the pressure forces exerted over the plume 'footprint' for a touchdown or slumped plume. These forces arise from two distinct physical mechanisms: the destruction of momentum associated with the impact of a dense plume upon the ground surface; and the pressurisation associated with the gravity-limited rate of lateral plume spreading.

Take first the case of a plume impacting the ground surface (Figure 5.10). The assumption of an elastic collision applied to the plume as a whole requires that the impact pressure force be at right angles to the momentary orientation of the centroid axis. This ensures conservation of kinetic energy for a system without entrainment or other disturbing influences such as gravity. Focus next upon that proportion of the descending plume impinging upon level ground in time $dt > 0$.

If the footprint is of width ℓ then the impinging momentum flux is correspondingly,

$$\mathbf{dP} = dA\ \rho\ u(\cos\phi, 0, \sin\phi);\ dA = \ell\ u\,|\tan\phi|\,dt \tag{27}$$

in which dA is the sectional area 'absorbed' into the ground surface.

We assume further that the magnitude of the impact force is such as to destroy completely the momentum-flux impinging at any instant upon the ground. The impact pressure force is therefore,

$$\mathbf{Impact}^{F(s)}_{Amb} = \ell\ \rho\ u^2\,|\tan\phi|\,(\sin\phi, 0, -\cos\phi);\ \sin\phi \geq 0 \tag{28}$$

This formula differs somewhat from that expected from the control-volume analysis, in that both horizontal and vertical moments undergo continuous change. The pressure force integral implies a change solely in the vertical momentum. Additionally consideration of the destruction of horizontal momentum yields that flows in the negative x-direction are induced for impact angles in excess of 45°.

Certainly, for vertical incidence, the spreading pattern is axi-symmetric about the point of impact except inasmuch as this is modified by the ambient wind. For steeply descending plumes, therefore, upwind spreading, vortex formation, and flow separation make a simple transition described in terms of a continuous mean-flow at least difficult. However, for shallow incidence, such upwind spreading is typically absent, so that a 'top-hat' transition remains entirely feasible.

The form of the impact force $\mathbf{Impact}^{F(s)}_{Amb}$ implies a transition between 'steeply descending' and 'shallow incidence' plumes at an angle of descent $\phi = 45°$. This is precisely the value observed experimentally by Karman (1986). We restrict attention, therefore, to plume touchdown at angles ϕ less than 45°. Steeply descending plumes will require either empirical matching of airborne and slumped plumes (Karman 1986), or else matching to a 'spreading pool' model, possibly analogous to the HGSYSTEM area source slumping model HEXABOX.

In addition, in the absence of air entrainment or drag forces, such as would describe shallow incidence impact of a liquid jet, the above impact force implies that the mean jet/plume speed remains constant throughout the impact process. This is consistent with a direct application of Bernoulli's theorem, gravity and ground drag being negligible, and is consistent with the impact of a liquid jet on a curved vane (Fox 1974). For this case the horizontal impact force evidently arises from pressure components developed along the curved surface of the deflecting vane. For the actual case of ground impact we may 'square the above circle' by regarding the jet/plume as existing above a recirculating flow the common interface of which is the analogue of the physical vane. In the immediate vicinity of first ground impact, therefore, the top-hat model represents not the complete flow but only the non-recirculating portion. Plume impact may then be modelled as a simple (elastic) collision.

Gravity-Slumping Pressure Forces

Consider next the pressure force induced over the plume 'footprint' by the interaction of ('top') entrainment and gravity-'slumping'. This pressure arises from the fact that entrainment may increase the cross-sectional mass-flux at a rate incompatible with a prescribed gravity-spreading unless the centre of mass is also raised. Such a raising of the centre of mass against gravity can be accomplished only by means of a pressure force acting over the plume footprint. The absolute magnitude of this pressure is small; its integrated effect significant. Let us begin (refer Figure 5.11) with the gravity-spreading relation (van Ulden 1983, Raj and Morris 1987) for a rectangular, 'slumped' jet

$$\tfrac{1}{2}dD/ds = (k/u)\sqrt{g\,h(1 - \rho_\infty/\rho)} \qquad (29)$$

Notation: h plume height, D plume width, g acceleration due to gravity, (ρ,u) mean density and flow-speed, ρ_∞ ambient density, k (0.85-1.20) empirical coefficient, s centre-line displacement.

We seek a formulation for the vertical momentum equation such that this gravity-slumping behaviour is asymptotically recovered for dense, advected plumes. For such a plume the spatial rate of change of vertical momentum is undoubtedly small, that is the sum of vertical forces is approximately zero. We interpret Raj's formula for gravity spreading as a statement of the approximate balance of a buoyancy force, and the reactive pressure force driven by the interaction of slumping and entrainment. Given, therefore, that the buoyancy force has the form,

$$\mathrm{Buoy}_{\mathrm{Amb}}^{A(s)} = h\, D\, g\, (\rho - \rho_\infty) \qquad (30)$$

we propose a reactive pressure force,

$$\mathrm{Foot}_{\mathrm{Amb}}^{F(s)} = (1/k^2)\, D\, \rho\, u^2\, [\tfrac{1}{2} dD/ds]^2 \qquad (31)$$

proportional to the local footprint width, and to the square of the lateral spreading velocity.
In the case of a semi-elliptic cross-section we must reinterpret the lateral spreading velocity, and effective plume height h in terms of the plume width D and centroid height z.
The height h is for a rectangular section exactly twice the centroid height which allows the identification $h = 2z$. Additionally the rectangular section has area hD equal to that of a semi-ellipse $(3\pi^2/16)zD$ of centroid z and footprint width D.

This results in the final expression, modified for the semi-elliptic geometry

$$\mathrm{Foot}_{\mathrm{Amb}}^{F(s)} = (3\pi^2/32)^3\, (1/k^2)\, \ell\, \rho\, u^2\, [\tfrac{1}{2} dD/ds]^2, \; k = 1.15 \qquad (32)$$

We follow van Ulden (1983), rather than Raj and Morris (1988) in the choice of the gravity-spreading coefficient. Further work is, however, necessary in order optimally to determine the coefficient value for a semi-elliptic, slumped plume.

This revised formulation will evidently reproduce the gravity spreading behaviour 'hard-wired' by Raj and Morris (1988). It is, moreover, physically meaningful for an asymptotically neutral or buoyant plume/jet for which significant departures from gravity-spreading must be expected. In particular the original spreading formula is not defined for a buoyant plume. Initially dense, subsequently buoyant, plumes occur frequently for the release of pressurised liquid HF or other liquid gases, to ambient atmospheres of moderate humidity (> 50 %) and temperature (perhaps 20 °C).

Gravity Current Collapse

Gravity spreading as formulated by van Ulden (1983) and Puttock (1988) assumes the existence of a (relatively) sharp interface between plume and undisturbed air. Recent experiments by Linden and Simpson (1988) indicate that the leading vortex of such a gravity current is not unconditionally stable but may be disrupted by locally enhanced turbulence. Following gravity current collapse the cloud edge is more diffuse; lateral spreading much reduced.

Study of the HTAG ('Heavier than Air Gas') data set (Petersen and Ratcliff 1989), reveals evidence for the existence of such gravity current collapse for uniform ambient turbulence and increasingly weak gravity-head. We propose a collapse criterion and post-collapse spreading rate (essentially) as follows:

$$\tfrac{1}{2}dD/ds = (2\,\rho_\infty\, u_*\, h)/(3\, k\, C_D\, u\, D)\, Ri_*\, \Phi(Ri_*) \qquad (33)$$

$$\sqrt{\rho_\infty/\rho}\,\frac{D}{h} > \frac{16}{3\kappa}\sqrt{Ri_*}\,\Phi(Ri_*) \qquad (34)$$

$$\Phi(Ri_*) = \begin{cases} \dfrac{1}{\sqrt{1-3Ri_*/5}} & Ri_* < 0 \\ 1 & 0 \le Ri_* < \dfrac{189}{80} \\ \max\left(\dfrac{Ri_*}{7}, \dfrac{10}{17}\sqrt{1+4Ri_*/5}\right) & Ri_* \ge \dfrac{189}{80} \end{cases} \qquad (35)$$

with $Ri_* = g\, h\, (\rho - \rho_\infty)$ and $h = 2z$.

Notation: h plume height, D plume width, g acceleration due to gravity, (ρ, u) mean density and flow-speed, ρ_∞ ambient density, κ is the Von Kármán constant, C_D (with value 5.0) empirical (spreading) coefficient, s centre-line displacement, u_* friction velocity, Ri_* (bulk) Richardson number ; $\Phi(Ri_*)$ heavy gas entrainment function.

Spreading, 'post collapse', is represented in the HGSYSTEM plume models by the limit of the vertical momentum equation for which the corresponding 'footprint' force is simply

$$Foot^{F(s)}_{Amb} = (3\pi^2/64)^3\,(3\, k\, C_D/\Phi(Ri_*))\, \ell\, \rho\, u\, u_*\, (D/z)\, dD/ds \qquad (36)$$

$$\sqrt{\frac{\rho_\infty}{\rho}\,\frac{D}{z}} > \frac{1024}{9\pi^2}\sqrt{Ri_*}\,\Phi(Ri_*)/\kappa \qquad (37)$$

with $C_D = 5.0$ and $Ri_* = 2\, g\, z\, (\rho/\rho_\infty - 1)/u_*^2$

The possibility exists that a gravity current may reform following initial turbulent collapse. Intuition suggests that such reformation may occur, but that the collapsed state is 'metastable', that is vortex (re-) formation may be considerably delayed. In the absence of detailed experimental evidence, we may presume gravity current collapse irreversible.

Ground-surface Drag

Finally we consider the drag force exerted at the ground surface by an impacting or slumped plume. This force has the formal definition

$$\mathrm{Drag}^{F(s)}_{\mathrm{Amb}} = (d/ds)\iint_{F(s)} (\Sigma_{xz} - \Sigma^{\infty}_{xz})\, dA \qquad (38)$$

and results from differences in the mean horizontal and undisturbed wind speeds in the neighbourhood of the ground surface. The surface stress associated with the wind profile is $\rho_\infty u_*^2$, in which u_* is the friction velocity.

Equivalently Σ^{∞}_{xz} is proportional to the square of the velocity gradient du_∞/dz at the roughness height $z_r > 0$.

Profile information regarding the vertical variation in flow-speed within the impacting or slumped plume is therefore necessary in order to estimate the drag force. For an assumed neutrally buoyant plume and a logarithmic velocity profile the friction velocity associated with a plume of velocity at centroid height z is u/u_∞ times that of the unperturbed wind. This suggests (for a neutral plume) the drag function

$$\mathrm{Drag}^{F(s)}_{\mathrm{Amb}} = \ell\, \rho_\infty\, u_*^2\, [(u/u_\infty)\cos\phi - 1][(u/u_\infty)\cos\phi + 1], \text{ with } u_\infty > 0 \qquad (39)$$

in which ℓ is the footprint width.

For high speed flows we expect the (established) shear profile within a dense gas plume to be governed by surface roughness analogously to that in a neutral boundary layer. The surface stress is simply ρu_*^2, in which u_* is set by the known (mean) jet velocity at the centroid height. Substitution then yields the drag function in the presence of dense gas effects

$$\mathrm{Drag}^{F(s)}_{\mathrm{Amb}} = \ell\, \rho_\infty\, u_*^2[\sqrt{\rho/\rho_\infty}\ (u/u_\infty)\cos\phi - 1][\sqrt{\rho/\rho_\infty}\ (u/u_\infty)\cos\phi + 1] \qquad (40)$$

Density stratification damps turbulence and affects both friction velocity and plume drag. The drag force might be presumed proportional to some power of the Richardson number correction $\Phi(Ri_*)$ proposed by Witlox (1988) in the context of heavy-gas entrainment. Now the suppression of entrainment at a dense gas interface is largely due to gravity-driven 'recapture' of disturbed dense gas rather than to a lowering of turbulent energies within the system as a whole. This suggests that the influence of density stratification upon ground drag is rather small. We presume the effect negligible.

5.B.8. The Entrainment Function

We consider in this section the form of the entrainment function appropriate to each of the plume regions; airborne, touchdown, and slumped plume. The entrainment function is taken (barring interactions) to be the sum of contributions arising from different physical mechanisms; jet entrainment, cross-wind entrainment, gravity-slumping entrainment, and airborne or heavy-gas passive entrainment. These mechanisms are present to varying degree in each of the plume regions.

Jet Entrainment

For the discharge of (neutrally buoyant) gas jets to quiescent of co-flowing ambient the form and magnitude of the entrainment function is well established (Briggs 1984; Morton, Taylor and Turner 1956). It assumes for the 'top-hat' formulation the symbolic form

$$\mathrm{Entr}_{jet} = e_{jet}\,\pi\,D\,\rho_{\infty}\left|u - u_{\infty}\right| \text{ with } e_{jet} = 0.08 \tag{41}$$

This form (or related variants) has been found satisfactory in addition for the early release of two-phase propane jets (McFarlane 1988, Cowley and Tam 1988), and for ammonia releases (Wheatley 1987a, 1987b).

For dense two-phase jets in cross-flow, we propose the correlation

$$\mathrm{Entr}_{jet} = e_{jet}\,\eta(\rho/\rho_{\infty})\,L^{free}_{surface}\,\rho_{\infty}\left|u - u_{\infty}\cos\phi\right| \tag{42}$$

with $\eta(\rho/\rho_{\infty}) = [1 + (4/3)(\rho/\rho_{\infty} - 1)]/[1 + (5/3)(\rho/\rho_{\infty} - 1)]$

Jet entrainment is thus *proportional to the absolute difference between the jet speed and the aligned component of the ambient wind.*

Entrainment takes place over that part of the plume perimeter exposed to the ambient air. The form, excepting the small density correction, has been found satisfactory by several authors (Petersen 1978; Ooms 1972; Hoot, Meroney and Peterka 1973) in combination with various cross-wind formulations for the description of buoyant and dense gas plumes released orthogonal to an imposed wind.

It, other than the densimetric correction, is used by Raj and Morris (1987) for their gravity-slumping jet. It is closely analogous (asymptotically equivalent) to a 'shear' entrainment formulation based upon Prandtl closure of the turbulent kinetic equation proposed by McFarlane (1988). This formulation showed good agreement with large scale experimental data gathered by Cowley and Tam (1988).

Cross-wind Entrainment:

Crosswind entrainment is associated with the formation in the wake of a rising or falling plume of trailing vortices in response to the deflection by the release plume of ambient air. This mechanism is absent for release to a quiescent atmosphere, or for a wind aligned release, and is assumed to be maximum for releases at right angles to the ambient wind. This suggests immediately the functional form,

$$\mathrm{Entr}^{\mathrm{cross}}_{\mathrm{wind}} = e^{\mathrm{cross}}_{\mathrm{wind}}\, L^{\mathrm{free}}_{\mathrm{surface}}\, \rho_\infty\, u_\infty \left|\sin\phi\right| \tag{43}$$

(Morton, Taylor and Turner 1956; Hoot, Meroney and Peterka 1973; Hoult, Fay and Forney 1969).

By contrast Ooms (1972), and later Petersen (1978,1987) have found good agreement for Gaussian models with the modified form

$$\mathrm{Entr}^{\mathrm{cross}}_{\mathrm{wind}} = e^{\mathrm{cross}}_{\mathrm{wind}}\, L^{\mathrm{free}}_{\mathrm{surface}}\, \rho_\infty\, u_\infty \left|\cos\phi\, \sin\phi\right| \tag{44}$$

when used in conjunction with non-zero airborne drag correlation

$$\mathbf{Drag}^{A(s)}_{\mathrm{Amb}} = e^{\mathrm{drag}}_{\mathrm{Amb}}\, L^{\mathrm{cross}}_{\mathrm{wind}}\, \rho_\infty\, u_\infty^2 \sin^2\phi\, (\sin\phi, 0, -\cos\phi) \tag{45}$$

This formulation is reported by Li, Leijdens and Ooms (1986), and by Havens (1988) to be a successful predictor not only of buoyant and neutral plumes, but of dense emissions as well. Several other formulations have been tried (Schatzmann 1979, Spillane 1983, Frick 1984) and are reported as satisfactory in predicting plume rise and lateral spread (Schatzmann and Policastro 1984a, 1984b).

We have encoded various cross-wind entrainment terms within the (ideal-gas) plume model PLUME, and find, following Briggs (1984), that the cases of neutral and buoyant plume rise are adequately represented by the $|\sin\phi|$ correlation and a coefficient value $e^{\mathrm{cross}}_{\mathrm{wind}}$ of 0.60. By contrast, the dense plume data-base of Hoot, Meroney and Peterka is incompatible with *any* uniform choice for the crosswind entrainment coefficient.

Except in the immediate vicinity of the source, plume development is well represented by the Boussinesq approximation (Schatzmann and Policastro 1984b). It follows that rising dense plumes, and descending buoyant plumes should exhibit essentially the same behaviour in response to an imposed cross-wind. This suggests strongly that the same functional form be chosen to represent both dense and buoyant plumes, and that in the limit of great dilution the simple $|\sin\phi|$ dependence be recovered.

We find that cross-wind entrainment is weakened by high exit velocities and for rising dense plumes by density excess. Analysis of buoyant (Petersen 1978), and dense (Hoot, Meroney and Peterka 1973) gas-plume data suggests the functional form

$$\mathrm{Entr}^{\mathrm{cross}}_{\mathrm{wind}} = \mathrm{Cu}^{\mathrm{cross}}_{\mathrm{wind}}\, \eta(\rho/\rho_\infty,\phi)\, L^{\mathrm{free}}_{\mathrm{surface}}\, \rho_\infty u_\infty \sqrt{u_\infty / u}\ |\sin\phi| \tag{46}$$

with $\eta(\rho/\rho_\infty,\phi) = [1 + \mathrm{C}\rho^{\mathrm{cross}}_{\mathrm{wind}} \max(0,(\rho/\rho_\infty - 1)\sin\phi)]^{-1}$ and the coefficients $\mathrm{Cu}^{\mathrm{cross}}_{\mathrm{wind}} = 0.60$, $\mathrm{C}\rho^{\mathrm{cross}}_{\mathrm{wind}} = 7.50$.

The coefficient $\mathrm{C}\rho^{\mathrm{cross}}_{\mathrm{wind}}$ is matched to dense gas maximum rise-height, and the release velocity correction is suggested by an analysis of (early) buoyant plume rise. This expression, when used in conjunction with the above jet entrainment, is a satisfactory predictor of buoyant (Petersen 1978), and of dense plume-rise (both maximum rise-height and its downwind displacement).

Plume 'touchdown' is also satisfactory, though the validation is complicated by differences between the plume width of a 'top-hat' model, and the 'visible edge' data presented by Hoot, Meroney and Peterka (1973). The model adequately reproduces the downward releases of buoyant gas conducted by Li, Leijdens and Ooms (1986), and is of comparable accuracy to the truncated Gaussian model of Ooms and Duijm (1984), and to the similar model proposed by Havens (1988) after Morrow and co-workers (1982).

It should be emphasised that this entrainment term is *empirical*. It is a satisfactory predictor of both dense and buoyant plumes released orthogonal to a laminar cross-wind. Nonetheless it is rather likely that an improved correlation can be developed should plume centre-line touchdown data become available.

Gravity Slumping Entrainment

By 'gravity-slumping' entrainment we intend the absorption of ambient air within a 'slumped' plume as the result of lateral expansion in response to density differences between (dense) plume and ambient. This phenomenon was studied by van Ulden (1974) in the context of the initial development of a cylindrical (area) source of dense gas. Van Ulden (1974) proposed the entrainment relation,

$$\mathrm{Entr}^{\mathrm{grav}}_{\mathrm{slump}} = \tfrac{1}{2} e^{\mathrm{grav}}_{\mathrm{slump}}\, \pi D \rho_\infty h\, (dD/dt), \text{ with } e^{\mathrm{grav}}_{\mathrm{slump}} = 0.05 \tag{47}$$

Notation: h plume height, D plume diameter, dD/dt slumping rate.

Entrainment is proportional to the spreading velocity (½dD/dt), to the ambient density (ρ_∞) and to the area (πhD) of the plume 'edge'.
Almost all of the adjacent air is, for such cylindrical slumping, displaced by rather than entrained within the expanding cloud 'edge'. The analogue of van Ulden's entrainment relation for the (steady) state geometry of the slumped plume is

$$\mathrm{Entr}^{\mathrm{grav}}_{\mathrm{slump}} = e^{\mathrm{grav}}_{\mathrm{slump}}\, \rho_\infty\, z\, u \left| \cos\phi \right| (dD/ds) \tag{48}$$

in which we have assumed an equivalent cloud height which is twice that of the plume centroid.
We have also adopted this formula for the slumped plume.

Puttock (1988), in the model HEGABOX (available in HGSYSTEM version 3.0), proposed an entrainment coefficient $e^{\mathrm{grav}}_{\mathrm{slump}}$ = 0.85, this in accordance with observations on cylindrical collapse conducted at Thorney Island (McQuaid 1984).
The coefficient value, $e^{\mathrm{grav}}_{\mathrm{slump}}$ = 0.85, may reflect a contribution to entrainment associated with turbulence generated in the cylindrical collapse, turbulence which must decay as the plume is advected downwind. This suggests that the entrainment coefficient $e^{\mathrm{grav}}_{\mathrm{slump}}$ appropriate to a semi-elliptic plume may have a value considerably less than 0.85.

Alternatively some dependence of $e^{\mathrm{grav}}_{\mathrm{slump}}$ upon such flow parameters as the local (bulk) Richardson number or upon the local versus initial spreading-rate (Eidsvik 1978) might be investigated.

Conventionally (Ooms 1972, Petersen 1987, Schatzmann 1978, Briggs 1984) such lateral entrainment is absent from the airborne plume: indeed its inclusion results for the approximate equations of motion in an *exponential* growth in plume width. The touchdown plume is physically and geometrically intermediate between airborne and slumped plume. In this region forces are first developed whose interaction with buoyancy results in the subsequent (slumped plume) gravity current. Plausibly gravity current entrainment is weak in this intermediate zone. Certainly this is consistent with the observations of Puttock (1988) who found it necessary to 'switch off' gravity-current entrainment for an interval following initial (cylindrical source) release. This delay is required for the formation of a vortex system at the cloud leading 'edge'.
For the touchdown plume, therefore, we propose the interpolated form

$$e^{grav}_{slump} = [1 - 2z_c/D/|\cos\phi|]\, e^{grav}_{slump}\, \rho_\infty\, z\, u\, |\cos\phi|\, (dD/ds) \qquad (49)$$

in which z_c and D denote centre and diameter of the circular segment cross-section. This formulation is of necessity preliminary, and may require modification of 'tuning' in the light of subsequent validation of analysis.

Slumped Plume: Heavy Gas Entrainment

The dilution of a 'severely slumped plume' is dominated by 'top' entrainment of ambient air in response to ambient turbulence when modified by density stratification. The circumstances of such 'severely slumped' plumes are precisely those for which the heavy-gas advection model HEGADAS was designed.

As the HGSYSTEM plume models are required to merge smoothly with the far-field HEGADAS model, it is appropriate to take the 'top' entrainment formulation used by the latter, modified to allow for the different cross-sectional geometry's.

We are led immediately to the entrainment relation,

$$Entr^{heavy}_{gas} = [\Phi(Ri_*)]^{-1}\, L^{free}_{surface}\, \kappa\, \rho_\infty\, u_* \qquad (50)$$

$$\text{with } \Phi(Ri_*) = \begin{cases} \dfrac{1}{\sqrt{1-3Ri_*/5}} & Ri_* < 0 \\ 1 & 0 \le Ri_* < \dfrac{189}{80} \\ \max\left(\dfrac{Ri_*}{7}, \dfrac{10}{17}\sqrt{1+4Ri_*/5}\right) & Ri_* \ge \dfrac{189}{80} \end{cases} \qquad (50a)$$

and $Ri_* = 2\, g\, z\, (\rho - \rho_\infty)$. Relation (50a) is of course equal to relation (35).

The Richardson number correction to the turbulent entrainment is a modification to the HEGADAS formulation suggested by Witlox (1988) following a critical analysis of McQuaid's wind-tunnel data.

Airborne Plume: Passive Entrainment

In addition to 'jet' and 'crosswind' mechanisms, entrainment within the airborne plume is influenced by the state of ambient turbulence. Asymptotically it is this mechanism which is predominant, and which results in the far field in the Pasquill/Gifford correlations for the Gaussian standard deviations (Plate 1982; Stern, Boubel, Turner and Fox 1984) $\sigma_y(x,z)$, and $\sigma_z(x,z)$, as functions of the distance x downwind of release and (Pasquill 1976) of the (effective) plume height z. Additionally the ambient turbulence in the surface layer (Plate

1982; Stern, Boubel, Turner and Fox 1984) is governed (at any rate approximately) by Monin-Obukhov similarity theory, so that the entrainment function should be expressible in terms of the surface roughness, Monin-Obukhov length, and the plume centroid height above the ground surface.

Three approaches seem possible in formulating the passive entrainment function for the airborne plume. First we may attempt direct 'matching' from a plume-rise model in which passive entrainment is neglected to a Gaussian Pasquill-Gifford model for the far-field. Conservation of the fluxes of entrained mass, pollutant mass, horizontal momentum excess, prescribe the location of a virtual point source needed by the Gaussian model. This approach has clear computational advantages; it removes the need for the 'step by step' downwind integration of a set of ordinary differential equations describing plume motion. It takes advantage of well established empirical correlations for the far-field.

Notwithstanding, we may attempt to introduce within the range of plume rise and fall an approximate passive entrainment function, the effect of which will be to correct somewhat the predictions made in the absence of turbulent diffusion. The range of application will be such that the passive entrainment term is at most of co-magnitude with contributions from 'jet' and from 'crosswind'. Reference to the literature reveals essentially two procedures for the determination of the passive entrainment function; procedures based upon 'matching' to the Pasquill/Gifford correlations (Bloom 1980), and methods based upon an analysis of Monin-Obukhov similarity (Ooms 1972). Of these methods the former class may be criticised in that they rely on function forms constructed from far-field data, yet they are used in the near field when effects of buoyancy and release momentum are yet significant. We prefer the latter class, and in particular propose a (previously unpublished) formulation developed by Disselhorst (1987).

$$\mathrm{Entr}^{\mathrm{turb}}_{\mathrm{amb}} = (1 - \ell/D)\,\pi\, e^{\mathrm{turb}}_{\mathrm{amb}}\ \rho_\infty\, \varepsilon^{1/3}\,[\ell_y^{\,4/3}+\ell_z^{\,4/3}] \tag{51}$$

$$\begin{aligned} \ell_y &= \min[D/2,\ 0.88(z+z_r)(1-7.4\,\kappa\zeta)/(1-5\kappa\zeta)], && P/G = \{'A','B','C'\} \\ &\quad \min[D/2,\ 0.88(z+z_r)] && P/G = \{'D'\} \\ &\quad \min[D/2,\ 0.88(z+z_r)/(1+0.1\zeta)] && P/G = \{'E','F'\} \end{aligned} \tag{52}$$

$$\begin{aligned} \ell_z &= \min[D/2,\ 0.88(z+z_r)(1-7.4\,\kappa\zeta)/(1-5\kappa\zeta)] && P/G = \{'A','B','C'\} \\ &\quad \min[D/2,\ 0.88(z+z_r)] && P/G = \{'D'\} \\ &\quad \min[D/2,\ 0.88(z+z_r)/(1+4\zeta)] && P/G = \{'E','F'\} \end{aligned} \tag{53}$$

$$\varepsilon = \begin{cases} (1 - 5\,\kappa\zeta)u_*^3/\kappa/(z + z_r) & P/G = \{\text{'A','B','C'}\} \\ u_*^3/\kappa/(z + z_r) & P/G = \{\text{'D'}\} \\ (1 + 4\kappa)u_*^3/\kappa/(z + z_r) & P/G = \{\text{'E','F'}\} \end{cases} \qquad (54)$$

and $e^{turb}_{amb} = 1.0$, $\zeta = (z + z_r)L$, $L = u_*^3/\kappa/(g/T_g)/(u_*T_*)$.

Notation: z_r surface roughness, L Monin/Obukhov length, u_* friction velocity, κ Von Kármán constant, T_g ground (absolute) temperature, u_*T_* surface/air heat-flux, ε dissipation rate of turbulent kinetic energy, (ℓ_y, ℓ_z) turbulent (transverse horizontal, vertical) eddy length-scales; ℓ plume 'base'-length, D plume 'diameter', z centroid height; P/G Pasquill/Gifford atmospheric stability class.

This formulation differs from that proposed by Disselhorst in three ways. First the cross-section of an airborne plume is circular and not elliptic: nonetheless the different horizontal and vertical length scales within the atmosphere are represented. Second the atmospheric boundary layer is presumed effectively infinite: this should prove unproblematical for near ground releases of dense gas. Third the entrainment term is in the touchdown region given a linear scaling in $1-\ell D$ in order to vanish identically at (and beyond) the point of first plume slumping.

Interactions

Heavy-gas and jet entrainment are *not* independent mechanisms; each modifies the level of turbulence by inducing vertical gradients of velocity. These velocity gradients are (in general) antagonistic; the presence of dense gas requires a positive, of a (strong) jet a negative, gradient at the cloud surface.

We take the combined effect of jet and heavy-gas entrainment as the greater of the two contributions when acting in isolation. Further, pursuing the analogy with HEGADAS, we regard the heavy-gas entrainment as taking place across the plume 'top', with jet entrainment acting over both 'top' and 'side'. This maximum entrainment is (for reasons of continuity) partitioned amongst heavy-gas and jet mechanisms in the same proportion as would have arisen from the addition of the contributions Entr_{jet} and $\mathrm{Entr}^{heavy}_{gas}$:

$$\mathrm{Entr}^{jet}_{\substack{heavy\\gas}} = (\ell/L^{free}_{surface})\,\max(\mathrm{Entr}_{jet},\mathrm{Entr}^{heavy}_{gas}) + (1 - \ell/L^{free}_{surface})\,\mathrm{Entr}_{jet} \qquad (55)$$

$${}_{jet}\mathrm{Entr}^{jet}_{\substack{heavy\\gas}} = [\mathrm{Entr}_{jet}/(\mathrm{Entr}_{jet} + \mathrm{Entr}^{heavy}_{gas})]\,\mathrm{Entr}^{jet}_{\substack{heavy\\gas}} \qquad (56)$$

$${}^{heavy}_{gas}\mathrm{Entr}^{jet}_{\substack{heavy\\gas}} = [\mathrm{Entr}^{heavy}_{gas}/(\mathrm{Entr}_{jet} + \mathrm{Entr}^{heavy}_{gas})]\,\mathrm{Entr}^{jet}_{\substack{heavy\\gas}} \qquad (57)$$

The concepts of 'top' and 'side' require elucidation: we take the 'top' to have a length equal to the length ℓ of intersection between cross-section and level ground; the 'side' we identify with the balance $L^{\text{free}}_{\text{surface}} - \ell > 0$ of the 'free surface' or perimetric length.

The interaction between passive and gravity-slumping entrainment is treated similarly; interaction arises inasmuch as the contribution of passive entrainment induces lateral expansion which itself induces entrainment represented by gravity slumping. Such 'feedback' of entrainment is clearly a-physical, and results, for an 'airborne' plume, in the exponential increase of plume diameter and dilution. The assumptions are summarised below

$$\text{Entr}^{\text{pass}}_{\substack{\text{grav}\\\text{slump}}} = \max(\text{Entr}_{\text{pass}}, \text{Entr}^{\text{grav}}_{\text{slump}}) \tag{58}$$

$$_{\text{pass}}\text{Entr}^{\text{pass}}_{\substack{\text{grav}\\\text{slump}}} = [\text{Entr}_{\text{pass}}/(\text{Entr}_{\text{pass}} + \text{Entr}^{\text{grav}}_{\text{slump}})]\ \text{Entr}^{\text{pass}}_{\substack{\text{grav}\\\text{slump}}} \tag{59}$$

$$^{\text{grav}}_{\text{slump}}\text{Entr}^{\text{pass}}_{\substack{\text{grav}\\\text{slump}}} = [\text{Entr}^{\text{grav}}_{\text{slump}}/(\text{Entr}_{\text{pass}} + \text{Entr}^{\text{grav}}_{\text{slump}})]\ \text{Entr}^{\text{pass}}_{\substack{\text{grav}\\\text{slump}}} \tag{60}$$

5.B.9. The atmosphere model.

In the HGSYSTEM version 3.0 plume models, the same profiles for ambient wind speed and temperature are used as in the HEGADAS model. See Appendix 7.A.A for a description of these profiles.

5.B.10. Plume cross-sectional over-lap: curvature limited entrainment

The co-ordinate system used in formulating the 'top-hat' model of plume development determines and is determined by the physical interaction of the released jet and the ambient wind.

The co-ordinate system is not universal but exists only within a limited distance from the plume axis. Circumstances may arise in which plume curvature, whether in response to strong cross-winds, or to ground impact, results in the predicted 'over-lap' of successive plume cross-sections. Such behaviour is certainly rare for gas (including heavy gas) releases, and is largely absent from the wind-tunnel data sets of Hoot, Meroney and Peterka (1973) (dense gases), and of Petersen (1978) (buoyant plumes). Nevertheless, in view of the higher density and lower velocity to be expected in the near-field following release of pressurised dense jets, it seemed expedient to include provision for such plume 'overlap' within the HGSYSTEM plume models.

This section outlines the method employed by the HGSYSTEM plume models in treating such behaviour: the method adopted is *not* universally effective, but is successful in the clear majority of cases.

We begin by analysing the conditions under which plume overlap occurs in each of the three regions; airborne, touchdown, and slumped plume. Incipient overlap is defined by a geometrical relation in which a representative plume 'width' is compared with the axis curvature $d\phi/ds$. The results are as follows:

Airborne Plume

$$D/2 \, |d\phi/ds| = 1 \qquad (66)$$

Touchdown Plume

$$\begin{aligned} &-z/|\cos\phi| \, d\phi/ds = 1, \text{ for } d\phi/ds < 0 \\ &[D/2 - (z - z_c)/|\cos\phi|] \, d\phi/ds = 1, \text{ for } d\phi/ds < 0 \end{aligned} \qquad (67)$$

Slumped Plume

$$\begin{aligned} &-z/|\cos\phi| \, d\phi/ds = 1, \text{ for } d\phi/ds < 0 \\ &[\max(1,e) \, D/2 - z/|\cos\phi|] \, d\phi/ds = 1, \text{ for } d\phi/ds<0 \\ &e = (3\pi/2)\,(z/D)/|\cos\phi| \end{aligned} \qquad (68)$$

Notation: D plume (effective) 'diameter', z centroid height, e eccentricity (ratio minor to major axis for semi-ellipse), z_c centre height (circular segment), ϕ axis-inclination, s centre-line displacement, $d\phi/ds$ centre-line curvature.

These conditions define the limits imposed by cross-section geometry upon the integration of the pollutant source and ambient atmosphere implied by the conservation laws, and by the (empirically determined) entrainment function. Should these limits be exceeded we are faced with two alternatives: alter the geometry of the cross-section, or modify the entrainment function itself.

Modification of the sectional geometry is the more complex option: we must *simultaneously* satisfy the original entrainment equation and a consistency relation requiring that plume 'overlap', while incipient, does not actually occur within the zone of high axis-curvature. Introduction of variable geometry (within the three plume regions already recognised) substantially increases the number and complexity of geometrical transitions that must be represented within a computer based model. Such high curvature regions are, in any case, quite rare, or have quite limited geometrical extent, so that the need for such an increase in complexity did not seem, a priori, justified.

As an alternative to the modification of plume geometry, we may alter the entrainment function in regions of high curvature so as to prevent the occurrence of plume overlap. Concretely we replace the entrainment relation, d/ds(dm/dt) = Entr, by whichever of the geometrical constraints for incipient plume overlap is appropriate for the present cross-sectional shape. This revised equation system is of necessity geometrically consistent, and may be matched by continuity arguments to the previously existing plume structure. In addition the entrainment rate implied by the geometrical constraint may be calculated as the derivative d/ds(dm/dt). This parameter is then compared with the entrainment rate that would have occurred for the same plume description in terms of sectional mean velocity, density, and the like, from the empirically determined entrainment function Entr.
The model reverts to this usual description, should the 'curvature limited' entrainment exceed that calculated from the empirical entrainment function. This procedure introduces a minimal change into the basic model consistent with the existence of 'curvature limited' behaviour. The procedure rests upon the idea that excessive plume curvature is the result of too rapid air entrainment, and that the reduction of air entrainment to the maximum value compatible with plume geometry will permit integration to continue through the high curvature zone and to recover the basic model at some greater downwind displacement.

The success of this device of 'curvature limited' entrainment rests on the ability of the curvature limited model to recover normal entrainment rates. However it may occur that the corollary entrainment rate d/ds(dm/dt) inferred from a curvature limited model actually decreases *more rapidly* than does the associated empirically determined entrainment rate (Entr) for the *same* plume description.
Should this occur termination of the curvature limited zone will occur following detection of the a-physical entrainment step d/ds(dm/dt) ≤ 0. The plume models will terminates with an error message.

5.B.11. The HGSYSTEM plume models: algorithmic structure.

In order to solve the set of ordinary differential equations and non-linear algebraic which result from our plume modelling, a numerical solver capable of treating systems of this complexity is required.

SPRINT (Software for PRoblems IN Time) is such a solver: it was developed by Shell Research and by Leeds university (Berzins, Dew, and Furzeland 1983; Berzins and Furzeland 1985). SPRINT is effective for the solution of the differential/algebraic system in each plume region. It employs, for the solution of the algebraic constraints, a technique which is efficient for starting values near to the solution (values as are typically found for successive ODE steps). It may, however, prove inadequate for the determination of the 'initial conditions' needed at the release orifice, post flash, at touchdown, or at first plume slumping. Initial values are needed not only for the variables themselves, but also and equally importantly, for the first derivatives d/ds of all variables. These derivatives are typically discontinuous at the several model region boundaries, boundaries at which the assumed geometrical shape or phase composition of the developing plume change abruptly.

This difficulty with initial conditions is well known (Berzins, Furzeland and Scales 1988) and, for the HFPLUME model, it is made even more difficult due to the severe non-linearity introduced by the complex thermodynamic interaction of hydrogen fluoride and moist air.
The 'starting' problem, and in particular the calculation of initial derivative values 'immediately post transition' may be formulated as a non-linear algebraic problem for which we may employ a 'state of the art' non-linear equation solver. Such a solver, NAESOL (Non-LineAr Equation SOLver), has recently been developed at Thornton Research Centre (Scales 1994). This solver, which incorporates advanced search strategies, and provision for the solution of ill-conditioned or locally singular problems, typically succeeds where SPRINT would fail.

5.B.12. Validation studies, entrainment formulae

Several components of the model encoded in the HGSYSTEM plume models have been subject to independent experimental test. This section summaries the results of these validation studies, noting successes and limitations. Suggestions are made for further work in this area. The plume models as available in HGSYSTEM have *not* been tailored to data arising from the Goldfish experiments (Blewitt, Yohn, Koopman and Brown 1987; Blewitt, Yohn and Ermak 1987; Blewitt 1988), or other prototypical data: they have rather been *assembled* of separately validated models for plume entrainment and thermodynamics. Its success , when coupled with HEGADAS, in predicting the Goldfish experiments should be viewed in that light.

Buoyant plumes: crosswind entrainment and plume-path

Petersen (1978) carried out an extensive set of wind tunnel tests in which plume-path and concentration decay were examined as a function of distance downwind of a vertical release into a (near uniform) cross-wind. We consider those (19) experiments conducted for 'low' ambient turbulence in the Meteorological (boundary layer) Wind Tunnel at Colorado State University. High temperature air releases were simulated by the (isothermal) release of helium/air mixtures. The plumes were made visible by passing the stack gases over $TiCl_4$ (titanium tetrachloride) prior to release.

We have compared the experimental results obtained by Petersen with model runs in the limit of negligible ambient turbulence and with the entrainment formulation

$$\mathrm{Entr} = (\pi D)\,[e_{jet}\,\eta_{jet}\,\rho_\infty\,|u - u_\infty\cos\phi| + Cue^{cross}_{wind}\,\eta^{cross}_{wind}\,\rho_\infty\,u_\infty\,\sqrt{u_\infty / u}\,|\sin\phi|\,]$$

$$\eta_{jet}(\rho/\rho_\infty) = [1+(4/3)(\rho/\rho_\infty - 1)]/]1 + (5/3)\,(\rho/\rho_\infty - 1)] \qquad (69)$$

$$\eta^{cross}_{wind}(\rho/\rho_\infty,\phi) = [1 + C\rho e^{cross}_{wind}\,\max\{0, \rho/\rho_\infty - 1)\,\sin\phi\}]$$

with coefficents $e_{jet} = 0.08$, $Cue^{cross}_{wind} = 0.60$, $C\rho e^{cross}_{wind} = 7.5$

We compare the experimental rise-heights z_k with those $z(x_k)$ predicted to occur at the experimental (horizontal) displacement x_k downwind of release. The results are summarised in Figure 5.12. Agreement is satisfactory, with the predicted values almost always within 15% of those observed. The function form, and coefficient values for jet and crosswind entrainment are essentially those (0.08 and 0.60) recommended by Briggs (1984) on the basis of extensive data concerning neutral and buoyant plumes released at right angles to an imposed wind.

Dense plumes: crosswind entrainment and plume-path

Hoot, Meroney and Peterka (1973) conducted experiments in the (boundary layer) wind tunnel at Colorado State University the purpose of which was the characterisation of dense plume dispersion. Dense gas was formed by mixing air and Freon 12; releases were directed upwards and at right angles to the ambient wind; plumes were made visible by impinging the premixed (dense gas) jet on the surface of titanium tetrachloride ($TiCl_4$).

We consider a series of releases into a laminar crosswind, for which the velocity profile (Hoot, Meroney and Peterka (1973) Figure 4) is essentially constant above 3 inch from the tunnel floor.

We have compared the experimental results obtained by Hoot, Meroney and Peterka (1973) with predictions obtained in the limit of negligible ambient turbulence. The entrainment formulation are as above.

Comparison is made between observed and predicted maximum (centre-line) rise-height, and between (visible leading edge) touchdown and the impact of 'top-hat' leading-edge, or extrapolated plume centre-line, the tunnel floor. Initial conditions and observed rise heights and touchdown distances are as recorded in HMP (Hoot, Meroney and Peterka (1973)) (Report: Figure 2). In addition, comparison is made with horizontal displacement of maximum plume rise correlated by HMP's formula

$$x/D_0 = (u_\infty u_0)/(gD_0)(\rho_0/\rho_\infty - 1) \qquad (70)$$

The results of a comparison between the predictions of the PLUME model and HMP date are presented in Figures 5.13 through 5.16. Generally the agreement is good, with (maximum) rise-height fitted to within perhaps 10%, maximum-rise displacement.

As regards plume 'touchdown' the situation is more complex. HMP measured the horizontal displacement from release of the point of 'visible plume edge' touchdown. This differs significantly from (extrapolated) plume centre-line touchdown, and with the touchdown of the integral averaged plume width. It is well known (Briggs 1984) that the 'momentum' and 'concentration' widths of plume differ significantly. A 'top-hat' model, which represents mass and momentum entrainment with a single plume width, cannot accurately predict concentration width. Neither is it possible to identify the 'visible plume edge' with any fixed proportion of the equivalent Gaussian (concentration) width. The systematic dilution on the plume centre-line must imply that the 'visible edge' is an increasingly small proportion of the Gaussian width. Ultimately, of course, the visible plume must dissipate entirely. In the circumstances we are content to compare 'visible edge' data with predicted centre-line (Figure 5.15) and 'top-hat' edge displacements at 'touchdown' (Figure 5.16). The centre-line displacement is systematically larger, the 'top-hat' edge smaller, than visible edge touchdown observed by HMP.

Considerable scatter is evident: this reflects the sensitivity of plume touchdown to small variations in entrainment taking place in weakly descending (marginally dense) plumes. We consider this comparison satisfactory. Further improvements in the modelled entrainment must await more accurate experimental data on (extrapolated) centre-line touchdown. This latter could be deducible from photographs of visible plume-path taken (but not published) by Hoot, Meroney and Peterka.

In addition a comparison has been made with the small but well instrumented data set of Li, Leijdens and Ooms (1986). These authors measured the detailed vertical profiles that resulted from the downward release of heated air into an essentially uniform air stream. Differences between air and plume density are everywhere small, so that these experiments should be analogous to weakly dense plumes released upwards. The results are presented in Figure 5.17. Agreement is satisfactory, as regards both plume path and width. Accuracy is comparable or better to that achieved by Havens (1988), but is inferior to that of Li, Leijdens and Ooms using their elliptic sectioned Gaussian model. Nevertheless the overall predicative accuracy of the entrainment formulation advanced here is judged sufficient for purpose. Certainly the very large experimental scatter, and range of correlation based predictions should be borne in mind (Petersen 1987).

AEROPLUME validation

Post (1994) describes several validation test done with the HGSYSTEM 3.0 plume model AEROPLUME. Comparison with data is favourable including measurements for the distance to Lower Flammability Limit (LFL) for pressurised liquid propane releases.

5.B.13. Comparison with models of Wheatley, Raj and Morris, and Havens

It is useful to contrast the models of Morris and Raj (1987) for grounded jet, Wheatley (1986) for a two-phase jet, and Havens and Spicer (1988) for a dense gas plume with that here proposed for the representation of two-phase/dense gas releases (AEROPLUME) or HF releases (HFPLUME). Each of these models have limitations which restrict, more or less severely, the range of applicability. Certainly none will span the range of release conditions encompassed by AEROPLUME/HFPLUME.

The free jet model of Wheatley

This model (Wheatley 1987a, 1987b) was developed in order to predict the downwind distribution of concentration and temperature resulting from a pressurised release of liquid ammonia. The model structure is: steady state, no atmosphere gradients, (isobaric) thermal equilibrium, entrainment dominated by jet/ambient shear, negligible gravity slumping.

Though the model (TRAUMA) was originally 'tailored' for liquid ammonia releases, its thermodynamic structure permits the release of several reactive liquids and in particular anhydrous HF. No provision is made for the impact of jet upon the ground, either in respect of induced drag, or of geometrical distortions. Model applicability is thus limited under prototypical conditions to a downwind range of perhaps 10m, and to HF concentrations in excess of some 1% by volume HF.

The model differs from HFPLUME in that complete 'atomisation' of the released liquid is not *assumed*, but is rather *checked* against a criterion first developed by Ohnesorge (1936) for thermodynamically stable liquid jets. Maximum stable droplet size and gravitational settlement of droplets (Clift, Grace and Weber 1978) are considered in the context of droplet 'rain-out'; a simple (inequality) condition is developed for the absence of droplet rain-out. The analysis takes no account of droplet evaporation. The restricted downwind range of Wheatley's model make it suitable for the near-field prior to plume touchdown. No provision is made for other than horizontal releases. Overall the accuracy and range of validity of this model (comparable to HFPLUME) is, we judge, insufficient for a confident 'matching' to either heavy gas or passive dispersion models in the far field.

The grounded jet model of Morris and Raj:

Raj and Morris (1987) proposed a 'top-hat' (sectionally averaged) model for a ground affected (rectangular) jet. The range of validity extends from (plume) touchdown through momentum dominated jet, towards heavy gas dispersion. The model structure takes account of wind shear and atmospheric stability, and incorporates ground drag and gravity slumping effects. The cross-section is vertical. The equation system comprises horizontal momentum, conservation of pollutant mass-flux, a (differential) entrainment relation, and a gravity spreading law. Thermal equilibrium is assumed throughout. The entrainment relation is proportional to the mean difference (over 'top' or 'side') between ambient wind-speed and jet velocity.

Entrainment is further proportional to the ambient density and to a dimensionless entrainment coefficient which on the basis of gas jets has an anticipated magnitude $e \approx 0.08$. This is analogous to the formulations in the HGSYSTEM plume models, except that all parameters are referred in these latter cases to the centroid height. The drag force comprises two parts, a shear force exerted at the 'top' surface, and a 'drag' at the ground. Drag on either surface is assumed proportional to the square of the difference at the bounding surfaces between jet velocity and wind speed. Account is taken of density differences inasmuch as the drag at the jet 'top' is assumed proportional to the *ambient* density, whereas that at the ground is linear in the jet mean density.

This model is strongly empirical, however, in that both ground and atmosphere drag are assigned adjustable coefficients for matching with experimental data. Additional entrainment terms, representing ambient atmosphere entrainment, and lateral spreading entrainment (Puttock 1988) are entirely absent. The several empirically adjustable coefficients are obtained (and the model tuned) by comparison of model predictions against an extremely small data set, the Desert Tortoise 4 Ammonia Release (Ermak, Chapman, Goldwise, Gouveia and Rodean 1987).

In spite of these limitations it seems likely that the model of Raj and Morris represents a significant improvement on that of Wheatley for a free jet. The key difference rests in the explicit representation of gravity slumping in the formula

$$\frac{dD}{ds} = \frac{k}{u}\sqrt{gh(\rho/\rho_\infty - 1)}\text{, with } k = 1.15 \qquad (71)$$

This permits a reasonable description of gravity slumping for a near horizontal release in which horizontal and vertical motions are largely decoupled. Entrainment is dominated by jet/atmosphere shear. The structure is, however, incompatible with existing integral-averaged plume models, and cannot represent the early interaction between impacting plume and ground that accompanies 'touchdown'. Neither can the early (airborne) jet be followed, so that for predictions near the source a 'free' jet model, such as AEROPLUME, HFPLUME or TRAUMA, must be matched to that of Raj and Morris (1988).

The problem, mathematically, is that a gravity slumping formula has replaced the vertical momentum equation in the limit of horizontal jet flow: the solution (section 5.B.7) is to introduce pressure forces, acting at the ground surface, such as allow recovery of gravity slumping and plume descent in the appropriate asymptotic limits. Such a formulation we expect to be of comparable or greater accuracy for horizontal pressurised releases, whilst permitting extrapolation to vertical releases, and releases inclined to the ambient wind. The formulation of the drag forces at upper and lower jet edge is complex, and highly empirical. Formulations based on an analysis of the turbulent averaged equations of motion lead rather directly (section 5.B.7) to a drag force expressed in terms of ambient parameters at the centroid height, the form of which introduces no empiricism beyond that required for heavy gas (ambient) entrainment. The formulation of the HGSYSTEM plume models is therefore consistent throughout the free jet, touchdown, and slumped plume regions, and contains entrainment mechanisms relevant to all. The HGSYSTEM plume models is uniformly valid from point of release to far within the heavy gas advection regime.

The atmosphere plume model of Havens and Spicer:

Havens and Spicer (Havens 1988) have proposed that the model of Ooms, Mahieu, and Zelis (1974) be used for the representation of dense gas releases prior to plume touchdown. The model is a variant of the simple integral average models in that a truncated Gaussian ('similarity') profile is imposed upon velocity, density, and concentration within the developing plume. The model also includes an initial zone model, in which are adopted empirical correlations spanning the region prior to the establishment within the plume of (approximately) Gaussian conditions. This initial zone model is uncertain, even in the context of gaseous releases (Keffer and Baines 1963, Kanotani and Greber 1972); it is doubtful whether this additional complexity is necessary or desirable.

Specific comments may be made regarding such (truncated Gaussian) formulations. The centre-line concentration is artificially heightened by the process of profile 'cut-off' whereby the mass in the Gaussian 'tail' is redistributed toward the plume centre. The use of a cut-off is not necessary for such a self-similarity theory and may be eliminated by a reformulation of the integral equations of motion (Schatzmann 1978, McFarlane 1988).

Li, Leijdens and Ooms (1986) employed a 'drag' force in order to reproduce the observed plume path for a set of 3 buoyant jets released downwards; the use of such a drag force is controversial (Briggs 1984); the data set severely limited. Coefficient values and the functional form of the entrainment function are uncertain (Petersen 1978, Schatzmann 1978); there is considerable scatter in the experimental data (Petersen 1987).

The benefits of truncated Gaussian over simpler 'top-hat' models seem to us unproved, even in the context of gas plumes. For reactive, initially two-phase releases, solution of such models requires numerical integration of the energy equation at each downwind advance of the discretized differential system for plume motion; it is not possible to introduce the several simplifications to the system thermodynamics that allow explicit integration of the enthalpy excess over the plume cross-section (Havens 1987). For complex reactive flows, and in particular for pressurised releases of anhydrous HF, the computational cost of a Gaussian model seems prohibitive. Additionally the model requires initial zone information appropriate to pressurised gas or two-phase, or atomised liquid phase releases.

In practical terms what is required is a model prior to plume touchdown passing integral averaged information to a grounded jet model (Raj and Morris 1987), a slumping pool model (Raj and Morris 1987), or (perhaps) a heavy gas advection model (Colenbrander and Puttock 1988). Details of concentration behaviour off-axis cannot readily be passed from model to model; nor is this information likely to be accurate. *A sectionally-averaged or 'top-hat' model seems to be a reasonable compromise between computational complexity and predicative accuracy.* Development of the energy equation for such a model presents no difficulty (Davidson 1986); neither are problems found with the inclusion of reaction chemistry (Forney and Droescher 1985).

> The touchdown model of Havens and Spicer has the merit of simplicity:
> 'The Ooms model' .. ' is terminated when the lower edge of the plume impinges the ground. The resulting downwind distance, plume centre line concentration and

> temperature, and plume radius ($b_j\sqrt{2}$) are used as input to DEGADIS. The ground level gas source input to DEGADIS is a circular area source with radius ($b_j\sqrt{2}$) and concentration and temperature equal to the centre-line values output from Ooms model.' (Havens 1988a, 1988b)

Insufficient detail is given to permit full consideration of the touchdown assumptions. We presume however that the DEGADIS circular source has an 'evaporation rate' such as to conserve mass- and excess-enthalpy flux at the plane of transition. No account is taken of the momentum excess in either horizontal or vertical direction developed in the course of plume rise and fall. Substantial vertical velocities must imply enhanced (impact) spreading; differences in horizontal velocity between plume and wind imply transition to a grounded jet model, or to some intermediate touchdown model. It seems essential to take some account of these velocity (momentum) differences in the vicinity of plume touchdown. We suggest transition to a spreading pool model (fed from above) or to a slumped plume model in the manner of the HGSYSTEM plume models. Alternatively some empirical correlation between plume and heavy-gas advection might be developed.

For releases which result in much delayed plume touchdown, (> 1 km, say) we agree with Havens that the use of Ooms model is compromised by the much earlier touchdown of the leading plume edge. A possible solution is to include an 'image' plume as a model of the (horizontal) ground. However dilution is likely to be such that plume behaviour more closely approximates passive dispersion than that appropriate to heavy-gas advection models such as DEGADIS or HEGADAS. We suggest that for these cases transition should be made to a Gaussian far-field dispersion model (Hanna 1982) based upon asymptotic matching of plume and Pasquill/Gifford standard deviations σ_y and σ_z. Discussion of 'image' plume dynamics illustrates the additional complexity imported with Gaussian rather than 'top-hat' models in plume touchdown.

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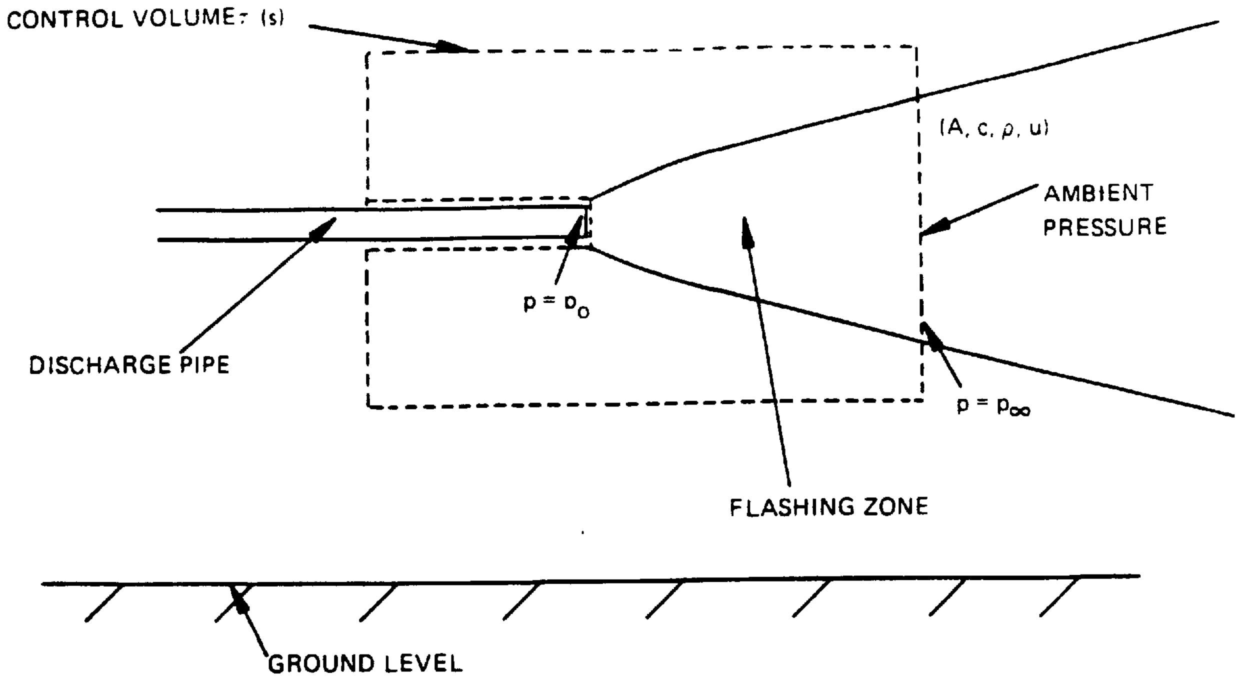


FIG. 5.1 – The zone of external flashing. On release, fluid expands to ambient pressure. Thermal equilibrium assumed. Entrainment and interphase slip taken to be negligible.

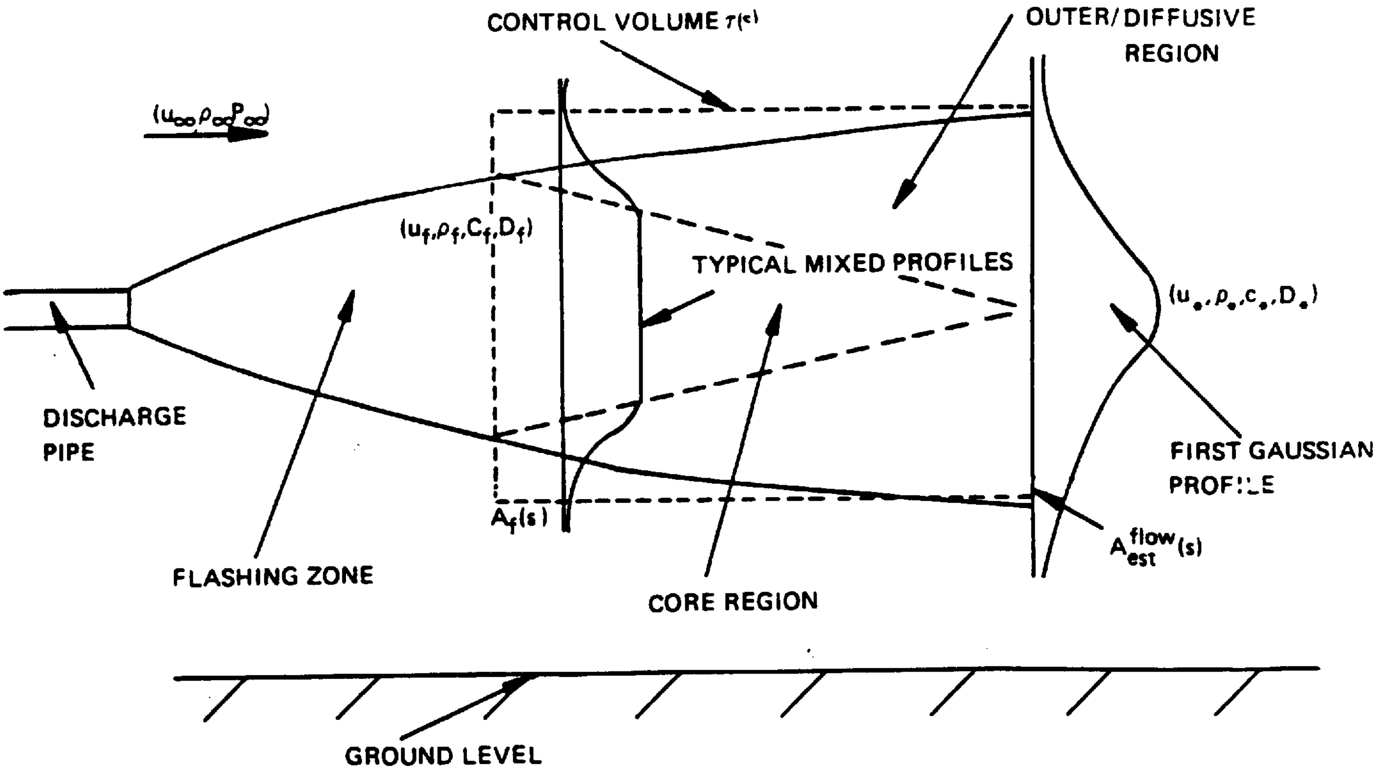


FIG. 5.2 – The zone of flow establishment. Transition region in which initially "top-hat" profiles are eroded by entrainment into outer region. Zone ends when undisturbed inner core region disappears to leave Gaussian profiles and self-similar flow.

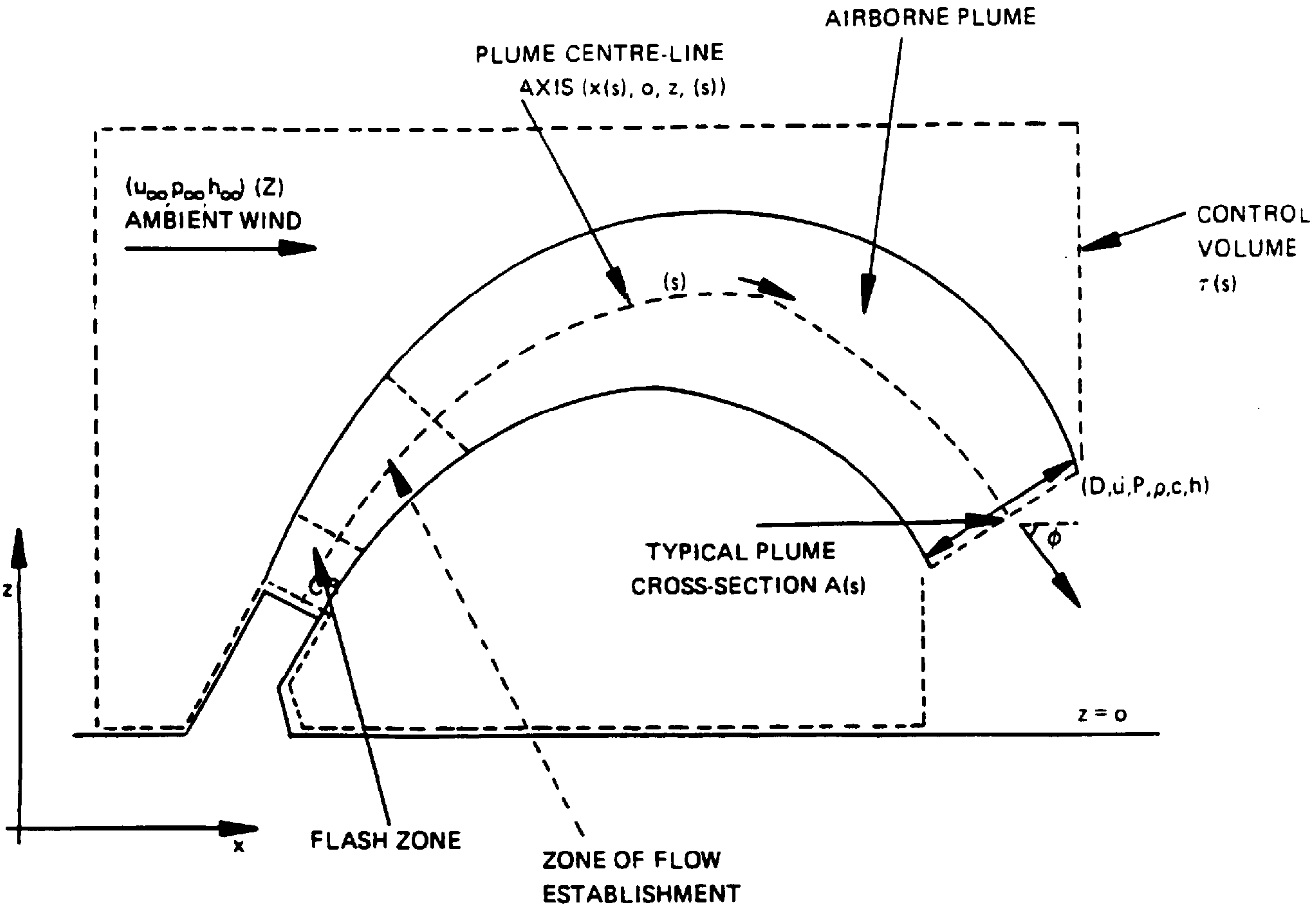


FIG. 5.3. – The airborne (established) plume. Negligible ground effect. Radial symmetry about plume centre-line.

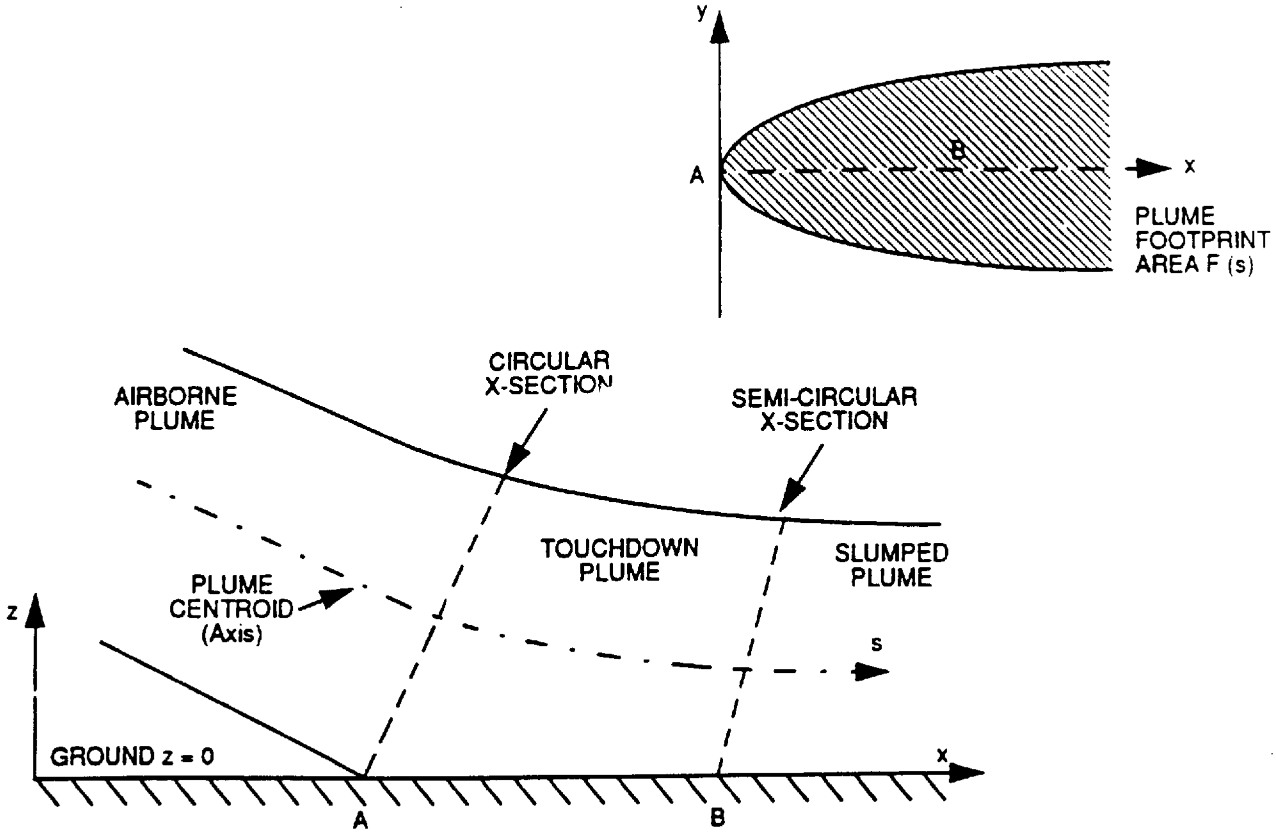


FIG. 5.4 - The touchdown plume. Transition of plume from circular X-section to semi-circular X-section in the touchdown region

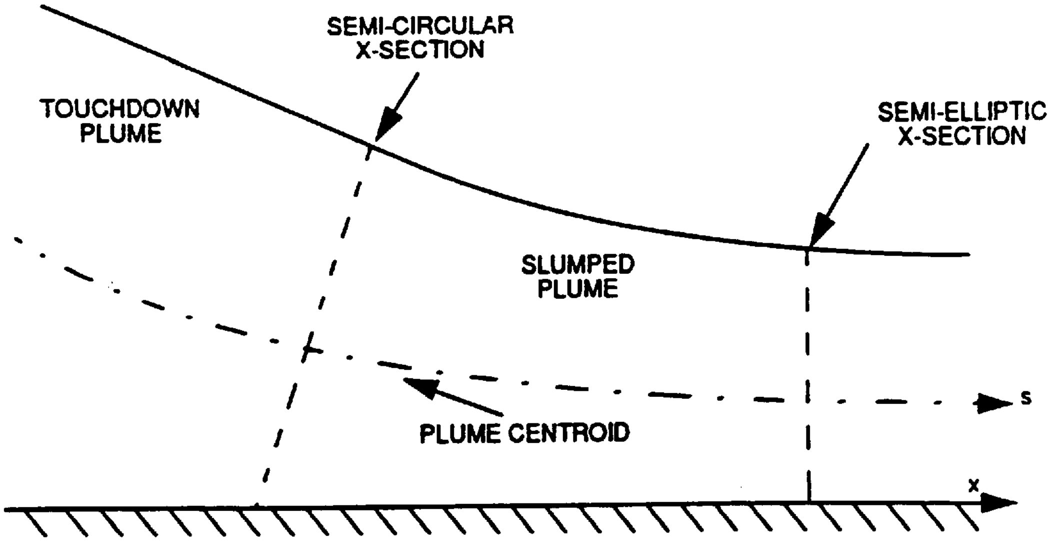


FIG. 5.5 - The slumped plume. Semi-elliptic X-section due to lateral gravity spreading

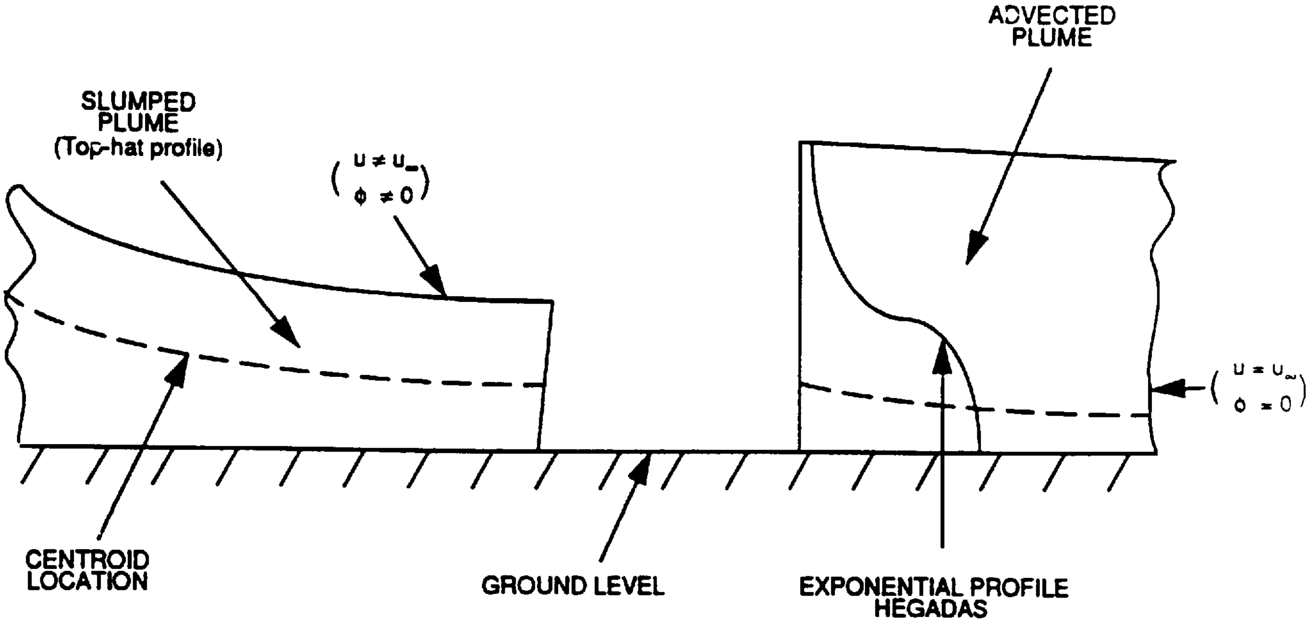


FIG. 5.6 - Transition to advected dense gas plume (HEGADAS). Criteria for transition are small plume excess velocity over ambient, and small jet entrainment

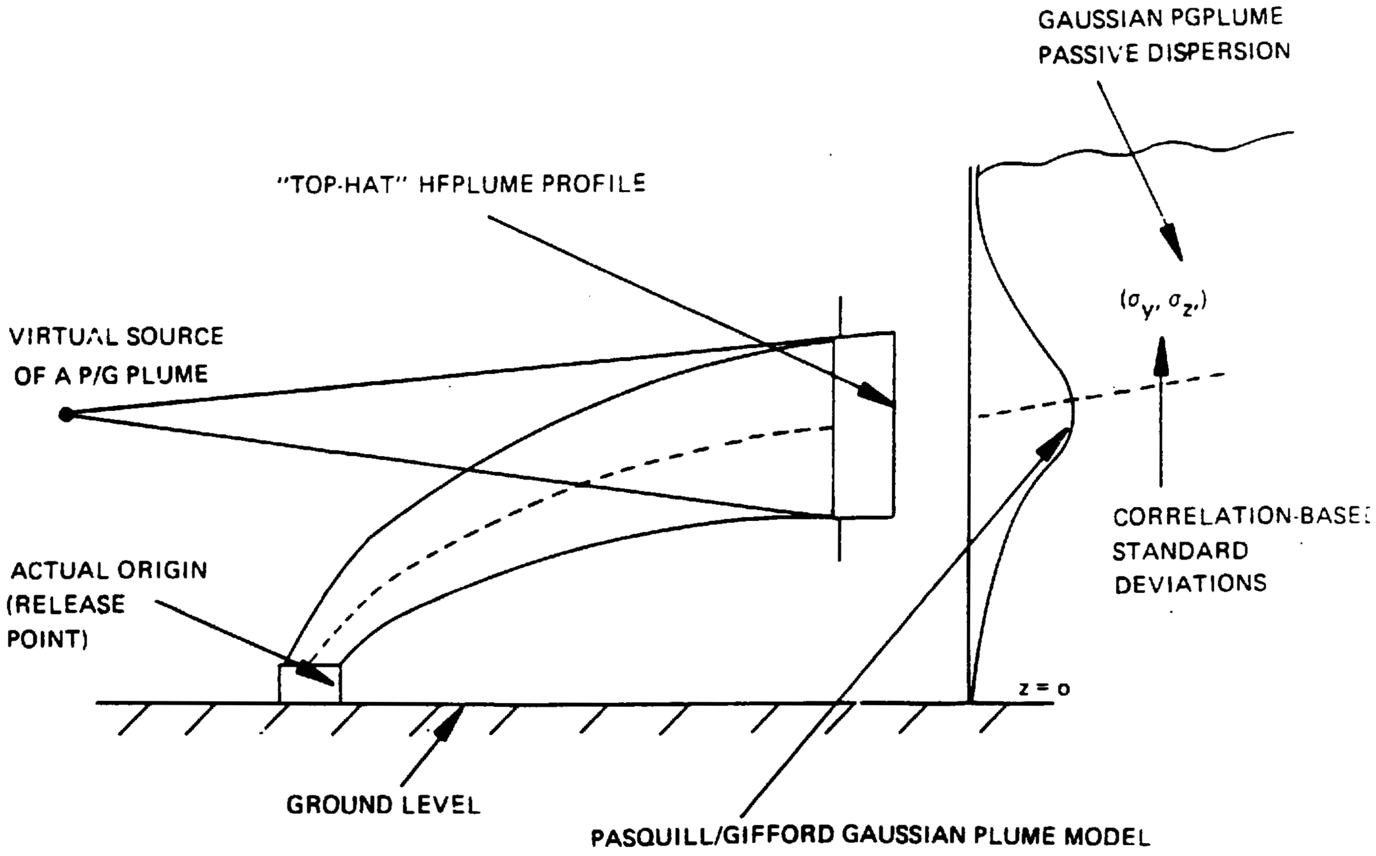


FIG. 5.7. – Transition to passive dispersion as an elevated Gaussian plume, when velocity excess over ambient is small and buoyancy/shear entrainment weak compared with passive entrainment.

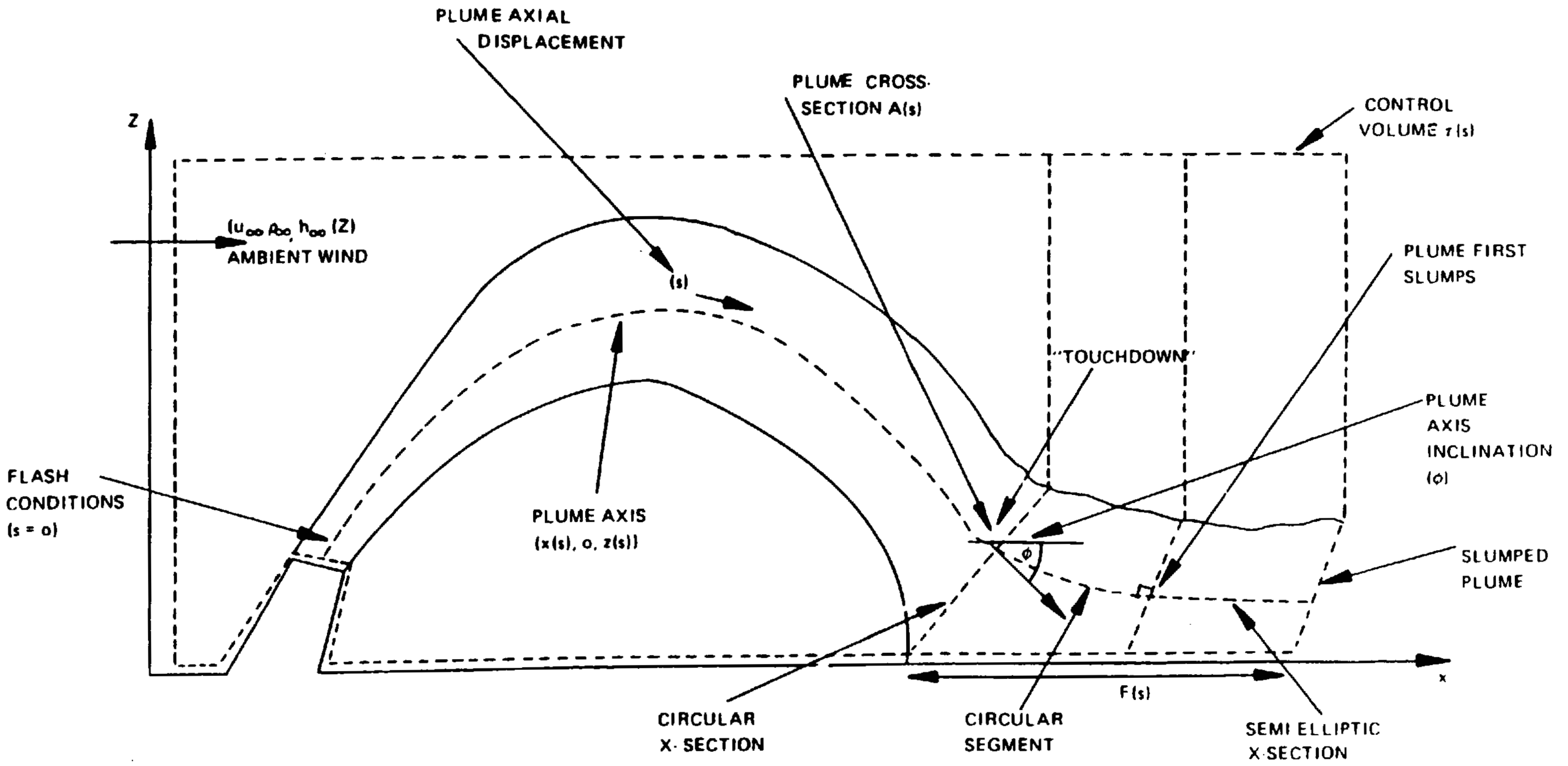
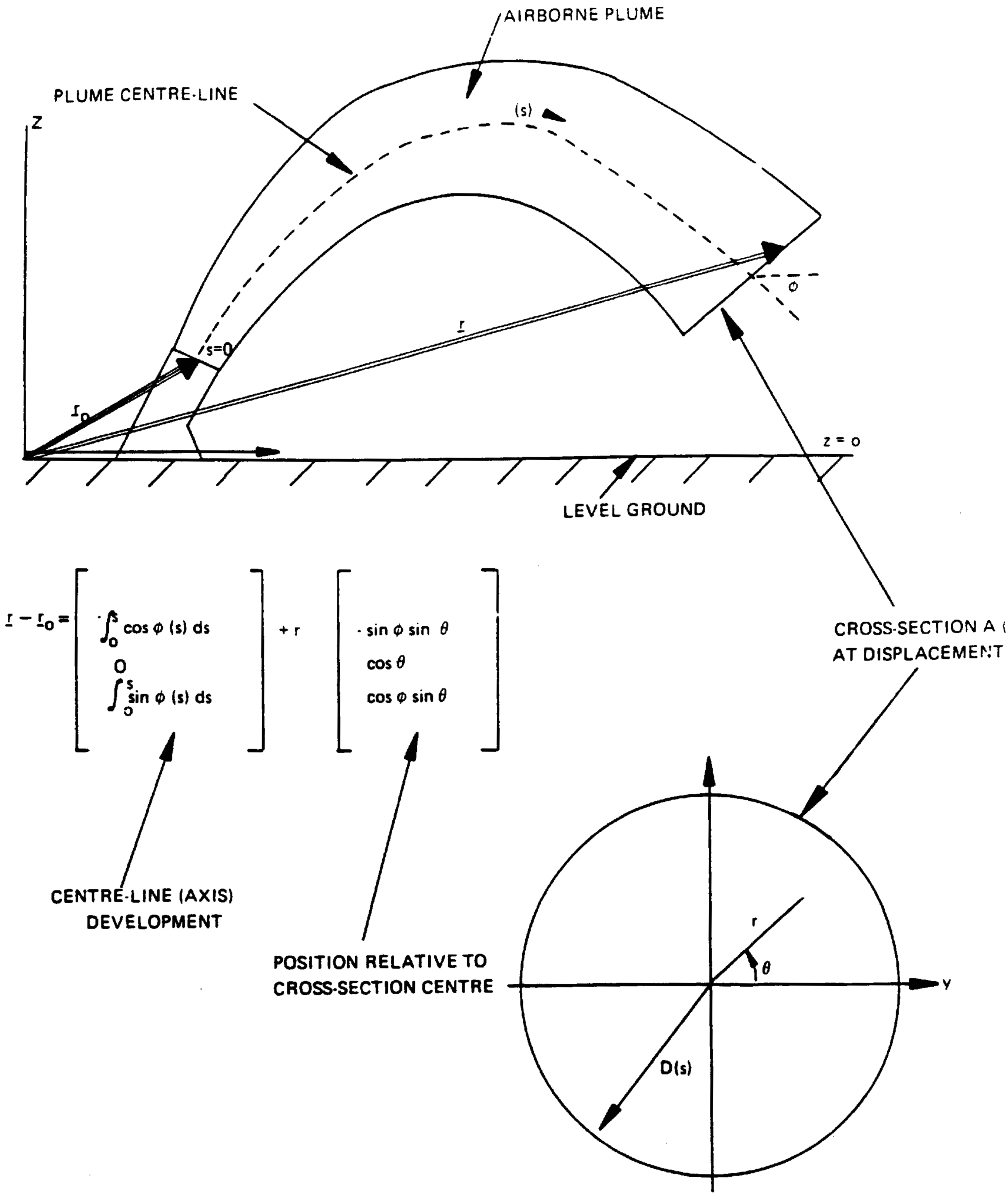


FIG. 5.8. — Illustration of the control volume $\tau(s)$, the plume coordinate system (s,r,Θ), and the cross-sectional geometry in the stages of plume development.



$$\underline{r} - \underline{r}_0 = \begin{bmatrix} \int_0^s \cos\phi(s)\,ds \\ 0 \\ \int_0^s \sin\phi(s)\,ds \end{bmatrix} + r \begin{bmatrix} -\sin\phi\sin\theta \\ \cos\theta \\ \cos\phi\sin\theta \end{bmatrix}$$

FIG. 5.9. – The plume coordinate system.

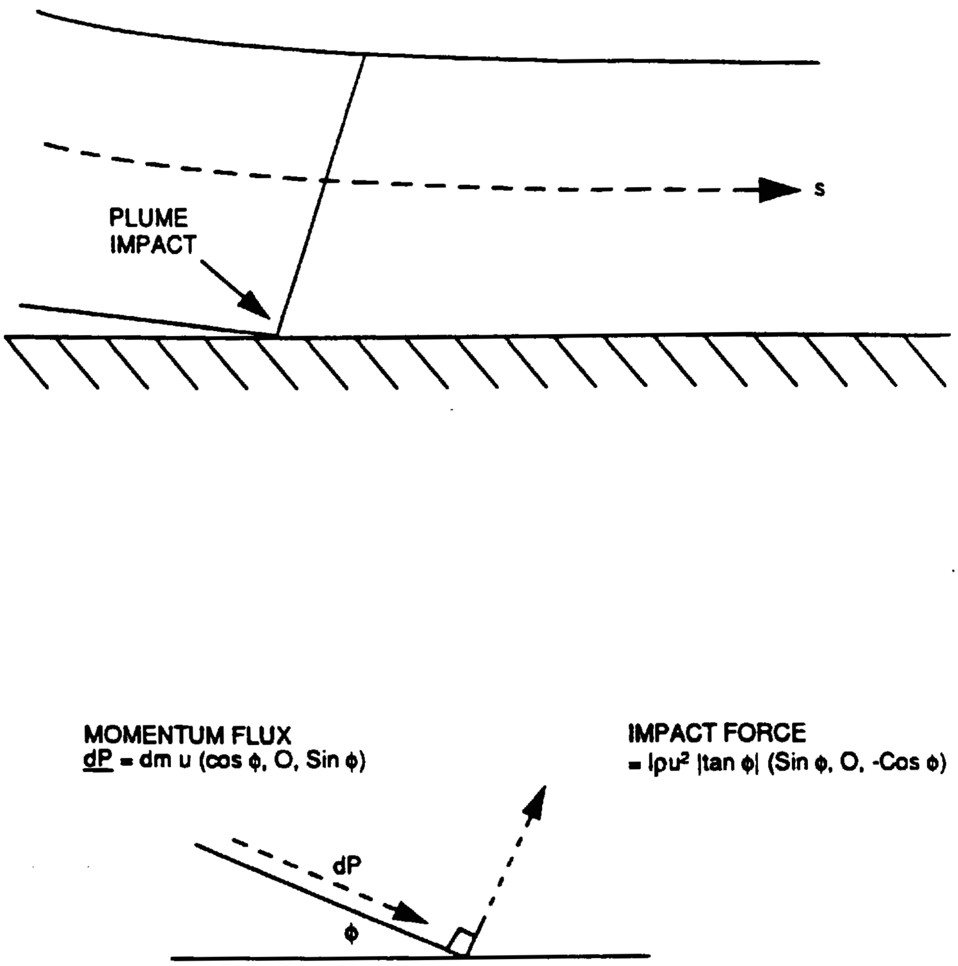


FIG. 5.10 - Plume Impact Pressure Forces. Fluid momentum impacting the ground is destroyed, exterting force per unit axis length of $I u^2 |\tan\phi|$. Kinetic energy conserved in elastic impact

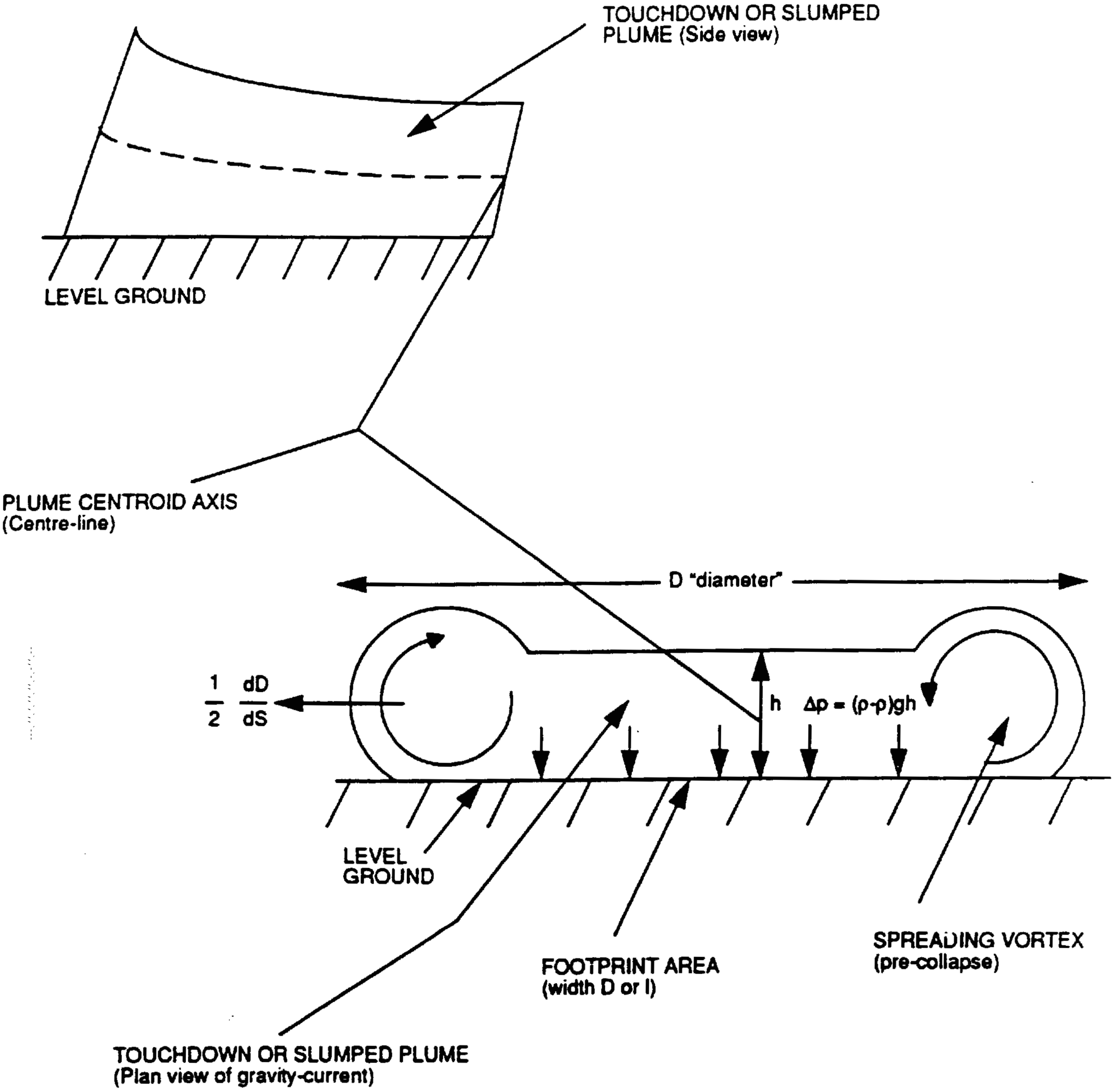


FIG. 5.11 - Gravity slumping and footprint area pressure forces. Lateral gravity spreading of heavy gas dominates slumping of plume

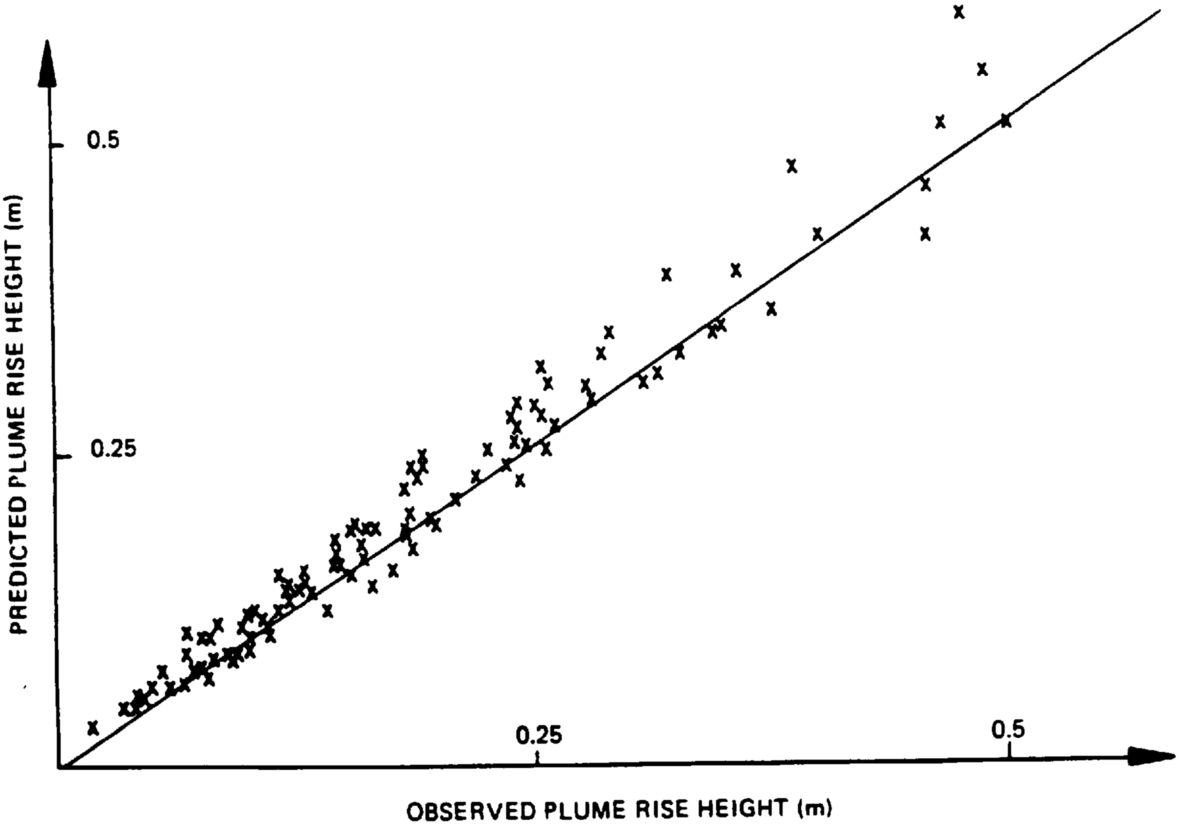


FIG. 5.12. – Comparison of the predicted plume rise height of buoyant plumes with the experimental data of Petersen (1978).

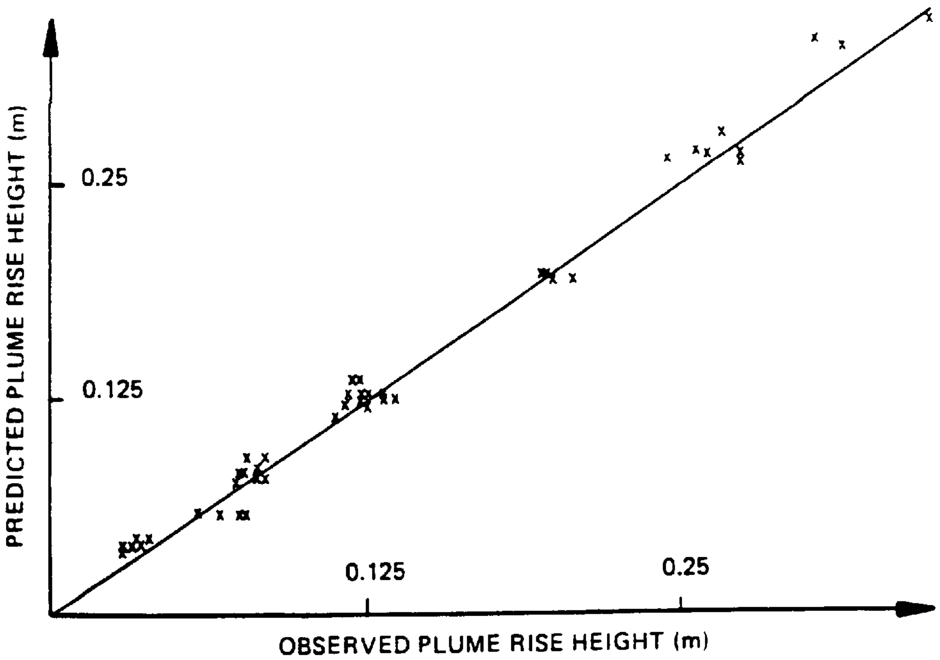


FIG. 5.13. – Comparison of the predicted plume rise height with experimental dense gas wind-tunnel data of Hoot, Meroney and Peterka (1973).

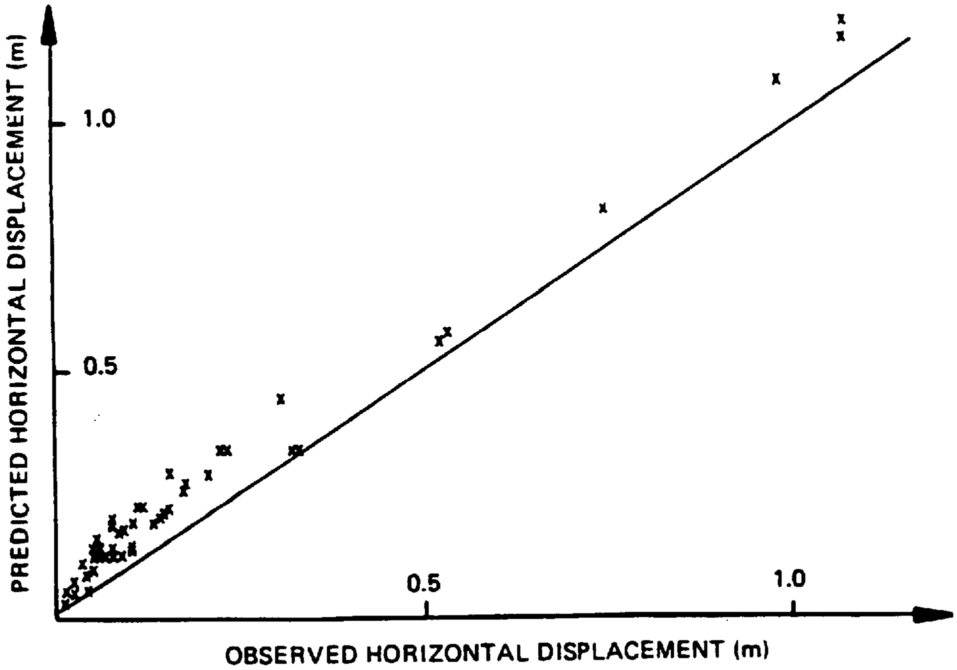


FIG. 5.14. – Comparison of the predicted location of maximum plume rise with experimental dense gas wind-tunnel data of Hoot, Meroney and Peterka (1973).

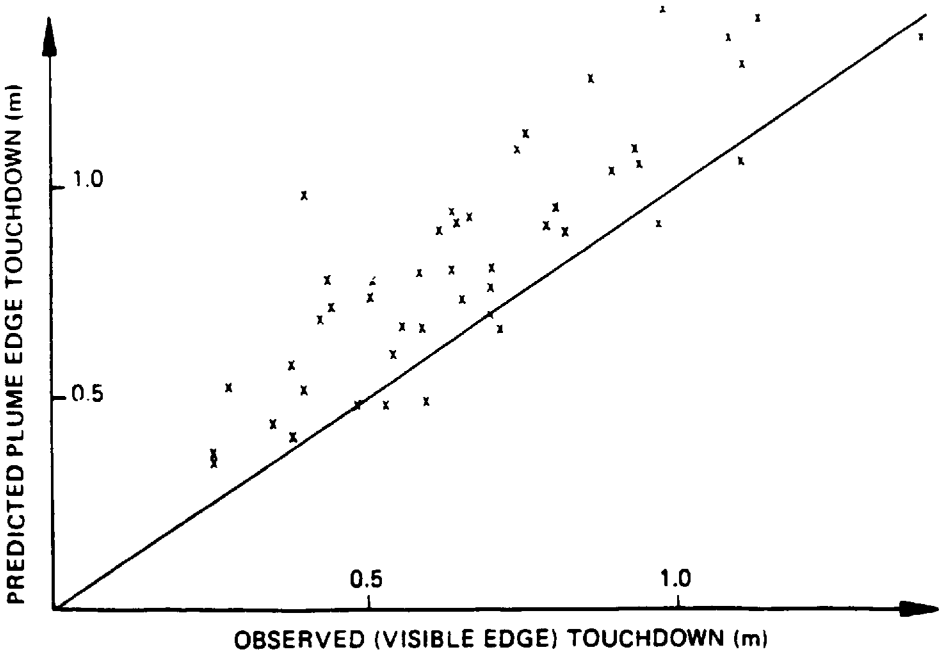


FIG. 5.15. – Comparison of the predicted point of plume touchdown with experimental (visible edge) touchdown of Hoot, Meroney and Peterka (1973).

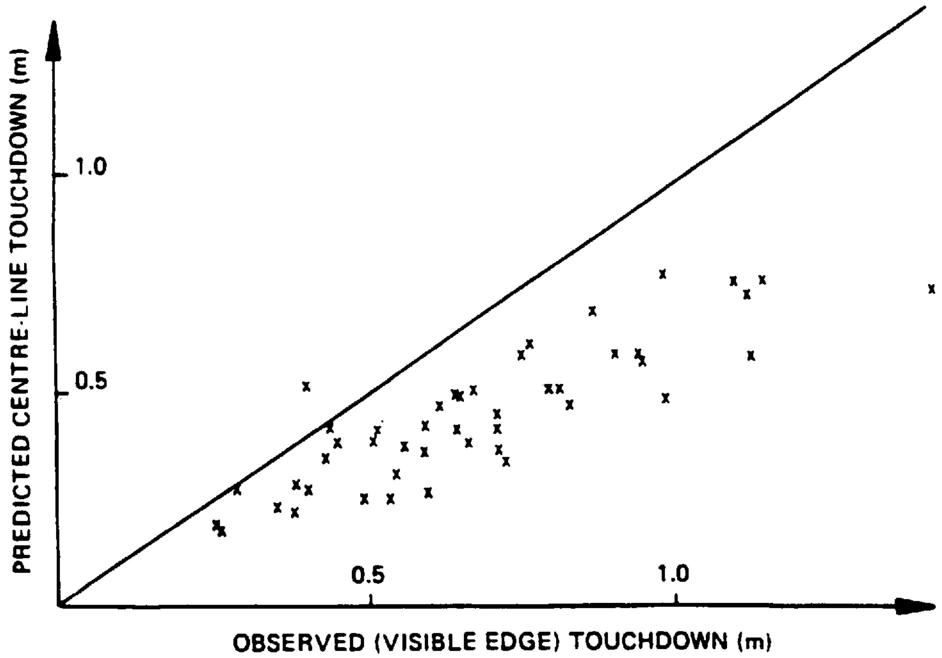
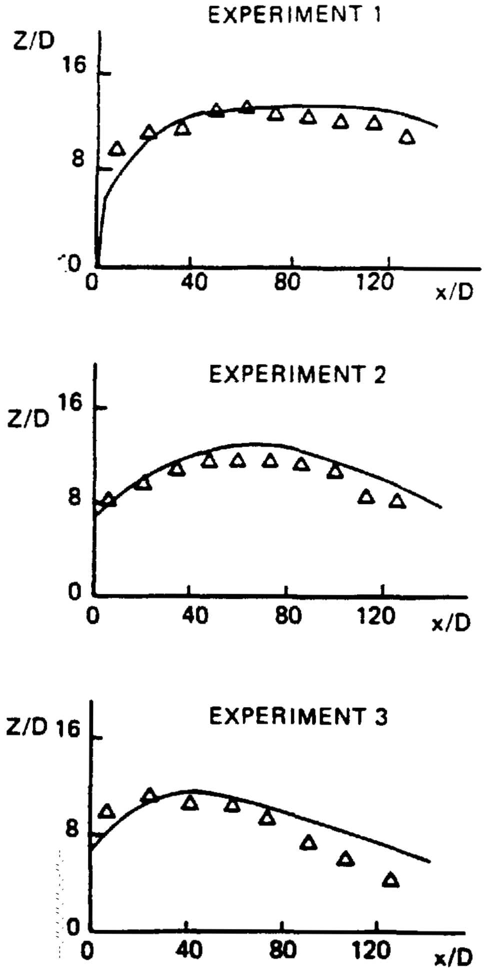
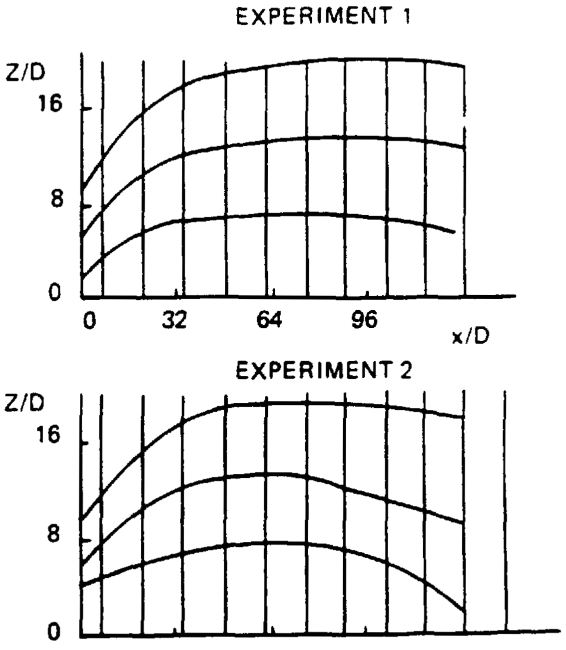


FIG. 5.16. – Comparison of predicted Centre-line touchdown with experimental Visible Edge touchdown data of Hoot, Meroney and Peterka (1973).



Measured and predicted plume paths (Δ: experiments; – :prediction).



Experimental conditions (T_a: tunnel temperature; T_c stack plume exit temperature)

	D (m)	U_a (m s^{-1})	U_c (m s^{-1})	T_a (K)	T_c (K)	Re	Fr
Experiment 1	0.025	0.92	5.16	293	353	8600	3.45
Experiment 2	0.025	0.97	5.75	292	393	9580	3.84
Experiment 3	0.020	0.85	3.68	291	393	4900	3.68

D orifice diameter
U_a ambient wind speed
U_c centre-line speed

x horiz. distance
z (downward) vertical distance

FIG. 5.17. – Comparison of predicted centre-line plume trajectory and plume width with data from experiments 1, 2 and 3 of Li Leijdens and Ooms (1986).

6. THE PGPLUME MODEL FOR FAR-FIELD DISPERSION

CONTENTS

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6. THE PGPLUME MODEL FOR FAR-FIELD DISPERSION

6.1. Introduction

The influence upon plume dispersion of release conditions and of complex reaction dynamics decreases with increasing downwind distance, and becomes negligible when compared with ambient turbulence in the far-field. Inasmuch as the formulation of ambient turbulence within the HGSYSTEM plume models (AEROPLUME/HFPLUME for HGSYSTEM version 3.0 and PLUME/HFPLUME for HGSYSTEM version 1.0) is rather uncertain, it is inappropriate to extrapolate these plume models far downwind of release.

For the regime of passive advection considerable (empirical) success has been obtained by means of a Gaussian plume/'image'-plume model. Local concentrations are prescribed in terms of horizontal and vertical standard deviations, each expressed as a function of distance downwind of the source. Atmosphere stability is described by the familiar Pasquill/Gifford classes 'A' through 'F;'. The correlations apply properly to extended and level terrain (Pasquill 1961, Gifford 1975). More recent developments allow correction of the standard correlations for surface roughness (Hanna 1982), for concentration averaging time (plume meander) (Hanna, Briggs and Hosker 1982), for release duration (Blewitt, Yohn, and Ermak 1987), and for the influence of the nearby ground (Pasquill 1976).

We may choose either to modify the entrainment function within the HGSYSTEM plume models, or else to link these models to the well established Pasquill/Gifford Gaussian plume model.

Modifications might incorporate the Pasquill/Gifford standard deviations into the entrainment function (Bloom 1980; Petersen and Cermak 1980); or else represent surface layer structure implied by observation and Monin-Obukhov similarity (Ooms 1972; Schatzmann 1978; Disselhorst 1984) in such a way as to reproduce observed far-field behaviour.

The choice of method is governed by computational efficiency and by the need to ensure *accurate* reproduction of well-known far-field effects. We link HFPLUME to a Pasquill/Gifford model by asymptotic matching, in which a virtual source for a Pasquill/Gifford model is located by requiring the continuity of mass, momentum, and energy fluxes between near and far-field descriptions at a (given) matching plane. Subsequent dispersion is then obtained by function evaluation, rather than by the numerical solution of a set of ordinary differential equations. The matching procedures are broadly analogous to those proposed in the context of heavy gas dispersion by Raj and Morris (1987).

The HGSYSTEM model which can describe the far field passive dispersion is called

PGPLUME. All HGSYSTEM plume models (AEROPLUME and HFPLUME in version 3.0 of HGSYSTEM) can make a transition (link) to PGPLUME if appropriate.

6.2. Far-field Dispersion: Pasquill/Gifford Models

The dispersion of a trace contaminant from a ground or an elevated point source over flat homogeneous terrain is well described by an (essentially empirical) plume/'image'-plume model of the general form (Stern, Boubel, Turner and Fox 1984; Hanna 1982; Briggs and Hosker 1982):

Point-local concentration

$$c(\Delta x,y,z)/c_* = \psi(y,z;\sigma_y,\sigma_z,z_{PG}) \qquad (1)$$

$$c_* = dm/dt_0/[2\,\pi\,u_\infty\,\sigma_y\,\sigma_z] \qquad (2)$$

where $\psi(y,z;\sigma_y,\sigma_z,z_{PG}) = \exp(-y^2/(2\sigma_y{}^2))\,[\exp(-(z - z_{PG})^2/(2\sigma_z{}^2)) + \exp(-(z + z_{PG})^2/(2\sigma_z{}^2))]$ (3)

and $\sigma_y,\sigma_z = (\sigma_v,\sigma_z)(\Delta x = x_{PG} - \langle x\rangle,z_{PG};\tau,z_{cm},z_r)$

$z \geq 0;\ \Delta x \geq 0$

$-\infty < y < \infty$

$z_{cm},\ z_{PG},\ \sigma_y,\ \sigma_z \geq 0$

Notation: Δx displacement downwind of a (virtual) point-source of pollutant mass-flux dm/dt_0 at co-ordinates $(x_{PG},0,z_{PG})$; c_* 'centre-line' mass-concentration at displacement Δx; $(x_{PG} + \Delta x,y,z)$ co-ordinates of a general point within the Pasquill/Gifford plume a distance z above ground, and a (horizontal) distance y off-axis; (σ_y,σ_z) standard deviations in horizontal and vertical directions (m); u_∞ mean wind-speed (m/s); z_{cm} plume centre-of-mass (centroid) height (m).

Pollutant is *advected* at the (vertical-mean) wind-speed u_∞. Cross-wind dispersion is described by vertical and horizontal standard deviations σ_z and σ_y respectively. Each standard deviation depends on the atmosphere stability (class), distance downwind of the source (Gifford 1976), the chosen concentration averaging time (Pasquill 1976), Hanna 1982), the surface roughness (Hanna and Briggs 1984), and the mean plume (centroid) 'height' (Pasquill 1976).

The standard Pasquill/Gifford standard deviations based upon a (reference) surface roughness z_r^{PG} = 3cm, ground-level source, and a (reference) averaging time τ_{PG} = 10 minutes (Hanna, Briggs and Hosker 1982) were given graphically for distances less than some 10-50 km downwind of release. These correlations were given numerical form by Turner and Busse

(1973), who proposed for σ_y^{PG} the dimensioned form (Stern, Boubel, Turner and Fox 1984),

Horizontal Standard Deviation

$$\sigma_y^{PG} = 465.116\,(\Delta x/10^3)\tan(\theta\,\pi/180) \tag{4}$$

$$\theta(\Delta x, PG) = \begin{array}{ll} 24.167 - 2.5334\ln(\Delta x/10^3) & PG = \text{'A'} \\ 18.333 - 1.8096\ln(\Delta x/10^3) & PG = \text{'B'} \\ 12.500 - 1.0857\ln(\Delta x/10^3) & PG = \text{'C'} \\ 8.3333 - 0.72382\ln(\Delta x/10^3) & PG = \text{'D'} \\ 6.2500 - 0.54287\ln(\Delta x/10^3) & PG = \text{'E'} \\ 4.1667 - 0.36191\ln(\Delta x/10^3) & PG = \text{'F'} \end{array} \tag{5}$$

with $0 \le \Delta x < 100$ km and PG = {'A','B','C','D','E','F'}

Notation: Δx downwind distance (m); PG Pasquill/Gifford stability class; σ_y^{PG} standard (Pasquill/Gifford) horizontal standard deviation (m).

In addition the vertical standard deviation σ_z^{PG} is assigned for each stability class a piece-wise power-law form (Turner and Busse 1973; Stern, Boubel, Turner and Fox 1984).

Vertical Standard Deviation

$\sigma_z^{'A'} = 122.80\Delta x^{0.9447}$	$\Delta x < 100$ m	$\sigma_z^{'B'} = 90.673\Delta x^{0.93198}$	$\Delta x < 200$ m
$158.08\Delta x^{1.0542}$	$100\text{ m} \le \Delta x \le 150$ m	$98.483\Delta x^{0.98332}$	$200\text{ m} \le \Delta x \le 400$ m
$170.22\Delta x^{1.0932}$	$150\text{ m} < \Delta x \le 200$ m	$109.30\Delta x^{1.09710}$	$400\text{ m} \le \Delta x \le 35$ km
$179.52\Delta x^{1.1262}$	$200\text{ m} < \Delta x \le 250$ m	5000m	$\Delta x > 35$ km
$217.41\Delta x^{1.2644}$	$250\text{ m} < \Delta x \le 300$ m	$\sigma_z^{'C'} = 61.141\Delta x^{0.91465}$	$0\text{ m} < \Delta x$
$258.89\Delta x^{1.4094}$	$300\text{ m} < \Delta x \le 400$ m	$\sigma_z^{'D'} = 34.459\Delta x^{0.86974}$	$\Delta x < 300$ m
$346.75\Delta x^{1.7283}$	$400\text{ m} < \Delta x \le 500$ m	$32.093\Delta x^{0.81066}$	$300\text{ m} < \Delta x \le 1$ km
$453.85\Delta x^{2.1166}$	$500\text{ m} < \Delta x \le 3.11$ km	$32.093\Delta x^{0.64403}$	$1\text{ km} < \Delta x \le 3$ km
5000	$\Delta x > 3.11$ km	$33.504\Delta x^{0.60486}$	$3\text{ km} < \Delta x \le 10$ km
		$36.650\Delta x^{0.56589}$	$10\text{ km} < \Delta x \le 30$ km
		$44.053\Delta x^{0.51179}$	$\Delta x > 30$ km

where the σ's are in m.

$$
\begin{array}{rll}
\sigma_z^{'E'} = & 24.260\Delta x^{0.83660} & \Delta x < 100 \text{ m} \\
& 23.331\Delta x^{0.81956} & 100 \text{ m} \le \Delta x \le 300 \text{ m} \\
& 21.628\Delta x^{0.75660} & 300 \text{ m} \le \Delta x \le 1 \text{ km} \\
& 21.628\Delta x^{0.63077} & 1 \text{ km} \le \Delta x \le 2 \text{ km} \\
& 22.534\Delta x^{0.57154} & 2 \text{ km} \le \Delta x \le 4 \text{ km} \\
& 24.703\Delta x^{0.50527} & 4 \text{ km} \le \Delta x \le 10 \text{ km} \\
& 26.970\Delta x^{0.46713} & 10 \text{ km} \le \Delta x \le 20 \text{ km} \\
& 35.420\Delta x^{0.37615} & 20 \text{ km} \le \Delta x \le 40 \text{ km} \\
& 47.618\Delta x^{0.29592} & \Delta x > 40 \text{ km}
\end{array}
\qquad
\begin{array}{rll}
\sigma_z^{'F'} = & 15.209\Delta x^{0.81558} & \Delta x > 200 \text{ m} \\
& 14.457\Delta x^{0.78407} & 200 \text{ m} \le \Delta x \le 700 \text{ m} \\
& 13.953\Delta x^{0.68465} & 700 \text{ m} \le \Delta x \le 1 \text{ km} \\
& 13.953\Delta x^{0.63227} & 1 \text{ km} \le \Delta x \le 2 \text{ km} \\
& 14.823\Delta x^{0.54503} & 2 \text{ km} \le \Delta x \le 3 \text{ km} \\
& 16.187\Delta x^{0.46490} & 3 \text{ km} \le \Delta x \le 7 \text{ km} \\
& 17.836\Delta x^{0.41500} & 7 \text{ km} \le \Delta x \le 15 \text{ km} \\
& 22.651\Delta x^{0.32681} & 15 \text{ km} \le \Delta x \le 30 \text{ km} \\
& 27.074\Delta x^{0.27436} & 30 \text{ km} \le \Delta x \le 60 \text{ km} \\
& 34.219\Delta x^{0.21716} & \Delta x > 60 \text{ km}
\end{array}
\tag{6}
$$

where the σ's are in m

In (5) and (6) $0 \le \Delta x < 100$ km and PG = {'A','B','C','D','E','F'}

Notation: Δx downwind distance (m or km); PG Pasquill/Gifford stability class; σ_z^{PG} standard (Pasquill/Gifford) horizontal standard deviation (m).

Plume standard deviations derive ultimately from the spectrum of turbulence within the ambient atmosphere. Short averaging times correspond to diffusion associated with small scale eddies: long averaging times are dominated by plume meander. The distribution of vertical and horizontal turbulence differ, with the vertical turbulence materially influenced by the proximity of the ground. Turbulent kinetic energy is further influenced surface roughness: greater roughness implies greater turbulent energy, and greater eddy diffusivity.

Hanna (1982), following Smith (1973, 1977) and McDonald (1978), suggested for σ_z a surface roughness effect $(z_r/z_r^{PG})^{0.2}$. Now surface roughness governs the friction velocity u^* (say), and the Monin-Obukhov length L, with the distribution of turbulence in horizontal (σ_u/u^*, and σ_v/u^*) and vertical (σ_w/u^*) directions universal functions of the scaled height z/L (Arya 1982). Plausibly the influence of surface roughness applies equally and proportionately to the horizontal standard deviation σ_y of a dispersing plume.

However, Roberts (Chapter 5.B), analysing extensive meteorological data (Draxler 1984), discerned *no* significant effect of surface roughness upon σ_y . Certainly for longer averaging times the dominant influence upon σ_y is plume meander, which is essentially uncorrelated with (local) surface roughness; we follow observation and take σ_y independent of the surface roughness.

The influence upon horizontal standard deviation of plume meander and concentration averaging time effect has the form of the power law $(\tau/\tau_{PG})^{0.2}$ (Hanna 1982). Vertical spectra differ from horizontal as the result of the geometrical influence of the ground, so that for long averaging times no further increase in σ_z with averaging time is to expected. For such times the vertical spectrum is fully active in determining turbulent diffusion. Equally for very short averaging times turbulent diffusion is dominated by small-scale eddies, the distribution of which is roughly homogeneous. This suggests that for short averaging times the functional dependence of both σ_z and σ_y on averaging time τ should be identical, whereas, near the ground, or for long averaging times, σ_z should be independent of τ. We propose, following Hanna (1982) and Pasquill (1976), the dimensioned forms

Effects of surface roughness, plume centroid height, and concentration averaging-time

$$\sigma_y = \sigma_y^{PG} (\tau/\tau_{PG})^{0.2} \tag{7}$$

$$\sigma_z = \sigma_z^{PG} (z_r/z_r^{PG})^{0.2} \{\min[\tau,\tau_{PG}]/\tau_{PG}\}^{0.2} \tag{8}$$

with $z_r > 0$; $z_{cm} > \geq 0$; $\tau \geq \tau_{match} > 0$

Notation: z_{cm} plume-section centroid (centre-of-mass) height (m); τ concentration averaging time (s); τ_{match} = 18.75 s, effectively 'instantaneous' averaging time (TNO 1990); $z_r > 0$, ground surface roughness; τ_{PG} reference averaging time (taken to be 600 s in PGPLUME); z_r^{PG} reference surface roughness height (taken to be 0.03 m (3 cm) in PGPLUME).

6.3. Local versus Integral Average Properties: Near/Far field Matching

The near-field models AEROPLUME and HFPLUME are idealised particularly in respect of the shape of the cross-wind profiles of concentration and temperature. Predictions are made not of *point-local* but of *average* behaviour within each plume cross-section, and take properly into account the several effects of source momentum, orientation, and dense gas dispersion in determining air entrainment and the development of the plume trajectory.

Far-field dispersion is similarly idealised. Predictions are made of local (particularly ground-level) concentrations; no account is taken of near source effects influencing plume trajectory. The far-field dispersion of plumes is independent of release conditions except inasmuch as they determine the downwind displacement, height above ground, and strength of an equivalent point source.

Consider an asymptotically neutral or marginally buoyant release downwind of release. In the near-field predictions are available of entrained air mass-flux, released pollutant mass-flux, and the excess (above ambient) fluxes of momentum and total energy. Sufficiently far from the source the conditions for passive dispersion of an inert pollutant are well met: chemical reaction (if pollutant is HF) has all but ceased ; the influences of release buoyancy and initial momentum largely spent.

At such distances the sectional-average predictions supplied by HFPLUME or AEROPLUME correspond closely to those of a matched Pasquill/Gifford (Gaussian) plume. Equating fluxes deduced from Gaussian far-field and 'top-hat' near-field models will then furnish a set of non-linear integral equations for the virtual source location, and will define the Pasquill/Gifford plume at the transitional or 'matching' plane and at greater distances downwind of release.

Matching Equations

$$< dm/dt >_0 = \int_0^\infty \int_{-\infty}^\infty c\,u \;\; dydz \tag{9}$$

$$< dm/dt >_{air} = \int_0^\infty \int_{-\infty}^\infty \left((\rho - c)u - \rho_\infty u_\infty\right) dydz \tag{10}$$

$$< dP_x / dt > = \int_0^\infty \int_{-\infty}^\infty \rho u (u - u_\infty) \;\; dydz \tag{11}$$

$$< dE / dt > = \int_0^\infty \int_{-\infty}^\infty \rho u \left(h + \tfrac{1}{2} u^2 - h_\infty - \tfrac{1}{2} u_\infty^2\right) \;\; dydz \tag{12}$$

Notation: $<dm/dt>_0$ mass-flux of pollutant; $<dm/dt>_{air}$ mass-flux of entrained air, $<dP_x/dt>$ mass-flux excess (horizontal) momentum; <dE/dt> mass-flux excess above ambient total-energy; (c,ρ,h,u) point-local mass-concentration pollutant, total density, specific enthalpy, and (horizontal) velocity; $(\rho_\infty,h_\infty,u_\infty)$ ambient air density, ambient air specific enthalpy, and wind speed.

The notation '<...>' refers to a *sectional-average value* such as is predicted by the HGSYSTEM near-field models AEROPLUME and HFPLUME.

The equation express the invariance between plume descriptions of $<dm/dt>_0$, the pollutant mass-flux, $<dm/dt>_{air}$, the entrained air mass-flux, $<dP_x/dt>$, the excess horizontal momentum, and <dE/dt>, the excess above ambient of total energy.

The pressure P_∞ within the plume is essentially that (hydrostatic) value within the undisturbed atmosphere.

Pasquill/Gifford Profiles

The assumption of a Gaussian plume/'image'-plume description of the far-field dispersion yields for the mass-concentration, and for the excess velocity the explicit profiles:

$$c/c_* = \psi(y,z;\sigma_y,\sigma_z,z_{PG})$$

$$(u - u_\infty)/(u_* - u_\infty) = \psi(y,z;\varepsilon\sigma_y,\varepsilon\sigma_z,z_{PG}) \tag{13}$$

$$\psi(y,z;\sigma_y,\sigma_z,z_{PG}) = \exp(-y^2/(2\sigma_y^2))\ [\exp(z - z_{PG})^2/(2\sigma_z^2)) + \exp(-(z + z_{PG})^2/(2\sigma_z^2))]$$

with $\sigma_y,\sigma_z = (\sigma_y,\sigma_z)(\Delta x = x_{PG} - \langle x\rangle, y = 0, z_{PG}; \tau = \tau_{match}, z_{cm} = \langle z\rangle, z_r)$
and $0 \le z$, $x \ge 0$, $-\infty < y < \infty$ and $\langle z\rangle$, $\sigma_y,\sigma_z \ge 0$.

Notation: ε^2 turbulent Schmidt number; $u_* - u_\infty$ 'centre-line' excess of horizontal velocity; $\langle z\rangle$ near-field centroid height; τ_{match} 'instantaneous' (concentration) averaging-time; z_r ground surface roughness.

The averaging time appropriate to the standard deviations σ_y and σ_z must be chosen for comparability with the near-field description underlying the entrainment assumptions of HFPLUME and AEROPLUME.

Such an averaging time is certainly short, and may be regarded as effectively 'instantaneous'. Reference to TNO(1990) yields for and 'instantaneous' average the effective averaging time $\tau_{match} = 18.75$ s.

Note that in addition to the expected profile for the mass concentration c(x,y,z), a second related profile has been introduced for the excess-velocity $(u(x,y,z) - u_\infty(x,y,z))$. This reflects the broad comparability of density and velocity differences in the near-field, and the desire to assign both influences equal weight in the criteria of matching.

The velocity profile is identical in form to the Gaussian image system proposed for concentration; the standard deviations are scaled by the far-field turbulent Schmidt number ($\varepsilon^2 = 1.35$) to reflect the different rates of mass and momentum diffusion (Rouse, Yih and Humphreys 1952; Ooms 1972).

Local Thermal Equilibrium

The assumption of thermal equilibrium the *point-local* thermodynamic relation

$$(h + \tfrac{1}{2}u^2 - h_\infty - \tfrac{1}{2}u_\infty^2) = (c/\rho)\ (\langle dE/dt\rangle/\langle dm/dt\rangle_0) \tag{14}$$

to be developed.

This equation may be motivated as follows: First consider the integral-averaged plume description, and in particular the total energy-flux <dE/dt> passing a given cross-section. The mean-flow may be assumed to result from the uniform mixing of a pure pollutant stream of mass-flux $<dm/dt>_0$ with an ambient air stream of mass-flux $<dm/dt>_{air}$.

The pure pollutant stream has therefore the specific enthalpy $<dE/dt>/<dm/dt>_0$ above ambient values.

Next abstract a unit mass of pollutant/moist-air mixture from within a plume cross-section.

The sample possesses a definite mass-fraction c/ρ of pollutant: it results from the intimate mixing of two parcels of material; the one (pure pollutant) of mass c/ρ, the specific energy content of which (relative to the ambient air) is $(<c>/<p>)(<dE/dt>/<dm/dt>_0)$; the other air of mass 1 - c/ρ and *zero* specific energy (because we define the energy relative to the ambient air).

The mixture specific total energy is correspondingly $h - h_\infty + \frac{1}{2}u^2 - \frac{1}{2}u_\infty^2$.

The point local relationship follows from energy conservation. The non-linear equation

$$< dE/dt >= \int_0^\infty \int_{-\infty}^\infty \rho u\left(h + \tfrac{1}{2}u^2 - h_\infty - \tfrac{1}{2}u_\infty^2\right)\, dydz \qquad (15)$$

is then satisfied identically.

The equation system for near/far-field matching then provides a set of three non linear equations in the 'centre-line' concentration c_*, the centre-line velocity-excess $u_* - u_\infty$, and in the virtual origin location $(x_{PG}, z_{PG} \geq 0)$.

An additional equation is therefore needed to close the equation system.

Model Closure: Centroid, Buoyant Potential Energy, and Angular Momentum

Recall the importance of the plume centroid of '*centre of mass*' in model formulation: this suggests that the plume centroid height be invariable between the near and far-field descriptions. The matching equation then becomes

$$< z >= \frac{\int_0^\infty \int_{-\infty}^\infty z(\rho - \rho_\infty)\, dydz}{\int_0^\infty \int_{-\infty}^\infty (\rho - \rho_\infty)\, dydz} \qquad (16)$$

This equation is straightforward; it accurately reflects the systematic rise in the Pasquill/Gifford centroid height with increasing downwind distance, a variation not followed by the virtual source.

It differs significantly in functional form from the other matching conditions, which represent the invariance between near and far-field descriptions of the material *fluxes* whether of pollutant, entrained air, excess (horizontal) momentum, or excess total-energy.

It is suggested that the final (closure) equation should express the invariance of some physically based *flux*. Such considerations lead, rather naturally, to the invariance of the buoyancy potential-energy flux

$$< dB/dt >= \int_0^{\infty}\int_{-\infty}^{\infty} \rho u g z(1-\rho_\infty/\rho)\, dydz \tag{17}$$

Equally some account should be taken of residual differences between plume and ambient velocities at the plane of matching; this in addition to the (hydrostatic) 'centre of gravity' effects governed by density differences alone. We suggest that the excess above ambient values of plume ***angular momentum*** be conserved.

Taking moments from the point of the matching plane of maximum ground-level concentration yields the equation

$$< dL_y/dt >= \int_0^{\infty}\int_{-\infty}^{\infty} \rho u z(u-u_\infty)\, dydz \tag{18}$$

Matching is not influenced by the choice of origin for L_y. This equation has the form of a physically derived flux, and is, in the limit of negligible velocity difference, equivalent to centroid invariance. Account is now taken of velocity differences on an equal footing with density differences analogously to the remaining conservation equations.

It is, however, *impossible* to satisfy buoyant-energy and angular-momentum flux conservation simultaneously.

This illustrates a general problem of matching, that only a *limited number* of physical invariants can be transferred between matched models, the limit being set by the Pasquill/Gifford far-field.

Introducing a velocity profile allows a rather better transfer of momentum related information than would otherwise have been possible; however it does not seem possible to introduce sufficient degrees of freedom to encompass $<dL_y/dt>$ and $<dB/dt>$ invariance.

In the circumstances we must *choose* which invariant will be conserved. Inasmuch as the buoyancy flux occurs explicitly as a major determinant of near-field behaviour, whereas the angular momentum is only implicitly calculated, we *prefer <dB/dt> invariance* for the calculation of the far-field.

Existence of Matched (Far-field) Solutions

It is a general feature of non-linear equations that physically appropriate solutions may not exist for certain ranges of the input parameters. Certainly, circumstances may arise under which the matching of a near-field description and a far-field Pasquill/Gifford model may be inappropriate: source momentum may be significant; heavy gas effects may predominate. Even under near passive conditions sufficient 'memory' of earlier (heavy gas, say) dispersion may be retained to prevent physically sensible matching: the solution space, in terms of the matching variables $\langle dm/dt\rangle_0$, $\langle dm/dt\rangle_{air}$, $\langle dP_x/dt\rangle$, $\langle dB/dt\rangle$ needs to be examined.
This discussion is deferred until an appropriate asymptotic analysis of the non-linear system has been carried out.

6.4. System Asymptotics: the Limit of Great Dilution

Inasmuch as the Pasquill/Gifford formulation applies to *passive* dispersion, significant departures between plume and ambient atmosphere at the plane of transition are inappropriate. It is not necessary to solve the matching equations in full generality; it suffices to examine the solution space in the limit of great plume dilution.
First order expansion about the ambient state $(\rho_\infty, T_\infty; P_\infty)$ yields estimates of the enthalpy and temperature excess above ambient, together with estimates of the centre-line concentration and velocity-excess. Vertical variation within the plume is neglected, with the wind-speed and ambient density assigned (mean) values $\langle u_\infty\rangle$ and $\langle \rho_\infty\rangle$ evaluated at the (near-field) centroid height $\langle z\rangle$.

First Order Approximation

$$(h - h_\infty)/(c_p^\infty\, T_\infty) = (T/T_\infty - 1) \tag{19}$$

$$1 - T/T_\infty = (\rho/\rho_\infty - 1) + (\mu_\infty/\mu_{pol} - 1)\, c/\rho_\infty \tag{20}$$

$$c_*/\rho_\infty = (\beta/(2\pi))\,(\langle c\rangle/\rho_\infty) \text{ with } \beta = \langle A\rangle/(\sigma_y\sigma_z) \tag{21}$$

$$u_*/u_\infty - 1 = (\beta\varepsilon^2/(2\pi))\,(\langle u\rangle/u_\infty - 1) \text{ with } \beta = \langle A\rangle/(\sigma_y\sigma_z) \tag{22}$$

$$\langle z\rangle = \sigma_z\sqrt{2}\{(1/\sqrt{\pi})\exp(-\eta^2) + \eta\,\mathrm{erf}(\eta)\};\text{ with } \eta = z_{PG}/(\sigma_z\sqrt{2}) \tag{23}$$

with $|\langle\rho\rangle/\rho_\infty - 1| << 1$, $|\langle c\rangle/\rho_\infty| << 1$, $|\langle u\rangle/u_\infty - 1| << 1$, $|u_\infty^2/(2c_p^\infty\, T_\infty)| << 1$

Notation: $\mathrm{erf}(\eta) = \left(2/\sqrt{\pi}\right)\int_0^\eta \exp\left(-\xi^2\right) d\xi$ the standard error function (Abramowitz and Stegun 1972); c_p^∞ ambient (moist) air (isobaric) specific heat; μ_∞ ambient air molecular mass; μ_{pol}

molecular mass pollutant; (<z>,<A>) near-field plume centroid height and cross-sectional area; (<c>,<ρ>) near-field (internal-average) pollutant mass-concentration and total-density; <u> near-field (mean) flow-velocity; $(u_\infty,\rho_\infty,T_\infty)$ mean wind-speed, atmosphere density and (absolute) temperature; (ρ,c,h,T) point-local density, concentration, specific enthalpy and absolute temperature; h_∞ atmosphere specific enthalpy.

Note that the virtual origin is *not* located by first order matching; the quantity $<A>/(\sigma_y\sigma_z)$ being undetermined. Second order asymptotic analysis yields the required equation:

Second Order Closure

$$<A>/(\sigma_y\sigma_z) = 4\pi[\Delta^2 h + 2h_\rho\delta_u(\delta_\rho+\delta_u)]/[I(1,1)\Delta^2 h + 2h_\rho\delta_u(I(1,\varepsilon)\delta_u + I(\varepsilon,\varepsilon)\delta_\rho)] \qquad (24)$$

where $\Delta^2 h = h_{\rho\rho}\delta_\rho{}^2 + 2h_{\rho c}\delta_\rho\delta_c + h_{cc}\delta_c{}^2 + 2h_\rho\delta_\rho{}^2 + 2h_c\delta_\rho\delta_c$

$$I(\varepsilon,\mu) = 2\varepsilon^2\mu^2/(\varepsilon^2 + \mu^2)\ \{1 + \exp[-2\varepsilon^2\mu^2/(\varepsilon^2 + \mu^2)\ (z_{PG}/\sigma_z)^2]\}$$

$$h_\rho = \rho_\infty/(c_p^\infty\ T_\infty)\ \partial(h - h_\infty)/\partial\rho\,\big|_{\rho = c}$$

$$h_c = \rho_\infty/(c_p^\infty\ T_\infty)\ \partial(h - h_\infty)/\partial c\,\big|_{c = \rho}$$

$$h_{\rho\rho} = \rho_\infty{}^2/(c_p^\infty\ T_\infty)\ \partial^2(h - h_\infty)\partial\rho^2\,\big|_{\rho = c}$$

$$h_{cc} = \rho_\infty{}^2/(c_p^\infty\ T_\infty)\ \partial^2(h - h_\infty)\partial c^2\,\big|_{c = \rho}$$

$$h_{\rho c} = \rho_\infty{}^2/(c_p^\infty\ T_\infty)\ \partial^2(h - h_\infty)/\partial\rho\partial c$$

$$\delta_\rho = <\rho>/\rho_\infty - 1;\ \delta_c = <c>/\rho_\infty;\ \delta_u = <u>/u_\infty - 1$$

together with the consistency constraints

$$|<u>/u_\infty - 1|\ |4\pi - \beta\varepsilon^2 I(1,\varepsilon)| \ll 4\pi,\ \beta = <A>/(\sigma_y\sigma_z)$$

$$|\{(<u>/u_\infty - 1)\ [4\pi - \beta\varepsilon^2 I(1,\varepsilon)]\} + \{(<\rho>/\rho_\infty - 1)\ [4\pi - \beta I(\varepsilon,\varepsilon)]\}| \ll 4\pi$$

The virtual origin is then located relative to the matching plane x= <x> at such height z_{PG} above ground, and such horizontal displacement $\Delta x = x_{PG} - <x>$ that the (leading order) area and centroid matching satisfies the equation set:

Virtual Origin Location

$$<z> = \sigma_z\sqrt{2}\{(1/\sqrt{\pi})\exp(-\eta^2) + \eta \operatorname{erf}(\eta)\} \text{ with } \eta = z_{PG}/((\sqrt{2}\cdot\sigma_z) \quad (25)$$

$$<A>/(\sigma_y\sigma_z) = 4\pi[\Delta^2 h + 2h_\rho\delta_u(\delta_\rho+\delta_u)]/[I(1,1)\Delta^2 h + 2h_\rho\delta_u(I(1,\varepsilon)\delta_u + I(\varepsilon,\varepsilon)\delta_\rho)]$$

with $\Delta^2 h = h_{\rho\rho}\delta_\rho{}^2 + 2h_{\rho c}\delta_\rho\delta_c + h_{cc}\delta_c{}^2 + 2h_\rho\delta_\rho{}^2 + 2h_c\delta_\rho\delta_c$

$$I(\varepsilon,\mu)=2\varepsilon^2\mu^2/(\varepsilon^2 + \mu^2)\{1 + \exp[-2\varepsilon^2\mu^2/(\varepsilon^2 + \mu^2)(z_{PG}/\sigma_z)^2]\}$$

$$\sigma_y,\sigma_z = (\sigma_y,\sigma_z)(\Delta x = x_{PG} - <x>, z_{PG}; \tau = \tau_{match}, z_{cm} = <z>, z_r)$$

Notation: $<x>$ downwind distance from release of the plane of matching; $<z>$ near-field plume centroid at matching; τ_{match} 'instantaneous' matching time; ε^2 turbulent Schmidt number; $<u>$ near-field (mean horizontal) velocity.

This non-linear system, though complex, has a *unique* solution for assumed monotone increasing standard deviations σ_y and σ_z and for $x_{PG} \leq <x>$, *provided* only that $<z>/\sigma_z \geq \sqrt{(2/\pi)}$; otherwise *no* solution exists.

In the absence of a solution we presume a ground-level (virtual) source, and solve for the *unique* root of the second order equation in $<A>/(\sigma_y,\sigma_z)$, $z_{PG} = 0$.

The solution is regular in the limit of passive dispersion, and where matching is dominated by densimetric or velocity differences; second order matching then yield the results

$$<A>/(\sigma_y,\sigma_z) \rightarrow 4\pi/I(1,1) \text{ when } <u> \rightarrow u_\infty$$

$$<A>/(\sigma_y,\sigma_z) \rightarrow 4\pi/I(1,\varepsilon) \text{ when } <\rho> \rightarrow \rho_\infty$$

$$<A>/(\sigma_y,\sigma_z) = 4\pi/I(1,1)$$

$$<\rho> = \rho_\infty$$

$$<u> = u_\infty$$

$$<c> \neq 0$$

Certain consistency conditions need be imposed on the quantities $<\rho>$ and $<u>$ at matching. The empirical form of σ_y is severely 'pathological' for $0 < (<x> - x_{PG}) << 10$ km, that is, *outside* the correlated range $10 \text{ m} < (<x> - x_{PG}) < 10$ km, say.
Aphysical solutions so arising are very unlikely to intrude upon asymptotic matching.

6.5. Prediction of (Steady) Far-field Dispersion

Having located the virtual origin, it remains only to evaluate for each downwind displacement $x \geq <x>$ the Pasquill/Gifford standard deviations σ_y and σ_z associated with the required concentration averaging-time $\tau \geq \tau_{match}$.
Note that the vertical standard deviation σ_z depends implicitly upon the local centroid (centre-of-mass) height z_{cm} via the equation

$$z_{cm} = \sigma_z\sqrt{2}\{(1/\sqrt{\pi})\exp(-\eta^2) + \eta\,\mathrm{erf}(\eta)\};\ \text{with } \eta = z_{PG}/(\sigma_z\sqrt{2}) \qquad (26)$$

The solution for the pair (σ_z, z_{cm}) is *unique*.
Note that for displacements for which $z_{cm} > 100$ m the dependence of σ_z upon z_{cm} is ended, and explicit calculation recovers first σ_z and then (if required) z_{cm}.
Armed with the 'width' parameters σ_y and σ_z, the *local concentration* at downwind distance $x > <x>$, height $z \geq 0$, and (horizontal) off-axis distance y is to leading order

$$c(x,y,z)/c_* = \psi(y,z;\sigma_y,\sigma_z,z_{PG}) \text{ with } c_* = dm/dt_0/[2\,\pi\, u_\infty\, \sigma_y\, \sigma_z] \qquad (27)$$

where $\psi(y,z;\sigma_y,\sigma_z,z_{PG}) = \exp(-y^2/(2\sigma_y^2))\,[\exp(-(z - z_{PG})^2/(2\sigma_z^2)) + \exp(-(z + z_{PG})^2/(2\sigma_z^2))]$

and $0 \leq z;\ x_{PG} < (<x>) \leq x;\ -\infty < y < \infty;\ z_{PG}, \sigma_y, \sigma_z \geq 0$

The local velocity excess is calculated similarly.

6.6. Transient Effects: Releases of Limited Duration

Thus far we have presumed that steady state conditions either exist or will develop throughout the asymptotic far-field. In practice, however, spill duration may be a few minutes; whereas the establishment of steady conditions at kilometre distances requires tens of minutes or even hours. Such different time scales are especially significant for high consequence, low probability events, for example catastrophic storage vessel failure: steady-state predictions are in such cases not merely conservative, but impossibly large. There is, therefore, a practical need for 'best estimate' values reflecting (more or less accurately) the influence of release duration upon peak concentrations in the far-field.

Downwind Diffusion

Limited duration 'puff', releases disperse both perpendicular and parallel to the ambient wind: dispersion occurs in response not only to eddy diffusion, but also (Hanna 1982) to the cumulative effect of wind-shear. We follow Ermak (1986, 1989), and Blewitt, Yohn, and Ermak (1987), in representing downwind dispersion (in the context of a Gaussian plume model) in terms of the plume standard deviation σ_x. The (time/meander-averaged) standard deviation attributable to downwind diffusion is taken to be (essentially) equal to the standard deviation σ_y, horizontal and perpendicular to the ambient wind. The effect of wind-shear is represented after Smith (1965), except that attention has been given to elevated as well as ground-level sources. The proposed formulation is as follows:

$$\sigma_x^2 = \sigma_y^2 + [2/(3\pi)]\, \sigma_z^2 \, \{(du_\infty/dz)\big|_{z_{cm}} (\Delta x/u_\infty)\big|_{z_{cm}}\}^2 \qquad (28)$$

Note that the gradient du_∞/dz is evaluated at the plume centroid height z_{cm} rather than at Smith's (1965) reference height of $\sigma_z/2$. This choice is representative of the (mean) wind-shear not only for grounded but also for elevated plumes. The coefficient $[2/(3\pi)]$ multiplying the wind-shear term ensures predictions identical to Smith (1965) for grounded plumes and neutral stability.

Prediction of Peak Concentrations

Gaussian plume modelling is based upon the (*steady-state*) solution of the diffusion equation for a fixed point-source, uniform wind, and constant (eddy-)diffusivities. This formulation suggests the Gaussian form upon which the highly successful Pasquill/Gifford model is constructed.

Perhaps encouraged by this success, Ermak (1986) formulated a transient release model based upon the general solution of the above diffusion equation in the (Green's function) form:

$$c(x,y,z;t) = \int_{-\infty}^{\infty} (dm/dt)(\tau)\, G(x,y,z;t-\tau)\; d\tau \qquad (29)$$

with $G(x,y,z;\tau) = G_x(x;\tau)\, G_y(y)\, G_z(z)$

$$G_x(x;\tau) = [\sqrt{(2/\pi)}/\sigma_x]\, \exp[-(x - x_{PG} - u_\infty\tau)^2/(2\sigma_x^2)]$$

$$G_y(y) = 1/[\sqrt{(2\pi)}\sigma_y]\, \exp[-y^2/(2\sigma_y^2)]$$

$$G_z(z) = 1/[\sqrt{(2\pi)}\sigma_z]\, \{\exp[-(z - z_{PG})^2/(2\sigma_z^2)] + \exp[-(z + z_{PG})^2/(2\sigma_z^2)]\}$$

and $\sigma_x(\tau) = \sqrt{(2K_x\tau)}$; $\sigma_y(\tau) = \sqrt{(2K_y\tau)}$; $\sigma_z(\tau) = \sqrt{(2K_z\tau)}$

Notation: dm/dt (momentary) mass release-rate (kg/s); $(x_{PG},0,y_{PG})$ location of the fixed (point) source; (K_x,K_y,K_z) eddy diffusivities parallel and perpendicular to the ambient wind; (x,y,z,t) co-ordinates and time following first release at which the (mass-) concentration c is to be evaluated.

Formally the plume standard deviations (σ_x, σ_y, σ_z) are functions of the elapsed *time* from the moment of release. We nevertheless follow Ermak (1986) in interpreting σ_x, σ_y, and σ_z as known (above specified) functions of the *distance* (x) downwind of a fixed source.
The (reinterpreted) solution c(x,y,z,t) forms a 'template' for a transient (Pasquill/Gifford) model or far-field diffusion. The solution c(x,y,z,t) is further simplified by presuming a *steady* source of *limited* duration. The source function dm/dt(t) assumes the form

$$\mathrm{dm}/\mathrm{dt}(t) = \begin{cases} 0 & -\infty < t < 0 \\ (\mathrm{dm}/\mathrm{dt})|_\infty & 0 < t < \tau_\infty \\ 0 & \tau_\infty < t < \infty \end{cases} \qquad (30)$$

with corresponding far-field concentration

$$c(x,y,z,t)/[G_y\, G_z\, (\mathrm{dm}/\mathrm{dt})|_\infty] = \tfrac{1}{2}\mathrm{erf}\{\eta/(\sigma_x\sqrt{2})\}\Big|_{\eta=\Delta x-u_\infty \min(0,t-\tau_\infty)}^{\eta=\Delta x-u_\infty t} \qquad (31)$$

Notation: $\Delta x = x - x_{PG}$ distance downwind of the (virtual) point source; $\mathrm{dm/dt}|_\infty$ (sustained) mass release-rate; $\mathrm{erf}(\eta) = \left(2/\sqrt{\pi}\right)\int_0^\eta \exp\left(-\xi^2\right) d\xi$ standard error function (Abramowitz and Stegun 1972).

For each downwind distance (x) the time (t) at which occurs the maximum concentration corresponds to the (unique) root of the (turning point) equation $\partial c/\partial t = 0$.
The maximum concentration at distance x downwind of release is therefore (Ermak 1986)

$$c_{max}(x,y,z)/[G_y\, G_z\, (\mathrm{dm}/\mathrm{dt})|_\infty] = \tfrac{1}{2}\mathrm{erf}\{(1/\sqrt{2})\, [\min(\Delta x, \tfrac{1}{2}u_\infty\tau_\infty) + \eta]/\sigma_x\}\Big|_{\eta=0}^{\eta=u_\infty\tau_\infty} \qquad (32)$$

with the steady-state value recovered in the limit of infinite release duration.
Release maximum and steady-state concentrations are then related by the (dimensionless) factor

$$c_{max}/c_{state}^{steady} = \mathrm{erf}\{\sqrt{2}\{\min(\Delta x, \tfrac{1}{2}u_\infty\tau_\infty) + \eta]/\sigma_x\}]\Big|_{\eta=0}^{\eta=u_\infty\tau_\infty} / \{1 + \mathrm{erf}[\Delta x/(\sigma_x\sqrt{2})]\} \qquad (33)$$

which provides an *approximate* correction for the combined effects of downwind diffusion and of release duration. The correction acts upon steady-state values estimated from asymptotic matching and by the straight forward use of standard Pasquill/Gifford formulae.

6.7. Conclusions

In the far-field the calculation of plume dispersion by means of an entrainment based (integral-averaged) description is both highly uncertain and seriously inefficient. Such models as exist currently (Bloom 1980) derive entrainment from an analysis of observed dispersion behaviour summarised in the Pasquill/Gifford curves; any satisfactory formulation of entrainment must, in the far-field, recover the observed results.

Such far-field performance is best achieved by means of (asymptotic) 'matching'; that is by preserving at some matching plane a set of physically derived fluxes generated in the near-field by an integral-averaged model. This results in the identification of a virtual (point) source, such that a Pasquill/Gifford plume at the matching plane is, as regards several physical fluxes, identical to that predicted near the actual source. Beyond the matching plane, dispersion behaviour is taken to be that derived for a Pasquill/Gifford model. Approximate correction may be made for limited duration releases and for downwind diffusion using an (error function) correction suggested by Ermak (1986). The formulation, though tentative, should provide an estimate of the 'conservatism' inherent in assigning steady-state predictions to high consequence, short duration releases.

Matching is achieved in the limit of large dilution, for which buoyancy effects, mis-alignment of plume and wind, and the influence of release momentum are negligible.
Matching takes proper account of differences in vertical and horizontal diffusion, and of the influence upon these of concentration averaging times, and the proximity of the ground. Once the virtual source is located concentrations, may be predicted for *any* required averaging time, and for any point downwind of the plane of matching.

In HGSYSTEM, the far-field passive dispersion is simulated using the PGPLUME model. PGPLUME is, in effect, a 'post-processor' to AEROPLUME and HFPLUME to be used beyond the limits of AEROPLUME/HFPLUME when the near-field dispersion remains 'airborne', or at least does not credibly merge into a heavy-gas advected plume in the manner of HEGADAS (see Chapter 7.A section 7.A.4.2. for linking between the HGSYSTEM plume models and HEGADAS).

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7. THE HEAVY GAS DISPERSION MODEL HEGADAS

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7. THE HEAVY GAS DISPERSION MODEL HEGADAS

In this chapter a technical description of the HGSYSTEM heavy gas dispersion model HEGADAS is given. As a reference description, in Chapter 7.A detailed technical information is given about the HEGADAS version (HEGADAS 5) which was available in HGSYSTEM version 1.0. This description still applies to the HEGADAS model as available in HGSYSTEM 3.0, apart from the changes that are described in Chapter 7.B and 7.C.

7.A. TECHNICAL DESCRIPTION OF THE HEGADAS MODEL

7.A.1. Introduction

Considerable quantities of flammable and toxic gases are produced, stored or transported throughout the world. Many of these gases are denser than air if released to the atmosphere. The gas may be heavier than air for several reasons; for example, because of high molecular weight (e.g. carbon dioxide CO_2), low temperature (e.g. liquefied natural gas, LNG), chemical transformations (e.g. polymerisation of hydrogen fluoride, HF), or the formation of liquid aerosols.

Safety considerations necessitate the assessment of the hazards that might ensue in the event of an accidental gas release. Such an assessment involves the study of the gas-dispersion processes, and should lead to an estimate of (or upper bound for) the gas concentration as a function of position relative to the source and time.

Among the most well-known large-scale tests are the Thorney Island field tests (McQuaid, 1984), the Burro field tests (Koopman et al., 1982), the Maplin field tests (Puttock, Colenbrander and Blackmore, 1984), and the Goldfish field tests (Blewitt, 1988).

A large number of heavy-gas dispersion models exist for predicting the dispersion of dense gas clouds; see, for example, Hanna and Drivas (1987) and Witlox (1991) for a review of vapour-cloud-dispersion models. Most heavy-gas-dispersion models are based on empirical similarity profiles for the concentration. These profiles are usually expressed in terms of the centre-line ground-level concentration, and vertical/cross-wind dispersion parameters. The latter quantities are determined from a number of basic equations describing gas-mass conservation, air-entrainment, cross-wind gravity spreading and cross-wind diffusion. Most models include a thermodynamical description, which assumes that the heavy gas is an ideal, non-reactive gas.

The Shell program HEGADAS ('HEavy GAs Dispersion from Area Sources) is a well developed and validated heavy gas dispersion similarity model. HEGADAS is a further improvement of a mathematical model developed by Te Riele (1977) for the prediction of gas concentrations in ground-level plumes emitted by area sources in steady-state situations. HEGADAS was originally developed by Colenbrander (1980, 1984) for both steady-state and transient releases. Colenbrander and Bond (1986) included the effects of heat and water vapour transfer from the substrate. This version of HEGADAS (called HEGADAS-4) is documented by Colenbrander and Puttock (1988) and Witlox (1988).

HEGADAS can be used both for steady-state calculations (using the HEGADAS-S version of the model) or for transient (time-dependent) calculations (using the HEGADAS-T model).

Chapter 7.A contains a detailed technical description of the version HEGADAS-5 of HEGADAS as it was available in HGSYSTEM version 1.0, and includes a large number of enhancements and extensions compared to HEGADAS-4. The description in Chapter 7.A serves as a reference point in the technical specification of HEGADAS-5. The HEGADAS version which is available in HGSYSTEM 3.0 is almost identical to HEGADAS-5. The main differences between HEGADAS-5 and the HGSYSTEM 3.0 version of HEGADAS are described in Chapter 7.B and 7.C.

HEGADAS-5 has in part been developed in a multi-sponsored project to produce a software package (HGSYSTEM) for modelling the release/dispersion of hydrogen fluoride (HF) and ideal gases. This project has been documented by the HGSYSTEM version 1.0 Technical Reference Manual (McFarlane, Prothero, Puttock, Roberts and Witlox, 1990) and the HGSYSTEM version 1.0 Program User's Manual (Witlox, McFarlane, Rees and Puttock, 1990). The latter documentation includes historical details not contained in Chapter 7 of this Manual.

The steady-state HEGADAS-5 model is also described in Witlox (1994a) and the transient model in Witlox (1994b). The interfacing of different HGSYSTEM modules is also discussed in Witlox and McFarlane (1994).

The two thermodynamical models available in the HGSYSTEM 3.0 HEGADAS model are described in full detail in Chapter 2.

The plan of this Chapter is as follows.

Section 7.A.2 describes the basic similarity model for *steady-state dispersion*. This model includes a new cross-wind gravity-spreading formulation, which accounts for the phenomenon of collapse of gravitational spreading, and a generalised cross-wind diffusion law for improved prediction of cross-wind diffusion far downwind (e.g. possible use of Briggs formula for cross-wind dispersion coefficient σ_y).

Section 7.A.3 describes the *time-dependent model* for dispersion downwind from either a horizontal ground-level source or a vertical transition plane with a near-field model.

Section 7.A.3.2 describes the new algorithm with which the concentrations are determined as a function of time and downwind distance.
Section 7.A.3.3 includes a new formulation which describes the spreading and evaporation of a horizontal ground-level pool (gas-blanket formulation).
Section 7.A.3.4 contains a new formulation with time-dependent dispersion calculations being started from a vertical transition plane (breakpoint); thus the heavy gas dispersion model can be interfaced with near-source jet/plume models in the case of time-dependent pressurised releases.
Section 7.A.3.5 contains an improved formulation which describes the inclusion of along-wind-diffusion effects for transient releases.

Section 7.A.4 describes the interfacing of the heavy gas dispersion model with pool evaporation models and near-source jet/plume models.
In HGSYSTEM version 3.0, the heavy gas dispersion model HEGADAS can be interfaced with the pool-evaporation model LPOOL and with the near-source jet/plume models AEROPLUME and HFPLUME.

Section 7.A.5 describes the validation of the HEGADAS model.

Section 7.A.6 summarises the major conclusions of Chapter 7.A.

7.A.2. Steady-state model

The HEGADAS-5 steady-state model is also described in Witlox (1994a).

7.A.2.1. Wind-speed and concentration similarity profiles

The HEGADAS model adopts a power-law fit of the ambient wind speed for the velocity u

$$u = u_0 \left[\frac{z}{z_0} \right]^{\alpha} \tag{2.1}$$

where z is the height and z_0 is a reference height at which the velocity is u_0. The exponent α is found by matching the power law against the atmospheric wind profile $u_a(z)$.
See Appendix 7.A.A for details of this matching and an expression for $u_a(z)$ in terms of the Von Kármán constant $\kappa = 0.41$, the ambient friction velocity u_*, the surface roughness z_R and the Monin-Obukhov length λ.

The HEGADAS model adopts a similarity profile for the concentration c (kg/m^3).

$$
\begin{aligned}
c(x,y,z) &= c_A(x)\cdot\exp\left[-\left[\frac{z}{S_z(x)}\right]^{\beta}\right] && |y| < b \\
c(x,y,z) &= c_A(x)\cdot\exp\left[-\left[\frac{|y|-b(x)}{S_y(x)}\right]^{2}-\left[\frac{z}{S_z(x)}\right]^{\beta}\right] && |y| > b
\end{aligned}
\qquad (2.2)
$$

In the above formula x, y and z are Cartesian co-ordinates with the x-, y- and z- directions corresponding to the downwind, crosswind and vertical directions, respectively.

The release of the gas is at a rectangular ground-level area source located at $-\frac{1}{2}L < x < \frac{1}{2}L$, $-B < y < B$, $z = 0$, with L being the source length and B the source half-width.

The parameter β in the concentration profile is at present taken to be $\beta = 1 + \alpha$.
Figure 7.A.1 illustrates the concentration profile (2.2), which is expressed in terms of the peak concentration c_A, the dispersion coefficients S_z, S_y and the half-width b.

7.A.2.2. Dispersion variables and effective cloud data

DISPERSION VARIABLES

The dispersion variables c_A, S_z, S_y, b in the concentration profile (2.2) need to be determined in order to evaluate the concentration as a function of downwind distance x, crosswind distance y and height z.
The amount of heat and water-vapour added to the cloud needs also be evaluated if heat and water-vapour transfer from the substrate is included.
Thus the following dispersion variables need to be calculated as a function of downwind distance.

1. the centre-line ground-level concentration c_A (kg of dry pollutant/m^3)

2. the vertical dispersion coefficient S_z (m) defining the decay of the concentration in the vertical direction

3. the crosswind dispersion coefficient S_y (m) defining the decay of the concentration along the Gaussian flanks of the crosswind concentration profile

4. the half-width b (m) of the middle part of the crosswind profile (along which the ground-level concentration equals c_A), as S_y increases, b eventually becomes zero and the cross-wind profile is purely Gaussian.

5. the heat H_e added from the surface (Joule/kmole of mixture)

6. the water-vapour y_{w3} added from the surface (kmole/kmole of mixture)

Instead of the centre-line ground-level concentration c_A (kg of dry pollutant/m³), HEGADAS also utilises as an alternative variable the centre-line ground-level molar pollutant fraction y_{pol}: c_A is related to y_{pol} by

$$c_A = m_{dp} \cdot (1-\eta_w) \cdot y_{pol} / V_m \tag{2.3}$$

where η_w is the mole fraction of water in the pollutant, m_{dp} the molecular weight of the dry pollutant (kg/kmole), and V_m the mixture volume at centre-line and ground level (m³/kmole).

For given values of y_{pol} and H_e, the thermodynamic model as described in Chapter 2, determines the thermodynamic data V_m, ρ_m, T_m, which are the volume, the density and the temperature of the mixture at centre-line and ground level.

EFFECTIVE CLOUD CHARACTERISTICS

In HEGADAS the equations for the above dispersion variables are expressed in terms of so called 'effective' characteristics of the cloud. At each downwind position x the gas cloud in HEGADAS is characterised by an effective cloud half-width B_{eff}, an effective cloud height H_{eff}, an effective cloud speed u_{eff}, an effective molar cloud flow M_{eff}^{mol} (kmole of mixture passing per second through vertical plane at downwind distance x), a uniform concentration chosen to be equal to c_A, and a uniform molar mixture volume chosen to be equal to V_m (m³/kmole).
The effective cloud characteristics B_{eff}, H_{eff}, u_{eff}, M_{eff}^{mol} can be expressed as functions of S_z, b and S_y by

$$B_{eff} = \frac{1}{c(x,0,z)} \int_0^\infty c(x,y,z)\, dy = b + \tfrac{1}{2}\sqrt{\pi} S_y \tag{2.4}$$

$$H_{eff} = \frac{1}{c(x,y,0)} \int_0^\infty c(x,y,z)\, dy = \frac{1}{\beta} \cdot \Gamma\left(\frac{1}{\beta}\right) \cdot S_z \tag{2.5}$$

$$u_{eff} = \left[\int_0^\infty c\, dz\right]^{-1} \int_0^\infty u \cdot c\, dz = \frac{\Gamma[(1+\alpha)/\beta]}{\Gamma[1/\beta]} \cdot u_0 \cdot \left(\frac{S_z}{z_0}\right)^\alpha \tag{2.6}$$

$$\begin{aligned} M_{eff}^{mol} &= \frac{1}{V_m \cdot c_A} \int_0^\infty \int_{-\infty}^\infty u \cdot c\, dz = \frac{2 \cdot u_0 \cdot \Gamma[(1+\alpha)/\beta]}{\beta \cdot z_0^\alpha \cdot V_m} \cdot (b + \tfrac{1}{2}\sqrt{\pi}) \cdot S_z^{1+\alpha} \\ &= 2 \cdot B_{eff} \cdot H_{eff} \cdot u_{eff} / V_m \end{aligned} \tag{2.7}$$

7.A.2.3. Dispersion equations

The 6 unknown HEGADAS dispersion variables c_A, S_z, S_y, b, H_e, y_{w3} are determined from the following six equations.

1. A *continuity equation* describing the conservation of gas mass flowing through a plane x = constant,

$$\begin{aligned} E &= \int_0^\infty \int_{-\infty}^\infty u \cdot c\, dz = \frac{2 \cdot u_0 \cdot \Gamma[(1+\alpha)/\beta]}{\beta \cdot z_0^\alpha} \cdot c_A \cdot (b + \tfrac{1}{2}\sqrt{\pi}) \cdot S_z^{1+\alpha} \\ &= c_A \cdot 2 \cdot B_{eff} \cdot H_{eff} \cdot u_{eff} = (1 - \eta_w) \cdot m_{dp} \cdot y_{pol} \cdot M_{eff}^{pol} \end{aligned} \tag{2.8}$$

where E is the prescribed source strength (kg of dry pollutant released per second).

2. An empirical *entrainment law* describing the vertical entrainment of air into the top of the gas cloud (kmole/sec per unit of cloud width and per unit of cloud length) and substrate water-vapour transfer,

$$\frac{1}{2 \cdot B_{eff}} \cdot \frac{d}{dx}\left[M_{eff}^{mol}\right] = u_e(u_T) / V_0 + Q_{wv} \tag{2.9}$$

with V_0 = 22.4 m^3/kmole the molar volume of ideal gas at 0 °C and 1 atmosphere, u_e the vertical air-entrainment velocity and Q_{wv} the molar water-vapour flux from the surface.

In equation (2.9) it is assumed that dilution of the cloud is caused by vertical mixing at the top of the cloud, with the vertical entrainment velocity of air given by u_e. equation (2.9) states that the increase of molar cloud flow in the downwind direction equals the sum of molar cloud entrainment of air through the top of the cloud (kmole/s/m^2) and the molar water-vapour transfer from the substrate (kmole/s/m^2).

The entrainment velocity u_e can be expressed in terms of an empirical entrainment function Φ,

$$u_e(u_T) = \frac{\kappa \cdot u_T}{\Phi(Ri_*(u_T))} \tag{2.10}$$

with

$$\Phi(Ri_*) = \begin{cases} \dfrac{(1 + 0.8 \cdot Ri_*)^{1/2}}{(1+\alpha)} & Ri_* > 0 \\ \dfrac{(1 - 0.6 \cdot Ri_*)^{-1/2}}{(1+\alpha)} & Ri_* < 0 \end{cases}$$

and with the bulk Richardson number $Ri_*(u_T)$ defined by

$$Ri_*(u_T) = g \cdot \frac{(\rho_m - \rho_{amb}(z = H_{eff}))}{\rho_{amb}(z = 0)} \cdot \frac{H_{eff}}{u_T^2} \tag{2.11}$$

where g is the gravitational acceleration (= 9.81 m/s^2), κ is the Von Kármán constant (= 0.41) and ρ_{amb} the density of the ambient air. See Appendix 7.A.A for the evaluation of ρ_{amb} as a function of the height z.

The velocity u_T equals the friction velocity u_* if substrate heat transfer is not taken into account. Otherwise it is a modification of the friction velocity u_* to account for air entrainment caused by convection as a result of the temperature difference between the substrate and a cold vapour cloud. See Appendix 7.A.C.3 for the evaluation of u_T.

Note that the Richardson number Ri_* is proportional to the density difference between the gas cloud and the air, and reduces to zero in the far-field, passive-dispersion region.
The function $\Phi(Ri_*)$ was determined empirically using experimental laboratory data. See Section 3 of Appendix 3 in the HGSYSTEM 1.0 Technical Reference Manual (McFarlane, Prothero, Puttock, Roberts and Witlox, 1990) for further historical details.

3. An empirical law describing the *gravitational spreading of the gas cloud* in the cross-wind direction. In this spreading law the following consecutive phases are distinguished:

- The initial phase of gravity spreading is governed by a simple spreading law by Van Ulden (1984),

$$\frac{dB_{eff}}{dt} = C_E \cdot \sqrt{g \cdot H_{eff} \cdot \left[1 - \frac{\rho_{amb}(z=0)}{\rho_m}\right]} \tag{2.12a}$$

  where $C_E = 1.15$ is the spreading constant. The above law expresses that a dense vapour plume will spread laterally due to the difference in density between itself and the surrounding air. There is no entrainment.

- As a result of detailed comparisons between predictions of HEGADAS and an extensive set of wind-tunnel simulations of dense-gas plumes, it was found that the well-defined gravity-current head at the edge of such a plume can be destroyed by boundary-layer turbulence. Thus equation (2.12a) is only applicable up to the downwind position, at which *collapse of gravity spreading* takes place. This position was found to be well given by the position at which the following collapse criterion is first satisfied,

$$\frac{B_{eff} / H_{eff}}{\sqrt{Ri} \cdot \sqrt{1 + 0.8 \cdot Ri_*}} \geq \frac{8}{3 \cdot \kappa} \tag{2.12b}$$

  with the Richardson number Ri given by

$$Ri = g \cdot \frac{(\rho_m - \rho_{amb}(z=0))}{\rho_m} \frac{H_{eff}}{u_*^2}$$

- The considerably reduced post-collapse lateral spreading was found to be well defined by

$$\frac{dB_{eff}}{dx} = \frac{1}{u_{eff}} \cdot \frac{dB_{eff}}{dt} = \frac{u_*}{u_{eff}} \cdot \frac{Ri \cdot \sqrt{1 + 0.8 \cdot Ri_*}}{3 \cdot \kappa \cdot C_D} \cdot \frac{H_{eff}}{B_{eff}} \tag{2.12c}$$

  where $C_D = 5$ is an empirical constant.

- The gravity spreading is neglected downwind of the point at which the crosswind profile becomes purely Gaussian (i.e. at the point at which b reduces to 0). If the gas becomes buoyant ($Ri_* < 0$) in the region $b > 0$, zero gravity spreading (B_{eff} = constant) is assumed.

The gravity-spreading law has been formulated by Roberts, Puttock and Blewitt (1990). Figure 2 compares the old HEGADAS-4 and new HEGADAS-5 models with the HTAG wind-tunnel experiments (Petersen and Ratcliff, 1989). Section 7.3.2 and Chapter 8 in the HGSYSTEM 1.0 Technical Reference Manual (McFarlane, Prothero, Puttock, Roberts and Witlox, 1990) include further details and experimental evidence for the gravity-spreading model.

4. The derivation of the differential equation for the *cross-wind dispersion coefficient* S_y is based on an empirical formula for the non-dense cross-wind dispersion coefficient σ_y. In HEGADAS-4, this formula was restricted to a power-law dependence of σ_y on the downwind distance x. The steps in a generalised formulation for the evaluation of S_y are described in detail in Appendix 7.A.B and can be summarised as follows:

   - A Gaussian cross-wind concentration profile $c = c_a \exp(-\frac{1}{2}(y/\sigma_y)^2)$ is considered with the non-dense cross-wind dispersion coefficient σ_y given as an empirical function $\sigma_y^e(x)$ of the downwind distance x. The inverse of this function is denoted by $x^e(\sigma_y)$.

   - The 2D cross-wind diffusion equation $u_x \partial c/\partial x = \partial/\partial y(K_y \partial c/\partial y)$ is considered. The cross-wind diffusion coefficient K_y is assumed to be proportional to the wind speed u(z), $K_y = k_y \cdot u$, with $k_y = k_y^e(W)$ a function of the cloud half-width $W = (\pi/2)^{\frac{1}{2}} \cdot \sigma_y$.

   - Insertion of the formulas for c and K_y into the diffusion equation can be shown to lead to $k_y^e(W) = \sigma_y \partial\sigma_y^e/\partial x[x = x^e(\sigma_y)]$ with $\sigma_y = (2/\pi)^{\frac{1}{2}} \cdot W$.

   The derivation of the above formula for k_y is based on a Gaussian cross-wind concentration profile. In the HEGADAS concentration profile (2.2) the cross-wind dispersion coefficient S_y corresponds to $2^{\frac{1}{2}} \cdot \sigma_y$; the concentration c is uniform in a middle part of half-width b and it exhibits Gaussian decay for $|y| > b$ only.
   Instead of the cloud half-width $W = (\pi/2)^{\frac{1}{2}} \cdot \sigma_y$, HEGADAS adopts the effective cloud half-width $B_{eff} = b + \frac{1}{2} \cdot \pi^{\frac{1}{2}} \cdot S_y$. Therefore, in the calculation of S_y in HEGADAS-5 the following generalised equation is adopted to describe passive diffusion in the crosswind direction,

$$S_y \frac{\partial S_y}{\partial x} = 2 \cdot k_y^e(B_{eff}) \qquad (b > 0) \qquad (2.13)$$

   Downwind of the position x_t at which b reduces to zero, S_y is taken to be defined by

$$S_y(x) = 2^{\frac{1}{2}} \cdot \sigma_y^e(x + x_v) \qquad (b = 0) \qquad (2.13^*)$$

   with x_v chosen such that S_y is continuous at x_t.

In HEGADAS equations (2.13) and (2.13*) are applied to the empirical formula $\sigma_y^e(x) = \delta \cdot x \cdot (1 + \gamma \cdot x)^{-\frac{1}{2}}$ recommended by Briggs (1973). In this formula $\gamma = 0.0001\ m^{-1}$ and δ is related to the averaging time t_{av} (seconds) by $\delta = \delta_{600} \cdot (t_{av}/600)$ with $\delta_{600} = 0.22$. 0.16, 0.11, 0.08, 0.06, 0.04 m^{-1} for stability classes A, B, C, D, E and F, respectively.

5. The *heat transfer* equation

$$\frac{1}{2 \cdot B_{eff}} \cdot \frac{d}{dx}\left[H_e \cdot M_{eff}^{mol}\right] = Q_H \tag{2.14}$$

describes the heat flux Q_H transferred from the substrate to the gas cloud (Joule/sec per unit of cloud width and per unit of cloud length). The term between brackets in equation (2.14) represents the cloud heat flow through the plane x = constant, caused by pick-up of heat from the substrate (Joule/sec).

HEGADAS takes into account both free and forced heat convection. See Appendix 7.A.C.1 for full details of the evaluation of the heat flux Q_H.

6. The *water-vapour transfer* equation

$$\frac{1}{2 \cdot B_{eff}} \cdot \frac{d}{dx}\left[y_{w3} \cdot M_{eff}^{mol}\right] = Q_{wv} \tag{2.15}$$

describes the water-vapour flux Q_{wv} transferred from the substrate to the gas cloud (kmole/sec per unit of cloud width and per unit of cloud length). The term between brackets in equation (2.15) represents the molar flow of water through the plane x = constant, caused by pick-up of water-vapour from the substrate (kmole/sec). See Appendix 7.A.C.2 for full details of the evaluation of the water-vapour flux Q_{wv}.

7.A.2.4. Solution to dispersion equations

The entrainment law (2.9), the cross-wind gravity-spreading equation (2.12a) or (2.12b), the cross-wind diffusion equation (2.13), the heat-transfer equation (2.14) and the water-vapour transfer equation (2.15) provide *five ordinary differential equations*.

In HEGADAS these differential equations are solved in terms of the basic solution variables, which are chosen to be the effective molar cloud flow M_{eff}^{mol}, the effective cloud half-width B_{eff}, the cross-wind dispersion coefficient S_y, the added heat H_e from the surface, and the mole fraction y_{w3} of water-vapour added from the surface. The right-hand side of the differential equations is evaluated as follows as a function of these basic variables:

- y_{pol} is set from M_{eff}^{mol} by applying the dry-pollutant conservation equation (2.8).

- V_m, ρ_m, T_m are set from y_{pol}, H_c using the relevant thermodynamic model (see Chapter 2); c_A is set from (2.3),

- S_z, H_{eff} are set from equations (2.8) and (2.5), b is found from (2.4)

- Q_H is set from equations (C.2), (C.4) and (C.7) and Q_{wv} from equation (C.10).

DISPERSION CALCULATIONS FROM GROUND-LEVEL POOL

For a ground-level pool (unpressurised release) the dispersion calculations are carried out as follows:

1. In HEGADAS-S the user-prescribed, so-called *'primary' gas source*, is assumed to be rectangular with specified length L_p (m), half-width B_p (m) and source strength E (kg of dry pollutant released per second).
   Above the pool HEGADAS assumes a uniform centre-line ground-level concentration c_A, zero cross-wind gravity-spreading (B_{eff} = constant), zero cross-wind diffusion ($S_y = 0$) and zero heat and water-vapour transfer from the substrate ($H_c = y_{w3} = Q_H = Q_{wv} = 0$, $u_T = u_*$).
   For given source dimensions L_p, B_p the maximum amount of dry pollutant that can be taken up by the atmosphere is found from equation (2.8) to be

$$E_{max}(B_p, L_p) = (1-\eta_w)\cdot m_{dp}\cdot M_{eff}^{mol}(x = \tfrac{1}{2}L_p) \qquad (2.16)$$

   The following two cases are now distinguished:

   - o If the specified source rate E is larger than the maximum take-up rate $E_{max}(B_p,L_p)$, all pollutant *cannot* be taken up directly by the atmosphere and a so-called 100 % *gas blanket or secondary pool* is assumed to form.
     The blanket dimensions B, L are chosen in such a way that the aspect ratio stays the same, $B/L = B_p/L_p$, and such that $E = E_{max}(B,L)$ is satisfied. To this purpose equation (2.9) is solved iteratively with different start values of L; $B = (B_p/L_p)\cdot L$ until equation (2.8) is satisfied at the downwind edge ($x = \tfrac{1}{2}L$) of the secondary pool.

o If $E < E_{max}(B_p,L_p)$ all released pollutant can be taken up directly by the atmosphere, a 100 % gas blanket *does not* form and the secondary pool equals the primary pool: $L = L_p$, $B = B_p$.
The mole fraction y_{pol} above the pool is less than one and is determined by solving equation (2.9) iteratively with different start values of y_{pol} until equation (2.8) is satisfied at the downwind edge ($x = ½L$) of the pool.

After y_{pol}, B and L have been determined as described above, the dispersion variables are calculated above the secondary pool ($-½L < x < ½L$):

- $B_{eff} = B$, $S_y = H_e = y_{w3} = 0$,
- V_m, ρ_m, T_m are set from y_{pol}, H_e using the relevant thermodynamic model,
- S_z is determined by solving the entrainment law (2.9) with $Q_{wv} = 0$, $u_T = u_*$.

2. The dispersion calculations downwind of the pool are carried out starting from the initial conditions at the downwind edge ($x = ½L$) of the pool. The entrainment law (2.9), cross-wind gravity-spreading equation (2.12a) or (2.12b), crosswind diffusion equation (2.13), and the heat and water-vapour transfer equations (2.14), (2.15) are solved stepping forward in the downwind distance x.

After b has reduced to 0, the crosswind spreading and diffusion equations (2.12a) or (2.12b), (2.13) are no longer solved and S_y is set from equation (2.13*).
The variables S_z, H_e, y_{w3} are calculated from the differential equations (2.9), (2.14) and (2.15) with B_{eff} taken to be constant and $M_{eff}^{mol} = 2 \cdot B_{eff} \cdot H_{eff} \cdot u_{eff}/V_m$,

$$\frac{d}{dx}\left[H_{eff} \cdot u_{eff} / V_m\right] = u_e(u_T) / V_0 + Q_{wv} \tag{2.9*}$$

$$\frac{d}{dx}\left[H_e \cdot H_{eff} \cdot u_{eff} / V_m\right] = Q_H \tag{2.14*}$$

$$\frac{d}{dx}\left[y_{w3} \cdot H_{eff} \cdot u_{eff} / V_m\right] = Q_{wv} \tag{2.15*}$$

Please note that the algorithm for b = 0 *has been changed* in the HEGADAS version as available in HGSYSTEM version 3.0. See Chapter 7.B. for a description of this new algorithm.

DISPERSION CALCULATIONS FROM TRANSITION POINT

For a pressurised release the momentum-dominated flow in the near field cannot be calculated by HEGADAS. Hence initial values of the dispersion variables at an appropriate transition point must be provided. Section 7.A.4.2 details how these data can be provided by a near-field model (e.g. HFPLUME or PLUME (HGSYSTEM 1.0) or AEROPLUME (HGSYSTEM 3.0)). Starting from these initial conditions the dispersion calculations are carried out as described in the above point 2.

PASSIVE LIMIT IN FAR FIELD

Both the entrainment law (for Richardson number Ri. → 0) and the crosswind spreading formulation (after b has reduced to 0) converge to the *passive-dispersion* limit in the far field. Moreover, the concentration profile becomes purely Gaussian after b has reduced to 0. Thus the HEGADAS formulation gives similar results to conventional passive-dispersion Gaussian models in the far field. The various phases in the dispersion of a steady ground-level release of propane (boiling liquid pool) are indicated in Figure 3.

SOLUTION OF DISPERSION EQUATIONS FOR HF; EQUIVALENT MOLES

When using the hydrogen fluoride chemistry and thermodynamics as described in Chapter 2.B, y_{pol}, H_e, y_{w3} and M_{eff}^{mol} are assumed to be associated with *equivalent moles* of mixture based on *all* HF being in the monomer state, and equations (2.7), (2.9), (2.9*), (2.14), (2.14*), (2.15), (2.15*) refer to equivalent moles. [Note that strictly speaking for equation (2.3) to be correct V_m should be the volume of the pollutant per equivalent mole and not volume of the pollutant per 'real' mole!].

7.A.3. Time-dependent model

The HEGADAS-5 transient model HEGADAS-T is also described in Witlox (1994b).

7.A.3.1. Introduction

The time-dependent (or transient) version HEGADAS-T of HEGADAS-5 can be used to model the time-dependent ground-level dispersion of a heavy gas cloud which moves with the ambient wind.

It can be used to model the dispersion downwind of either a time-dependent ground-level source (unpressurised release) or a vertical transition plane (or breakpoint; pressurised release). The dispersion variables at the transition plane are determined from a near-source jet/plume program (see Sections 7.A.4.2 and 7.A.4.3).

In HEGADAS-T the transient behaviour of the dense vapour cloud is approximated by a quasi-steady-state description in which so-called *'observers'* are released at the pool/transition-plane at a series of times. These observers travel with the wind. The concentration data are determined as a function of position and time by means of the following algorithmic steps.

1. For a ground-level source, the time-dependent pool dimensions and pool evaporation rate (primary pool) are user-specified or are provided from pool evaporation models (see Section 7.A.4.1). If the pool emission rate becomes larger than the maximum amount of gas which can be taken up by the air, a gas blanket forms (secondary pool).
   Observers are 'released' at a series of times upwind of the gas blanket. *These observers travel with the wind.* The blanket data observed by each observer are determined.

   For a vertical-plane transition from a near-source jet model, the values of the HEGADAS dispersion variables at the transition plane are determined by means of matching against the values of the dispersion variables for the jet model. The observers are released at the transition plane (breakpoint).

2. For each observer, the observed concentration is computed via steady-state HEGADAS calculations adopting the observed source data. Thus, by calculating the position of each observer at a given time t, the concentrations are determined at time t for a number of downwind distances from the pool/breakpoint.

3. A cloud shape correction is applied to the observer concentrations. This correction introduces downwind gravity spreading and reduces the calculated cross-wind gravity spreading in such a way that the amount of spreading in the downwind direction of the cloud as a whole equals the spreading in the cross-wind direction.

4. At a given time t, the actual concentration is determined from Gaussian integration with respect to the downwind distance x of the above observer concentrations. This Gaussian integration involves a downwind dispersion coefficient σ_x, which allows longitudinal diffusion to be taken into account.

Section 7.A.3.2 describes in more detail the new algorithm with which the concentrations are determined.

Sections 7.A.3.4.3 and 7.A.3.4.4 describe the models for a ground-level pool and a vertical transition plane, respectively.
Section 7.A.3.4.5 describes the along-wind-diffusion formulations adopted in the model.

See Appendix 7.A.E for the evaluation of the observer position as a function of time and see Appendix 7.A.F for details on the cloud shape correction.

7.A.3.2. Algorithm for evaluation of concentrations

In HEGADAS-4 the user had to specify the time interval Δt_{obs} with which observers were to be released. This procedure required the user to be familiar with the observer concept, since selection of too large a time step leads to inaccurate concentration predictions at the specified output times. This section describes the algorithm for evaluation of concentrations in HEGADAS-5 (as available in HGSYSTEM version 1.0).
In this algorithm Δt_{obs} is determined internally in the program to ensure accurate predictions (automated release of observers).

For a horizontal ground-level source, observers are released with a constant time interval Δt_{obs} at the upwind edge of the source. The observers travel with the wind in the downwind direction. While travelling over the time-varying source, each observer i (i = 1,2,...,M) 'sees' a source length L_i (m; in downwind direction), an averaged source half-width B_i (m; in cross-wind direction), a source strength E_i (kg/s) and a downwind edge of the source x_{dw}^i (m); see Section 7.A.3.3 for the evaluation of the observer source data.

Steady-state dispersion calculations based on these data yield the observer-dispersion data: ground-level centre-line wet-pollutant molar fraction $y^i_{pol}(x) = y_{pol}(x - x_{dw}^i + L_i/2;\ E_i,\ B_i,\ L_i)$, vertical dispersion coefficient $S_z^i(x) = S_z(x - x_{dw}^i + L_i/2;\ E_i,\ B_i,\ L_i)$, etc.
Here for example $y_{pol}(x;E,B,L)$ corresponds to a steady-state ground-level source with strength E, half-width B, length L and source centroid at $x = y = 0$.

For a vertical transition plane (breakpoint), observers i = 1,2,...,M are released with a constant time interval Δt_{obs} at the breakpoint. For each observer i, steady-state dispersion calculations are carried out based on the breakpoint data valid at the time the observer is released.

Let x_j^i be the position of observer i at the output time t_j ($j = 1,2,..N$; $t_1 < t_2 < ...< t_N$.).
Then $x_j^1 > x_j^2 > ... x_j^M$, i.e. *observers released earlier are located further downwind.*

The concentration data $y_{pol}(x,t_j)$, as a function of the downwind distance x at the output time t_j, are derived from the observer-dispersion data $c_j^i = y^i_{pol}(x_j^i)$, i = 1,2,...,N by the inclusion of a cloud-shape correction for gravitational spreading and the inclusion of downwind diffusion effects. Thus for an accurate evaluation of $y_{pol}(x,t)$, the release interval Δt_{obs} (determining the observer spacing) must be smaller if larger gradients of $y_{pol}(x,t)$ occur.

The observer concept in HEGADAS-T is a *quasi-steady-state solution method* for determining the concentration $y_{pol}(x,t)$ as a function of the downwind distance x and the time t. This method may be seen as a *first-order inclusion of time-dependent effects.* It produces accurate predictions for slowly varying time-dependent sources, but it may lead to less accurate predictions for rapidly time-varying sources.

CRITERION FOR CHOOSING NUMBER OF RELEASED OBSERVERS

In a HEGADAS-T run the concentrations calculated at each output time t_j must be accurate. This condition requires a sufficiently small spacing of the observers, i.e. a sufficiently small value of the observer-release interval Δt_{obs} such that the concentration curve $y_{pol}(x,t_j)$ can be evaluated accurately from the observer-dispersion data.
An observer spacing that is too large leads to concentration curves that are *too smooth* (peaks are eroded).

Consider the positions x_j^{i+1}, x_j^i, x_j^{i-1} ($x_j^{i+1} < x_j^i < x_j^{i-1}$) and the concentrations c_j^{i+1}, c_j^i, c_j^{i-1} seen by three adjacent observers i+1, i, i-1 (i = 2,...,M-1).
Let C_j^i be the estimate of the concentration at x_j^i based on linear interpolation of the data for observers i+1 and i-1 (*before* the inclusion of the cloud-shape correction and downwind-diffusion effects).
C_j^i thus equals

$$C_j^i = c_j^{i+1} + \left(x_j^i - x_j^{i+1}\right) \cdot \left(\frac{c_j^{i-1} - c_j^{i+1}}{x_j^{i-1} - x_j^{i+1}} \right) \tag{3.1}$$

This would have been the HEGADAS estimate of the concentration at x_j^i, if observer i would not have been released.

Thus the estimates of the absolute error $\varepsilon_j^{abs,i}$ and relative error $\varepsilon_j^{rel,i}$ at x_j^i are

$$\begin{aligned} \varepsilon_j^{abs,i} &= \left|C_j^i - c_j^i\right| \\ \varepsilon_j^{rel,i} &= \left|C_j^i - c_j^i\right| / c_j^i \end{aligned} \tag{3.2}$$

A convergence criterion for the observer concentrations must be chosen carefully. For smaller output times, the gas cloud may have very 'sharp' edges. The relative and absolute concentration errors near these edges will only be small for a very large number of observers and an excessive amount of computer time.
Hence, instead of demanding that the maximum value of the concentration error is small, it is more appropriate to demand that the *mean* concentration error is small. Effectively this means that the *predicted cloud volume* or *cloud shape* is accurately modelled.

The *peak* concentrations must be accurately predicted. Thus at each output time, error estimates for observers with larger concentrations should contribute more than those with minute concentrations. Hence it is more appropriate to demand small mean *absolute* concentration errors than small mean relative concentration errors.

The relative error in the predicted cloud volume or cloud shape must be small for every output time. Hence it is appropriate to scale the mean absolute concentration error at a given output time with the peak concentration at that time. Thus the following convergence criterion for the observer concentrations is adopted

$$\max_{1\le j\le N}\left[\frac{\dfrac{1}{M-2}\cdot\sum_{i=2}^{M-1}\varepsilon_j^{\mathrm{abs},i}}{\max\limits_{1\le i\le M} c_j^i}\right]<\varepsilon_{\mathrm{obs}} \qquad (3.3)$$

The above convergence criterion implies that for all times t_j ($j = 1,2,..,N$), the ratio of the mean error in the absolute concentration and in the peak concentration is smaller than the convergence tolerance ε_{obs}.
The default value of ε_{obs} adopted in HEGADAS-T equals $\varepsilon_{obs} = 0.05$. This value was found to lead to accurate concentration predictions without an excessive number of observers for most types of source conditions. [It is noted that the averaging of the concentration in the numerator of equation (3.3) is only applied to those observers which actually have seen (some part of) the source at time t_j.].

CRITERION FOR CHOICE OF OUTPUT TIMES

The maximum concentration over all times, $c_{max}(x)$ must normally be determined accurately. This condition requires a sufficiently close spacing between the output times t_1, t_2, ..., t_N, such that the envelope $c_{max}(x)$ of the curves $c(x,t_1)$, $c(x,t_2)$, ..., $c(x,t_N)$ is well defined.

The user can verify that this condition is satisfied by plotting a series of these curves in one graph. The plot file corresponding to each curve $c(x.t_j)$ can be generated by the interactive HEGADAS-T post-processor HTPOST (HGSYSTEM version 1.0) or the batch post-processor POSTHT (HGSYSTEM 3.0). See the relevant information on POSTHT in the HGSYSTEM 3.0 User's Manual.

HEGADAS-T ALGORITHM WITH AUTOMATED RELEASE OF OBSERVERS

In HEGADAS the time-dependent pool or transition data are specified with a fixed time step Δt.

Let n_{td} be the number of records and t_{st} be the start time; for a ground-level pool t_{st} equals the time at which the pool becomes active, and for a transition plane it equals the time at which pollutant first passes the transition plane.

Thus the data are specified at the input times $t_{st}+\Delta t$, $t_{st}+2\cdot\Delta t$, .., $t_{st}+n_{td}\cdot\Delta t$. Zero data are assumed for time $t > t_{st}+(n_{td}+1)\cdot\Delta t$.

Data are linearly interpolated between the input times.

The automation of the release of observers in HEGADAS-T is carried out by means of the following consecutive algorithmic steps:

1. For a ground-level source the primary-pool data and secondary-pool (gas-blanket) data are set as a function of time (see Section 7.A.3.3.1).
   The maximum blanket radius R_{max} is determined.
   The observers are released at $x = - R_{max}$. The minimum and maximum observer-start times for which a observer may see a pool (t^{st}_{min}, t^{st}_{max}) are determined.
   Observer-source data (secondary source data seen by the observer while travelling over the pool) are set for the maximum number of (currently) 161 observers (see Section 7.A.3.3.2). Observers 1, 2, .., 160, 161 are released at the times t^{st}_{min}, $t^{st}_{min}+\Delta t_{obs}$, .., $t^{st}_{max}-\Delta t_{obs}$, t^{st}_{max}, with the observer-release interval given by $\Delta t_{obs} = (t^{st}_{max} - t^{st}_{min})/160$.

   For a vertical transition plane, breakpoint data are set and observers are released at the times $t_{st}+\Delta t_{obs}$, $t_{st}+2\cdot\Delta t_{obs}$, .., $t_{st}+161\cdot\Delta t_{obs}$, where $\Delta t_{obs} = (n_{td}+1)*\Delta t/162$ (see Section 7.A.3.4).

2. a The initial observer release interval is currently chosen to be equal to IFREQ = 32, and dispersion data are set for the 6 observers 1, 33, 65, 97, 129, 161 (5 observer intervals).

   b If the convergence criterion (3.3) is satisfied for the current observers 1, 1+IFREQ, ..., 161-IFREQ, 161 go to step 3.

c If IFREQ = 1, terminate program with an error message saying that convergence can not be obtained with the maximum number of 161 observers.

d Double the number of observer intervals, i.e. set dispersion data for the additional, intermediate observers 1+IFREQ/2, 1+3·IFREQ/2, ..., 161-3·IFREQ/2, 161-IFREQ/2, and half observer frequency (IFREQ = IFREQ/2). Go to step 2b.

3. Carry out cloud shape correction of dispersion data for observers 1, 1+IFREQ, ..., 161-IFREQ, 161 (see Appendix 7.A.F) and include downwind-diffusion effects (see Section 7.A.3.5).

7.A.3.3. Dispersion from ground-level source

7.A.3.3.1. Secondary source

For finite-duration steady-state releases or slowly varying release rates the HEGADAS-T (version HEGADAS-4) formulation lead to erroneous oscillatory behaviour in the predictions of the dimensions of the gas blanket (secondary source).

This section introduces an improved formulation without oscillatory behaviour. See Section 7.5 in the HGSYSTEM 1.0 Technical Reference Manual (McFarlane, Prothero, Puttock, Roberts and Witlox, 1990) for further historical details.

In the model the primary source is assumed to be circular with a radius $R_p(t)$, m, and a dry-pollutant emission rate E(t), kg/s.

A 100 % vapour blanket is assumed to form if E(t) is larger than the maximum take-up rate $E_{max}[B=\frac{1}{2}\pi^{\frac{1}{2}}\cdot R_p(t), L=\pi^{\frac{1}{2}}\cdot R_p(t)]$ corresponding to an equivalent steady square pool that has the same area $\pi\cdot R_p^2(t)$ as the circular source (see equation (2.16)).

The gas blanket is taken to have a flat cylindrical shape of radius $R_g(t)$ and height $H_g(t)$. The blanket dimensions $R_g(t)$ and $H_g(t)$ are determined from the numerical solution of two differential equations representing a gravity-spreading law [analogous to the spreading equation (2.12a)] and blanket-mass conservation, respectively,

$$\frac{dR_g(t)}{dt} = C_E \cdot \sqrt{g \cdot \frac{\rho_E - \rho_a(z=0)}{\rho_E} \cdot H_g(t)} \tag{3.4}$$

$$\frac{dM(t)}{dt} = E(t) - E_{max} \cdot \left[B = \tfrac{1}{2}\pi^{\frac{1}{2}} \cdot R_g(t), L = \pi^{\frac{1}{2}} \cdot R_g(t)\right] \tag{3.5}$$

Here ρ_E is the dry-pollutant density, kg/m^3, g = 9.81 m/s^2 the acceleration of gravity and M(t) the blanket mass defined by

$$M(t) = \pi \cdot \rho_E \cdot R_g^2(t) \cdot H_g(t) \qquad (3.6)$$

At the onset of the formation of the gas blanket, say at time $t = t_0$, the blanket radius equals the primary source radius and the blanket mass equals zero. Thus in the numerical solution of equations (3.4), (3.5) the initial values $R_g(t_0) = R_p(t_0)$ and $M(t_0) = 0$ are adopted. The differential equations are subsequently solved stepping forward in time.

For $t > t_0$ the blanket radius $R_g(t)$ increases as a result of gravity spreading; see equation (3.4). Mass is added to the gas blanket because of material entering the pool [spill rate E(t)] and lost because of evaporation [evaporation rate $E_{max}[B=\frac{1}{2}\pi^{\frac{1}{2}} \cdot R_p(t), L=\pi^{\frac{1}{2}} \cdot R_p(t)]$; see equation (3.5). Note that the amount of evaporation increases with the blanket radius $R_g(t)$.

For $t > t_0$ the blanket radius $R_g(t)$ is initially small and therefore the evaporation rate is less than the spill rate. Hence the mass of gas in the blanket initially increases. Because of this accumulation of gas, the blanket continues to spread beyond the radius at which the evaporation rate would equal the spill rate, and thereafter the evaporation exceeds the source rate. The mass of gas in the blanket therefore decreases, eventually reaching zero.

Let $t = t_1$ be the time at which the blanket height reduces to zero, i.e. the time at which the entire gas blanket is taken up into the air.
If the source rate $E(t_1)$ is smaller than $E_{max}[B=\frac{1}{2}\pi^{\frac{1}{2}} \cdot R_p(t_1), L=\pi^{\frac{1}{2}} \cdot R_p(t_1)]$, the gas blanket disappears at time $t = t_1$ and the secondary pool is set equal to the primary pool.
If $E(t_1) > E_{max}[B=\frac{1}{2}\pi^{\frac{1}{2}} \cdot R_p(t_1), L=\pi^{\frac{1}{2}} \cdot R_p(t_1)]$, a zero-height gas blanket forms. This gas blanket is assumed to equal the steady-state blanket corresponding to the present spillage rate $E(t_1)$. Thus according to equation (3.5) the pool radius $R_g(t_1)$ of this blanket is determined from inversion of the formula $E(t_1) = E_{max}[B=\frac{1}{2}\pi^{\frac{1}{2}} \cdot R_p(t_1), L=\pi^{\frac{1}{2}} \cdot R_p(t_1)]$.

For $t > t_1$ a gas blanket with zero height is assumed to remain in existence as long as the gas-release rate does not increase [$dE(t)/dt < 0$] and the blanket radius exceeds the primary radius [$R_g(t) > R_p(t)$]. Let the end of this period be at time $t = t_2$. During the period $t_1 < t < t_2$ the blanket radius $R_g(t)$ is determined from the steady-state blanket corresponding to the release rate E(t), i.e. it is determined from inversion of the formula $E(t) = E_{max}[B=\frac{1}{2}\pi^{\frac{1}{2}} \cdot R_p(t), L=\pi^{\frac{1}{2}} \cdot R_p(t)]$.

At the end $t = t_2$ of the period the following two cases can be distinguished:

- The blanket radius $R_g(t)$ reduces to the primary radius $R_p(t)$ at $t = t_2$. In this case the zero-height gas blanket disappears and the secondary pool becomes equals to the primary pool.

- The release rate E(t) starts to increase at time $t = t_2$. In this case a finite-thickness gas blanket forms and equations (4.4), (4.5) are solved with the initial values $R_g(t_2)$ (unchanged blanket radius) and $M(t_2) = 0$.

Summarising the above results the following applies for the radius R(t) and the evaporation flux Q(t), kg/m^2/s of the secondary source:

$$
\begin{aligned}
&R(t) = R_g(t) && \text{(with gas blanket)}\\
&R(t) = R_p(t) && \text{(no gas blanket)}\\
&Q(t) = \frac{E_{max}\cdot\left[B = \tfrac{1}{2}\pi^{1/2}\cdot R_g(t_1), L = \pi^{1/2}\cdot R_g(t_1)\right]}{\left[\pi\cdot R_g^2(t_1)\right]} && \text{(with gas blanket)}\\
&Q(t) = \frac{E(t)}{\left[\pi\cdot R_p^2(t_1)\right]} && \text{(no gas blanket)}
\end{aligned}
\tag{3.7}
$$

The above formulation has been tested for a pool of boiling propane with a primary radius $R_p = 3$ m, a constant evaporation rate E = 30.0 kg/s and a release duration of 200 seconds. Figure 5 illustrates that the HEGADAS-5 model indeed eliminates the oscillatory gas-blanket behaviour of the former HEGADAS-4 model. Initially, a finite-thickness gas blanket forms. After this blanket has spread beyond the steady-state radius (≈ 15 m), the blanket mass diminishes until it is reduced to zero at time $t_1 \approx 25$ s. At this time the blanket radius is reset in the HEGADAS-5 model to the steady-state radius. In the HEGADAS-4 model the blanket radius is reset to the primary pool radius after each disappearance of the finite-thickness gas blanket.

7.A.3.3.2. Observer source data

The observers i = 1,2,... are released with a time interval Δt_{obs} upwind of the secondary pool, i.e. at $x = -R_{max}$, where R_{max} is the maximum blanket radius [= maximum value of R(t)].

The observers travel with the wind. Appendix 7.A.E describes the evaluation of the observer position $x^i(t)$ and observer speed $u^i(t)$ as a function of time. The observer velocity increases with downwind distance and for all observers their velocity at a given location x is the same ($u^i(x) = u^{i+1}(x)$).

This implies that at a given time t the velocity of observer i is greater than the velocity of the following observer i+1 ($u^i(t) > u^{i+1}(t)$).

Let us now consider one specific observer, say observer i, and let us follow this observer while it moves over the secondary pool. Let observer i encounter the upwind edge of the secondary source at $t = t_1^i$ and the downwind edge at $t = t_2^i$ and let $x^i(t)$ be the location of this observer at time t. As can be seen from Figure 6 the local secondary half-width of the source $B_{obs}^i(t)$ observed at time t is given by:

$$B_{obs}^i(t) = \sqrt{R^2(t) - \left(x^i(t)\right)^2} \tag{3.8}$$

The secondary source area A^i and the source rate E^i seen by observer i is found by evaluating the integrals

$$A^i = \int_{t_1^i}^{t_2^i} 2 \cdot u^i(t) \cdot B_{obs}^i(t)\, dt \tag{3.9}$$

$$E^i = \int_{t_1^i}^{t_2^i} 2 \cdot Q(t) \cdot B_{obs}^i(t) \cdot u^i(t)\, dt \tag{3.10}$$

The secondary source length L^i as seen by observer i is given by:

$$L^i = x^i(t_2^i) - x^i(t_1^i) \tag{3.11}$$

and thus we find an averaged observed secondary half-width of the source

$$B^i = ½ \cdot A^i / L^i \tag{3.12}$$

In this way we can determine, for each of the n observers travelling over the source (i = 1,...,n), the observed dimensions L^i and B^i, the locations $x^i(t_1^i)$ and $x^i(t_2^i)$ of, respectively, the upwind and the downwind edge of the secondary source and the take-up rate E^i.

7.A.3.3.3. Concentrations

From the observer source data the concentration distribution in the cloud can be determined at a specified time t_s. To this end the location $x^i(t_s)$ of each observer at time t_s is calculated and for each observer a steady-state calculation is done, using the pertinent parameters L_i,B_i,E_i and $x^i(t_2\ i)$. Thus the concentration distribution parameters $c_A(x^i(t_s))$, $S_y(x^i(t_s))$, $b(x^i(t_s))$, $S_z(x^i(t_s))$ are determined for $i = 1,\ldots,n$ and thus the concentration distribution $c(x'(t_s),y,z)$ given by equation (2.2).

It will be clear that in this quasi-steady state approach the gravitational spreading of the cloud in the wind direction cannot be taken into account, unlike in heavy gas dispersion box models for strictly instantaneous vapour releases (e.g. HEGABOX).
Thus, the width of the cloud calculated with the model presented here will be somewhat too large and the length too small, especially at very low wind velocities.
Some spreading in the wind direction is introduced in the gas blanket calculation, where we can use a radial spreading law because the centre of the gas blanket is assumed to remain stationary above the source at $x = 0$.
In addition, a correction algorithm has been devised for use at the end of the calculation, which redistributes part of the lateral gravity spread to longitudinal spreading. Appendix 7.A.F includes a description of this *cloud shape correction*.

For releases of short duration, dispersion in the wind direction may have a significant influence on the concentration level in the cloud.
Accordingly, the calculated concentrations are adjusted to take account of this dispersion in the x-direction. The method followed is described in Section 7.A.3.5.

7.A.3.4. Dispersion downwind of transition with near-source jet model

7.A.3.4.1. Transition data

If HEGADAS-T is to be run downwind of a vertical transition plane $x = x_{br}$ (breakpoint) with a near-source jet model, three data are to be specified at the breakpoint by the user for a number of times.
These data are the effective cloud half-width $B^{br}_{eff}(t)$ and any two of the following breakpoint values: the ground-level centre-line wet-pollutant molar fraction $y^{br}_{eff}(t)$, the effective cloud height $V^{br}_{eff}(t)$, and the dry-pollutant mass flow $E^{br}(t)$ through the transition plane (kg/s).
Breakpoint data at other times are derived by linear interpolation.

It is assumed that at the breakpoint the cross-wind concentration profile is uniform and does not have Gaussian flanks $[b = B^{br}_{eff}(t), S_y = 0]$. In addition, the amount of water-vapour y_{w3} and heat H_e added from the surface are taken to be zero $[y_{w3} = H_e = 0]$. From the specified breakpoint data described above, the dispersion variables y_{pol} and S_z at the breakpoint are then set using the equations described in Section 7.A.2.3.

7.A.3.4.2. Concentrations

The time-dependent values of the six dispersion variables y_{pol} (or c_A), S_z, b, S_y, H_e, y_{w3} determined at the breakpoint are used as starting values for the steady-state dispersion calculations for the observers, which are released with a fixed user-specified time interval Δt_{obs}. These calculations involve the solution of the dispersion equations described in Section 7.A.3.2. Thus, for each observer, dispersion data are obtained as a function of the downwind distance x.

In order to express the observer dispersion data as a function of position and time, a formula needs to be provided for the position of each observer as a function of time. See Appendix 7.A.A for a derivation of this formula. By use of this formula, the observer data are stored at those downwind positions, which correspond to a number of user-specified output times.

Appendix 7.A.B describes the subsequent application of the cloud shape correction for downwind gravity spreading to these data. After the cloud shape correction, downwind diffusion effects are taken into account as described in Section 7.A.4.
Note that the conditions at the breakpoint x_{br} remain satisfied during the inclusion of downwind diffusion. This is because zero diffusion ($\sigma_x = 0$) is assumed at $x = x_{br}$ in the along-wind-diffusion formulations.

EXAMPLES

First the problem is considered of a steady plume which starts to pass the transition plane at time t = 0. Figure 7 illustrates the HEGADAS-T predictions at time t = 100 seconds. As expected, the HEGADAS-T predictions at this time closely resemble the HEGADAS-S predictions for a corresponding steady release.
The formulation was also validated by a simulation of the first Goldfish experiment, in which the transition data were derived from the near-source jet/plume model HFPLUME.
Figure 8 shows that the time-dependent centre-line ground-level concentrations are predicted well by HEGADAS.
Chapter 9 in the HGSYSTEM version 1.0 Technical Reference Manual (McFarlane, Prothero, Puttock, Roberts and Witlox, 1990) includes full details.

7.A.3.5. Inclusion of along-wind-diffusion effects

The centre-line ground-level concentration $c_A = c_A(x,t)$ is calculated as a function of time t and distance x downwind of the source by means of *Gaussian integration of the observer concentrations* $C_A(\xi)$ at ξ,

$$c_A(x,t)=\int_0^{\infty}\frac{C_A(\xi)}{\sqrt{2\pi}\cdot\sigma_x(\xi)}\cdot\exp\left[-\frac{(x-\xi)^2}{2\sigma_x^2(\xi)}\right]d\xi \tag{3.13}$$

In the above equation ξ is the position at time t of an observer travelling with the wind in the downwind direction. At this position the observer observes the concentration $C_A(\xi)$, where $C_A(\xi)$ is calculated from a steady-state HEGADAS solution based on zero along-wind diffusion (see Section 7.A.3.2).
In (3.13) along-wind diffusion is taken into account by assuming that the concentration $C_A(\xi)$ spreads out around ξ according to a Gaussian distribution with a downwind dispersion coefficient $\sigma_x = \sigma_x(\xi)$.

Note that the position ξ of the observer in equation (3.13) corresponds to the observer position *after* the cloud shape correction for gravitational spreading in the wind direction has been applied (see Appendix 7.A.F).

The dispersion coefficient σ_x is usually considered to consist of two statistically independent components σ_{xs} and σ_{xt},

$$\sigma_x=\sqrt{\sigma_{xs}^2+\sigma_{xt}^2} \tag{3.14}$$

The component σ_{xs} is the spread induced by vertical wind shear and σ_{xt} is the turbulent spread caused by downwind-direction velocity fluctuations. Increasing the wind shear du/dz increases the relative speed at which the top and bottom of the cloud are advected, and so increased shear du/dz results in increased spread σ_{xs}. Since the wind shear increases with stability, the spread σ_{xs} increases with stability. This is confirmed by the experimental data of Nickola (1971).

LITERATURE REVIEW OF ALONG-WIND DIFFUSIONS FORMULATIONS

In the original HEGADAS-4 formulation the formula $\sigma_x = \sigma_x(\xi)$ did not take into account the change of wind shear and hence the formula was not altered as a function of the stability class.

The following provides an overview of along-wind-diffusion formulations in the literature.

1. Formula for σ_{xs} by Smith (passive flow).

Smith (1965) analysed the problem of shear diffusion of puffs released in the surface layer theoretically. Using the method of moments, he arrived at the following formula for σ_{xs} (source at ground level) valid for passive flow

$$\sigma_{xs} = \sigma_{xs}(\xi) = 12^{-1/2} \cdot \left(\frac{du}{dz}\right) \cdot t_{obs} \cdot \sigma_z \tag{3.15}$$

Here t_{obs} is the travel time of the puff from (the middle part of) the pool to the present puff position $x = \xi$, σ_z the vertical dispersion coefficient, and du/dz the vertical gradient of the horizontal wind speed u(z) at a certain reference height (see e.g. point 3 below).

2. Formula for σ_{xs} by Chatwin (neutrally stratified, passive flow).

Chatwin (1968) studied the passive dispersion of a puff in a neutral atmosphere. He arrived at the following formula for the downwind dispersion coefficient σ_{xs},

$$\sigma_{xs} = \sigma_{xs}(\xi) = 0.596 \cdot u_* \cdot t_{obs} / \kappa \tag{3.16}$$

Here $\kappa = 0.41$ is the Von Kármán constant and u_* the ambient friction velocity.
The derivation of equation (3.16) by Chatwin is based on a logarithmic formula for the ambient wind speed u valid for neutrally stratified flow only, and the linear formula $K_z = \kappa \cdot u_* \cdot z$ for the vertical diffusivity (or $u_e = u_*$ for entrainment velocity) valid for passive gases only. HEGADAS adopts the more general formula (A.1) in Appendix 7.A.A for the wind speed for stratified flow and the heavy gas, non-passive extension (2.10) of the formula for the entrainment velocity.

The analytical derivation of equation (3.16) by Chatwin consists of two parts. In the first part the velocity $d\xi/dt$ and position ξ of a puff (frozen puff, moving with the wind) as a function of the travel time t_{obs} are calculated (see equation (23) in Chatwin (1968)).
The extension of this calculation to stratified, heavy-gas flow can be done relatively easily. See Chaudry and Meroney (1972) for an extension of this calculation to stratified flow.

In the second part σ_{xs} is calculated by applying the Lagrangian similarity hypothesis valid for neutrally stratified flow. This calculation can easily be extended to neutral, heavy-gas flow with a constant Richardson number, and equation (3.16) can be shown to be still valid. However, it cannot be extended in a straightforward manner to the non-neutral case.

3. Formula for σ_{xs} and σ_{xt} by Ermak (stratified, passive flow).

The formulation of Ermak (1986) is a further development of an along-wind-diffusion formulation by Wilson (1981) for stratified, passive flow. By using a purely Gaussian profile for the concentration and a power-law for the ambient wind speed, he expresses the puff velocity $d\xi/dt$ as a function of the vertical spreading coefficient σ_z.
Using a stability-class dependent power-law fit of an empirical formula for $\sigma_z(\xi)$ recommended by Briggs (1973), he then expresses $t_{obs} = t_{obs}(\xi)$ as a function of ξ.

Following Wilson, Ermak evaluated (du/dz) in equation (3.15) at a reference height found from matching equations (3.15) and (3.16). Insertion of the expression $t_{obs} = t_{obs}(\xi)$ into equation (3.15) then leads to the evaluation of σ_{xs} as a function of ξ.
Assuming isotropic horizontal turbulent spread ($\sigma_{xt} = \sigma_{yt}$), Ermak determines σ_{xt} from a formula recommended by Briggs (1973).
Thus the following formulas are used by Ermak:

$$\sigma_{xs}(\xi) = \left\{ \frac{0.60 \cdot \sqrt{\pi} \cdot 0.34^{\alpha}}{(1-\alpha \cdot d) \cdot \Gamma(\tfrac{1}{2} + \tfrac{1}{2}\alpha)} \right\} \cdot \xi$$

$$\sigma_{xt}(\xi) = \frac{a_y \cdot \xi}{\sqrt{1 + b_y \cdot \xi}} \tag{3.17}$$

with d = 1, 1, 0.82, 0.66, 0.55, 0.55 and a_y = 0.22, 0.16, 0.11, 0.08, 0.06, 0.04 for stability classes A, B, C, D, E and F respectively; $b_y = 0.0001$, α is the wind-speed exponent, and Γ is the Gamma function.

4. Formulation by Wheatley for stratified, passive flow.

Wheatley (1988) derived in a more rigorous manner the concentration distribution of a passive puff in a stratified atmosphere from an approximate solution to the diffusion equation. He arrived at an ordinary differential equation for the downwind diffusion coefficient σ_x.

ALONG-WIND-DIFFUSION FORMULATIONS IN HEGADAS

As a result of the above literature review, the following two along-wind-diffusion formulations have been implemented into HEGADAS.

1. For *non-neutral stability* an adaptation of the formulation by Ermak has been implemented. In this formulation, $\sigma_x(\xi)$ is given by

$$\sigma_x(\xi) = \sqrt{\sigma_{xs}^2(x = \max[0, \xi - x_{br}] + \sigma_{xt}^2(x = \max[0, \xi - x_{br}])} \qquad (3.18)$$

In the above equation σ_{xs} and σ_{xt} are defined by equation (3.17) with the wind-speed exponent chosen equal to the exponent α adopted in the HEGADAS wind-speed profile (2.1).
Note that $\max[0,\xi\text{-}x_{br}]$ equals the middle x = 0 of the pool for a ground-level model and it equals the downwind position x_{br} for a vertical transition plane (breakpoint).

The formulation takes into account the effect of increased shear with increased stability. However, it has a number of deficiencies. The formulation is partially based on Chatwin's formula (3.16), which strictly speaking is valid only for neutral stability and passive gas dispersion.
Moreover, in the elimination of the time the (stability-class dependent) ambient wind speed and *not* the cloud speed is adopted, and downwind diffusion is *not* ignored in regions with high Richardson numbers.

It is noted that diffusion could be ignored in regions with high Richardson number by calculating for each observer the downwind position x_{cr}^{obs} at which the Richardson number reduces to a given critical Richardson number Ri_*^{cr} (x_{cr}^{obs} corresponds to middle of pool, if $Ri* < Ri_*^{cr}$ always) and replacing in equation (3.18) the argument $\max[0,\xi\text{-}x_{br}]$ by $\max[\xi\text{-}x_{cr}^{obs},\xi\text{-}x_{br}]$.
However, in this manner, the σ_x-formula is no longer a direct function of x and the formulation loses its simple nature.

For these reasons the formulation may be inaccurate, particularly if high cloud concentrations occur during the dispersion processes.

2. For *neutral stability*, a heavy gas adaptation of the formulation by Chatwin for passive, neutrally stratified flow has been implemented. In this formulation σ_x is not directly related to the downwind distance ξ, but is evaluated as a function of the actual travel time t_{obs} of the cloud.

In this formulation downwind diffusion is neglected in the region where the observed bulk Richardson number Ri_*^{obs} is larger than a user-specified value Ri_*^{cr} (default value Ri_*^{cr} = 10), say upwind of the point x_{cr}^{obs}. As in equation (3.18), downwind diffusion is also neglected upwind of the breakpoint $x = x_{br}$.

Thus x_{cr}^{obs} is reset to x_{br} if $x_{cr}^{obs} < x_{br}$ (with x_{br} taken to be at the middle of the observed pool in the absence of a breakpoint).

The actual concentration as a function of time t and downwind distance x is determined from equation (3.13). Here the downwind dispersion coefficient σ_x is set from equation (3.16) with the time t_{obs} taken to be the travel time of the observer from x_{cr}^{obs} to ξ, i.e. $t_{obs} = t - t_{cr}^{obs}$.

In the elimination of the time the actual true speed of the puffs (observers; cloud speed) as used in HEGADAS-T is adopted, and downwind diffusion is ignored in regions with Richardson number Ri_* larger than a user-specified value Ri_*^{cr}. Therefore, in the case of neutral conditions, the adapted Chatwin formulation is more compatible with the observer concept adopted in HEGADAS-T and gives more realistic predictions than Ermak's formulation.

In the high-density region $Ri > Ri_{cr}$, downwind diffusion induced by wind shear is assumed not to take place. However, in this region considerable gravitational downwind spreading occurs which is taken into account in HEGADAS-T by the cloud-shape correction.

It is still questionable what the ideal value is to be selected for Ri_*^{cr}. The default value $Ri_*^{cr} = 10$ presently used seems to be reasonable, but may induce insufficient downwind diffusion. A higher value for Ri_*^{cr} might be more appropriate. An appropriate value for Ri_*^{cr} could be found by fitting with experimental data.

EXAMPLE

Figure 9 depicts the application of the above along-wind diffusion formulations in HEGADAS-T simulations of the Goldfish 1 experiment (constant release rate of HF for $0 < t < 125$ seconds).

This figure also includes HEGADAS-S predictions for a corresponding steady pool and HEGADAS-S predictions with a finite-duration error-function correction. Note that the amount of downwind diffusion is lower for the adapted Chatwin's formulation lower than for the adapted Ermak's formulation.

The upper envelope of the Ermak's formulation resembles the peak-concentration prediction by the error-function formulation since identical σ_x formulas are adopted in both approaches; see Section 8.6.1 in the HGSYSTEM version 1.0 Program User's Manual (Witlox, McFarlane, Rees and Puttock, 1990) for further details.

7.A.4. Interfacing with pool-evaporation and near-source jet/plume models

The user needs to supply input parameters to the heavy-gas-dispersion program HEGADAS. Among these parameters, those input data describing the near-source conditions are often not known by the user a priori.

These input data can be obtained by using one of the other models included in the HGSYSTEM software package. The models in HGSYSTEM enable the user to model a wide range of release scenarios, i.e. pressurised or unpressurised release, release of HF gas or a non-reactive ideal gas (HGSYSTEM version 1.0)or aerosol mixture HGSYSTEM 3.0), steady-state or time-dependent (e.g. finite-duration) release rate of gas.

In the HGSYSTEM software package the program HEGADAS can be interfaced with the pool-evaporation program EVAP (HGSYSTEM 1.0) or LPOOL (HGSYSTEM 3.0) and the near-source jet/plume programs PLUME (HGSYSTEM 1.0) or AEROPLUME (HGSYSTEM 3.0) and HFPLUME.

The interfacing of HGSYSTEM modules is also discussed in Witlox and McFarlane (1994).

7.A.4.1. Interface with pool evaporation models

Liquid spillage may lead to the formation of a liquid pool. The geometry of the resulting liquid pool and the rate of evaporation can be calculated in HGSYSTEM 1.0 by the EVAP model for both steady and transient releases. EVAP calculates the (time-dependent) pool dimensions and pool evaporation rate as HEGADAS input. Chapter 4 in the HGSYSTEM version 1.0 Technical Reference Manual (McFarlane, Prothero, Puttock, Roberts and Witlox, 1990) includes full details on EVAP and its interface with HEGADAS.

In HGSYSTEM 3.0, EVAP has been replaced by the fully transient pool model LPOOL. Input for HEGADAS-T is generated by LPOOL. See the HGSYSTEM version 3.0 User's Manual and Chapter 4 for details on LPOOL. For releases that can be approximated as steady-state releases, the user can easily set the corresponding evaporation rate (GASFLOW or FLUX in the GASDATA input block for HEGADAS-S) in the HEGADAS-S input file. See HGSYSTEM 3.0 User's Manual for details on HEGADAS input parameters.

7.A.4.2. Interface with near-source models

For a pressurised release the heavy-gas-dispersion near the source is often momentum-dominated and HEGADAS cannot be applied in this region. Data at a near-source transition point can be derived from calculations by the near-source jet/plume models HFPLUME (for hydrogen fluoride releases) or PLUME (for non-reactive 'ideal' gas; HGSYSTEM 1.0) or AEROPLUME (two-phase releases; HGSYSTEM 3.0). See Chapter 5 for full details on the HGSYSTEM plume models.

TRANSITION CRITERION

The plume models (AEROPLUME, HFPLUME and PLUME) simulate cloud behaviour in a near-source region. The transition from the plume models to HEGADAS is chosen at the point where the cloud conditions become more appropriate to the physical assumptions in HEGADAS. The following criteria should be satisfied simultaneously:

- The plume jet speed u^{pl} is sufficiently close to the ambient wind speed u_a at the centroid height. The ambient wind speed is adopted in the HEGADAS program to approximate the velocity.
- The total plume entrainment is sufficiently close to the heavy-gas entrainment $\mathrm{Entr}_{gas}^{heavy}$, which is taken to be the entrainment in HEGADAS.

These criteria are included in the plume models by adding the following conditions

$$\left|u^{pl} / u_a - 1\right| < \mathrm{RULST} \quad \text{and} \quad 1 - \mathrm{Entr}_{gas}^{heavy} / \mathrm{Entr}_{total} < \mathrm{RELST} \tag{4.1}$$

In addition to these criteria, residual buoyancy should not 'disturb' momentary advection. See Section 6.2 in Witlox, McFarlane, Rees and Puttock (1990) for a complete description of the transition criteria. See the AEROPLUME <casename>.APZ file for information on all transition criteria for the specific AEROPLUME run. This file is normally deleted but by changing the AEROPLUME.BAT file it can be saved for inspection (see section 3.5 in the HGSYSTEM 3.0 User's Manual).

The successive regions of the jet/plume flow in the plume models are the 'airborne' region (elevated jet-flow/dispersion; circular plume cross-section), the 'touchdown' region (transitional region; cut-off circle cross-section) and 'slumped' region (ground-level dispersion; semi-elliptic plume cross-section).
The transition from the plume models to the ground-level dispersion program HEGADAS can only be made following touchdown.

PLUME MODEL VARIABLES

The plume models all assume a 'top-hat' model which assumes uniform, averaged data within the jet/plume. These data are a function of the downwind distance only. The basic unknowns in the plume models are the concentration of the pollutant (plume concentration), c^{pl}, the total mixture density (plume density), ρ^{pl}, the plume speed, u^{pl} and the plume enthalpy, h^{pl}. These four unknowns are determined from four conservation equations (excess of ambient quantities), i.e. conservation of gas-mass flow, total-mass flow, extra momentum and extra energy.

At the transition point the axis inclination of the plume will be nearly horizontal. Thus the area A^{pl} of the semi-elliptic cross-section of the plume is related to the plume diameter D^{pl} and the plume centroid z_c^{pl} by

$$A^{pl} = 3\cdot\pi^2\cdot z_c^{pl}\cdot D^{pl}/16 \tag{4.2}$$

See also section 5.B.6.

MATCHING OF PLUME MODEL VARIABLES WITH HEGADAS VARIABLES

The HEGADAS equations for the variables c_A, S_z, S_y, b, H_e, y_{w3} have been described in Section 2.3. These variables are set at the transition point from the plume model variables by means of appropriate matching criteria. These criteria transfer cloud characteristics and are described below.

The plume model formulation does *not* take into account heat transfer and water-vapour transfer from the ground. Thus it is consistent with the HEGADAS formulation to take H_e = y_{w3} = 0 at the transition point.

The plume models assume a uniform, averaged concentration within the jet. Thus it is consistent with the HEGADAS formulation to take S_y = 0, corresponding to a uniform concentration for $|y| < b$ and a zero concentration for $|y| > b$.
Thus the concentration c and the wind speed u adopted in HEGADAS are given at the breakpoint by (see equations (2.1) and (2.2))

$$c(x,y,z) = c_A \exp\left[-\left(\frac{z}{S_z(x)}\right)^{\beta}\right], \quad |y|<b, \quad u = u_0\left(\frac{z}{z_0}\right)^{\alpha} \tag{4.3}$$

with $\beta = 1 + \alpha$.

It remains to determine the variables c_A, S_z and b in equation (4.3). One might determine these variables by imposing the conservation equations adopted in the plume models.
Conservation of extra momentum is not applicable, because HEGADAS assumes the velocity to be the ambient wind speed (zero extra momentum).
Conservation of extra energy seems not to be appropriate because by setting $H_e = 0$ in HEGADAS we actually have ignored heat effects at the transition point.
Instead the following three conditions are imposed to determined the variables c_A, S_z and b:

- Conservation of pollutant mass flow.

  This means that the total flow of pollutant (kg/s), E, flowing through the transition plane $x = x_{br}$ is preserved. E is given by the following integral as a 'first' moment M_1 in concentration:

$$E = M_1 = \int_0^\infty \int_{-\infty}^{\infty} u\, c\, dy\, dz \qquad (4.4)$$

- Conservation of total plume mass.

  This means that the flow of total plume mass (kg/s) is conserved. The total mass flow M_{tot} is given by

$$M_{tot} = \int_0^\infty \int_{-\infty}^{\infty} u\, \rho\, dy\, dz \qquad (4.5a)$$

where ρ is the plume density.
However, an expression involving the concentration c is needed as this is one of the matching variables. For small concentrations, the total density ρ can be written as a function ρ(c) of c(z). Using a Maclaurin expansion around c = 0 for small c,

$$\rho(c) = \rho(0) + c\rho'(0) + \tfrac{1}{2}c^2\rho''(0) + \text{H.O.} \qquad (4.5b)$$

where H.O. stands for higher order terms. Inserting (4.5b) into (4.5a) it can be concluded that for $c \rightarrow 0$, conservation of total mass is implied by conservation of pollutant mass equation (4.4) (the term linear in c) and conservation of the 'second' moment M_2 of concentration (the quadratic term in c):

$$M_2 = \int_0^{\infty}\int_{-\infty}^{\infty} u\, c^2 \, dy\, dz \tag{4.5c}$$

- Plume centroid height.

The centroid height z_c is given by

$$z_c = \frac{1}{M_1}\cdot\int_0^{\infty}\int_{-\infty}^{\infty} u\, c\, z\, dy\, dz \tag{4.6}$$

Both the HEGADAS similarity profile (4.3) and the plume model top-hat profile for c and u are now inserted into the above conditions (4.4), (4.5) and (4.6). Subsequent matching leads to the following three conditions:

$$M_1 = A^{pl}\cdot c^{pl}\cdot u^{pl} = \frac{2}{\beta}\cdot\Gamma\left(\frac{1+\alpha}{\beta}\right)\cdot\frac{S_z^{1+\alpha}}{z_0^{\alpha}} b\cdot c_A\cdot u_0 \tag{4.7}$$

$$M_2 = A^{pl}\cdot\left(c^{pl}\right)^2\cdot u^{pl} = 2^{-\frac{(1+\alpha)}{\beta}}\cdot\frac{2}{\beta}\cdot\Gamma\left((1+\alpha)/\beta\right)\cdot\frac{S_z^{1+\alpha}}{z_0^{\alpha}} b\cdot\left(c_A\right)^2\cdot u_0 \tag{4.8}$$

$$z_c = z_c^{pl} = S_z\cdot\Gamma\left((2+\alpha)/\beta\right)/\Gamma\left((1+\alpha)/\beta\right) \tag{4.9}$$

In HEGADAS the exponent β in the vertical concentration profile is related to the wind-speed exponent α by $\beta = 1+\alpha$ (see equation 2.2). From HEGADAS simulations of experiments it is known that HEGADAS accurately predicts ground-level concentrations, but often badly predicts vertical variations of the concentration. Thus in the matching process it is not appropriate to adopt $\beta = 1+\alpha$ to obtain from the HFPLUME (uniform) data accurate estimates of the parameters c_A and b that determine the ground-level concentration. Instead, in particular in the far-field, a Gaussian concentration profile defined by $\beta = 2$ will be more appropriate.

Moreover the wind speed u(z) is approximated by the (uniform) centroid plume speed.

Thus $u(z) = u^{pl} = u_0\cdot(z/z_0)^{\alpha}$, $\alpha = 0$, $\beta = 2$ are inserted in the above matching conditions (4.7), (4.8) and (4.9). By eliminating z_c^{pl} and using equation (4.2), the following conditions are then derived:

$$c_A = \sqrt{2}\cdot c^{pl} \tag{4.10}$$

$$b = \frac{3 \cdot \pi}{16 \cdot \sqrt{2}} \cdot D^{pl} \qquad (4.11)$$

Finally the HEGADAS variable S_z is set from the gas-mass conservation equation (2.8) with the value of β taken to be consistent with the HEGADAS assumption $\beta = 1+\alpha$.

SENSITIVITY TO TRANSITION CRITERIA

Figure 10 illustrates the effect of the transition criteria (4.1) on the HFPLUME/HEGADAS predictions.

In agreement with equation (4.10) the HFPLUME (sectional-mean) concentration curves are almost parallel at the transition point to the HEGADAS (centre-line, ground-level) concentration curves.

The cloud half-width in Figure 10b equals $B_{eff} = 3 \cdot \pi \cdot D^{pl}/(16 \cdot \sqrt{2})$ in the HFPLUME region [compare equation (4.11)] and $B_{eff} = b + \frac{1}{2} \cdot \sqrt{\pi} \cdot S_y$ in the HEGADAS region [see equation (2.4)].

The concentration predictions are almost unaffected by the precise position of the transition point if RULST < 0.1 and RELST < 0.3. The values RULST = 0.1 and RELST = 0.3 are recommended and are default values in HGSYSTEM (versions 1.0 and 3.0).

7.A.5.3. Interface with near-source models (finite-duration release)

For the same reasons as for HEGADAS-S, the time-dependent model HEGADAS-T may not be applied to pressurised releases in the high-momentum near-source region. Thus HEGADAS-T should be only applied downwind of an appropriately chosen transition point or breakpoint $x = x_{br}$.

For *finite-duration releases* the program HEGADAS-T can automatically be interfaced with the near-source plume models. To this purpose the (steady-state) transition data are applied at the breakpoint x_{br} for a period corresponding to the release duration T_{dur}.

Thus at the breakpoint x_{br}, the dry-pollutant flow E (kg/s), the centre-line ground-level pollutant molar fraction y_{pol} (from equation (4.10) and the relevant thermodynamic model) and the cloud half-width b (m; from equation (4.11)) are applied for a period of T_{dur} (s).

Gas is being released at the release point $x = 0$ during the period $0 <$ time $t < T_{dur}$. In applying the above transition data at $x = x_{br}$ one must take into account the travel time T_{br} of the plume between the release point $x = 0$ and the transition point $x = x_{br}$. Thus the transition data are applied for T_{br} < time t < $T_{br} + T_{dur}$. The travel time T_{br} can be expressed in terms of the plume speed u = u(x) by the following formula,

$$T_{br} = \int_0^{x_{br}} \frac{1}{u_x(x)}\, dx \qquad (4.12)$$

where $u_x(x)$ is the horizontal component of the plume speed u^{pl}.

7.A.5. Validation

The physics or fundamentals of the HEGADAS model described in the previous sections were developed using experimental laboratory data. Parameters which quantify a particular physical process have been determined, where possible, from laboratory experiments which study that process in isolation. This has been carried out as follows.

- The empirical formula (2.10) for the entrainment velocity is based on data for a large number of wind tunnel experiments (see Section 7.A.2.3).

- The initial crosswind spreading law (2.12a) is based on experiments by Van Ulden (1984), and the subsequent collapse of gravity spreading given by equations (2.12b) and (2.12c) is based on experiments by Linden and Simpson (1988). The crosswind diffusion given by equations (2.13) and (2.13*) is based on empirical formulae for the non-dense crosswind dispersion coefficient σ_y introduced by Briggs (1973).

- The empirical formula (C.2 in Appendix 7.A.C) for the heat flux Q_H in the heat equation (2.14) is based on expressions for the forced and natural convection heat flux proposed by Holman (1981) and McAdams (1954).
  The water-vapour equation (2.15) is based on a theoretical approach by Rosner (1967). equations (2.14) and (2.15) have been validated by Colenbrander and Puttock (1984) by means of a series of three experiments involving cold nitrogen flowing across a water surface. See Section 5 of Appendix 3 of the HGSYSTEM 1.0 Technical Reference Manual (McFarlane, Prothero, Puttock, Roberts and Witlox, 1990) for further historical details.

- The hydrogen fluoride thermodynamics formulation described in Chapter 2.B. is based on experimental data by Schotte (1987,1988); see Figure 4.

The HEGADAS model was then validated against independent wind-tunnel and field data to ensure that it correctly describes the effect of these various physical processes in combination.

Thus an independence is maintained between the model formulation and the data which is used to verify the model (i.e. HEGADAS is not tuned to any particular field data set).
By using this approach, greater confidence can be given to the predictions from the HEGADAS model. The HEGADAS model was validated against the following wind-tunnel and field data.

1. Puttock, Colenbrander and Blackmore (1984) modelled continuous releases of liquid propane and LNG over water in the Maplin Sands field experiments (HEGADAS-2 version). Figure 11 illustrates the improved predictions for Maplin Spill 54 by the HEGADAS-5 version as available in HGSYSTEM 1.0.

2. Roberts (see Chapter 8 in the HGSYSTEM 1.0 Technical Reference Manual (McFarlane, Prothero, Puttock, Roberts and Witlox, 1990) for historical details) modelled wind tunnel data by Petersen and Ratcliff (1989) for steady, isothermal dispersion (HEGADAS-5; Figure 2). These experiments involved a wide range of surface roughnesses and gas/air density ratios.

3. Colenbrander and Puttock (1984) modelled transient releases of liquid propane and LNG over water in the Maplin Sands field experiments while including both heat and water-vapour transfer from the substrate (HEGADAS-4 version; Figure 12).

4. Puttock (1987) modelled instantaneous releases of Freon in Thorney Island experiments (Figure 13). He modelled the gravity-slumping in the near-field by the box model HEGABOX (see Chapter 8) and the dispersion further downwind was modelled by HEGADAS-T (HEGADAS-4 version).

5. Witlox (see Chapter 9 in the HGSYSTEM Technical Reference Manual (McFarlane, Prothero, Puttock, Roberts and Witlox, 1990) for full historical details) modelled steady and finite-duration pressurised releases of HF for the Goldfish experiments (Blewitt, 1988). He modelled the near-field momentum-dominated dispersion using the HGSYSTEM model HFPLUME and the dispersion further downwind by HEGADAS-5.
   Figures 14 and 15 illustrate the steady-state dispersion predictions for the Goldfish 3 experiment. Figures 8 and 9 illustrate the finite-duration dispersion predictions for the Goldfish 1 experiment.

The intended application of HEGADAS is to simulate postulated accidental releases of a hazardous pollutant in an industrial setting. However, there is no one set of experimental data against which all aspects of the model can be tested in its entirety. In verifying the models sensitivity analyses are the only method of testing the interaction of all components of the models and the validity of the several model assumptions. From these analyses it can be ensured that the results are physically reasonable. For the pressurised release of HF a detailed sensitivity analysis was carried out by Witlox. In this sensitivity analysis the near-field momentum-dominated dispersion was modelled by the HGSYSTEM model HFPLUME and the dispersion further downwind by HEGADAS.

The sensitivity to both input variables (meteorological data, source data, etc.) and model assumptions (interface criteria, crosswind-spreading and diffusion formulations, ..) were investigated. Two base cases were considered, one case with conditions similar to the Goldfish 2 experiment (high temperature, low surface roughness and humidity) and one with more typical rural conditions. See Chapter 10 in the HGSYSTEM 1.0 Technical Reference Manual (McFarlane, Prothero, Puttock, Roberts and Witlox, 1990) for full historical details.

7.A.6. Summary and conclusions

This report includes a complete technical description of the heavy-gas-dispersion model HEGADAS-5 as it was provided in HGSYSTEM version 1.0.

A number of enhancements and extensions to similarity models for heavy gas dispersion problems have been described, which have been incorporated into the HEGADAS-5 version of HEGADAS.

HEGADAS is based on an empirical similarity profile for the concentration, which is expressed in terms of the centre-line ground-level concentration and vertical/cross-wind dispersion parameters. The latter quantities are determined from a number of basic equations describing gas-mass conversation, air entrainment, cross-wind gravity spreading and cross-wind diffusion. The model includes the following new features:

1. A cross-wind gravity-spreading formulation, which accounts for the phenomenon of collapse of gravitational spreading (Section 7.A.2.3)

2. A generalised cross-wind diffusion law for improved prediction of cross-wind diffusion far downwind (e.g. possibility of Briggs formula for cross-wind dispersion coefficient σ_y; Section 7.A.2.3 and Appendix 7.A.B).

3. A thermodynamical description for HF, which takes into account the effects of polymerisation and the exothermic reaction of HF with the water-vapour in the moist air (Chapter 2.B).

4. A new algorithm for evaluation of the concentration data for transient releases (Section 7.A.3.2).

5. An improved formulation describing the spreading and evaporation of the pool (gas-blanket formulation) for transient releases (Section 7.A.3.3).

6. A new formulation with time-dependent dispersion calculations being started from a transition plane with a near-field jet model (Section 7.A.3.4). Thus the heavy-gas-dispersion model can be interfaced with near-source jet/plume models for time-dependent pressurised releases.

7. An improved formulation describing the inclusion of along-wind-diffusion effects for transient releases (Section 7.A.3.5).

8. A fully automated interface of the steady or transient heavy-gas dispersion model with pool-evaporation models (for unpressurised releases; Section 7.A.4.1) or with near-source jet/plume models (at a given transition point; for pressurised releases; Sections 7.A.4.2 and 7.A.4.3).

These model enhancements have been validated by simulating the HTAG wind-tunnel experiments (steady unpressurised release of ideal gases) and the Goldfish experiments (steady and finite-duration pressurised release of HF).
The program has also been evaluated by a sensitivity analysis (steady pressurised release of HF).

7.A.7. References

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7.A.8. Notation

This section contains a list of the major symbols used in the report. For each symbol the meaning and unit of the symbol is given, and the number of equation or section where it is defined. The sections and appendices are indicated without the 7.A prefix.

Symbol	Meaning and unit	Reference
$b(x)$	half-width of middle part of crosswind concentration profile (m); $b = 0$ after profile has become Gaussian	Eq. (2.2)
B	half-width of secondary ground-level pool (m)	Sect. 2.4
$B_{eff}(x)$	effective cloud half-width (m)	Eq. (2.4)
B_p	half-width of primary ground-level pool (m)	Sect. 2.4
$c(x,y,z)$	dry-pollutant concentration (kg/m^3)	Eq. (2.2)
$c_A(x)$	dry-pollutant centre-line ground-level concentration (kg/m^3)	Eq. (2.2)
c_p^α, C_p^α	specific heat (J/kg/K and J/kmole/K, respectively) of species α [α = dp, a, N, wl, wv, wi for dry pollutant, air, N-gas, water vapour, water liquid and ice]	App. C.2

E	dry-pollutant source emission rate (kg/s)	Eq. (2.8)
$E_{max}(B,L)$	maximum take-up rate (kg/s) of dry pollutant for ground-level source with half-width B and length L == emission rate of gas blanket with dimensions B,L	Eq. (2.16)
g	gravitational acceleration (= 9.81 m/s^2)	Eq. (2.11)
H^w_{cond}	heat of condensation of water (Joule/kmole)	App. D
H^w_{fus}	heat of fusion of water (Joule/kmole)	App. D
$H_e(x)$	heat added from the substrate to the pollutant/air mixture (J/kmole)	Sect. 2.2
$H_{eff}(x)$	effective cloud height (m)	Eq. (2.5)
L	length of secondary ground-level pool (m)	Sect. 2.4
L_p	length of primary ground-level pool (m)	Sect. 2.4
m_α	molecular weight of species α [α = dp, w, a, amb for dry pollutant, water, dry air and ambient air, resp.]	Sect. 2.2
$M^{mol}_{eff}(x)$	effective molar cloud flow (kmole/s of mixture flowing through vertical plane at downwind distance x)	Eq. (2.7)
P	total pressure (atm); in HEGADAS always taken to be 1	
$P_w^w(T)$	saturated vapour pressure of water (atm) at temperature T (in °C)	Eq. (A.13)
$Q_H(x)$	heat flux from substrate to cloud (J/s/m^2)	Eq. (2.14)
$Q_{wv}(x)$	water-vapour flux from substrate to cloud (kmole/s/m^2)	Eq. (2.15)
r_H	relative humidity of air (fraction; $0 < r_H < 1$)	Eq. (A.12)
R	gas constant = 0.082 atm/K/kmole = 8314.3 J/K/kmole	
$Ri_*(x)$	bulk Richardson number (-)	Eq. (2.11)
$Ri(x)$	Richardson number (-)	Eq.(2.12b)
$S_y(x)$	crosswind dispersion coefficient (m)	Eq. (2.2)
$S_z(x)$	vertical dispersion coefficient (m)	Eq. (2.2)
T_a	ambient temperature at ground level (°C)	App. A
$T_m(x)$	centre-line ground-level mixture temperature (°C)	App. A
T_{pol}	pollutant temperature (°C)	App. D
T_s	substrate temperature (°C)	App. C
$u(z)$	ambient wind speed (m/s)	Eq. (2.1)
$u_{eff}(x)$	effective cloud speed (m/s)	Eq. (2.6)
$u_T(x)$	modified friction velocity (m/s) to account for air entrainment caused by convected advents due to temperature differences between substrate and cloud	Eq. (C.11)
u_0	ambient velocity at reference height z0	Eq. (2.1)
u^*	ambient friction velocity (m/s)	Eq. (A.1)
V_0	volume of ideal gas at 0 °C and 1 atm. (= 22.4 m^3/kmole)	Eq. (2.9)
$V_m(x)$	centre-line ground-level mixture volume (m^3/kmole)	Eq. (2.3)

x	downwind distance from middle of pool (m)	Sect. 2.1
x_{br}	x co-ordinate of transition plane (breakpoint) between HEGADAS and near-source dispersion model	Sect. 5.2
y	crosswind distance from centre-line of cloud (m)	Sect. 2.1
$y_{pol}(x)$	centre-line ground-level pollutant molar fraction (-)	Eq. 2.3
$y_{w3}(x)$	water-vapour added from the substrate (kmole/kmole of mixture)	Sect. 2.2
z	vertical height above substrate (m)	Sect. 2.1
z_0	reference height for ambient velocity u_0 (m)	Eq. (2.1)
z^R	surface roughness (m)	Eq. (A.1)
α	exponent in power-law fit of ambient wind-speed (-)	Eq. (2.1)
β	exponent in concentration similarity profile (-)	Eq. (2.2)
η_w	mole fraction of water in pollutant (-)	Eq. (2.8)
κ	Von Kármán constant = 0.41 (-)	Eq. (A.1)
λ	Monin-Obukhov length (m)	Eq. (A.1)
$\rho_{amb}(z)$	ground-level density of moist ambient air (kg/m^3)	Eq. (A.10)
$\rho_m(x)$	centre-line ground-level mixture density (kg/m^3)	Sect. 2.2
$\sigma_x(x)$	downwind dispersion coefficient (m)	Eq. (3.13)
$\Phi(Ri_*)$	empirical entrainment function (-)	Eq. (2.11)

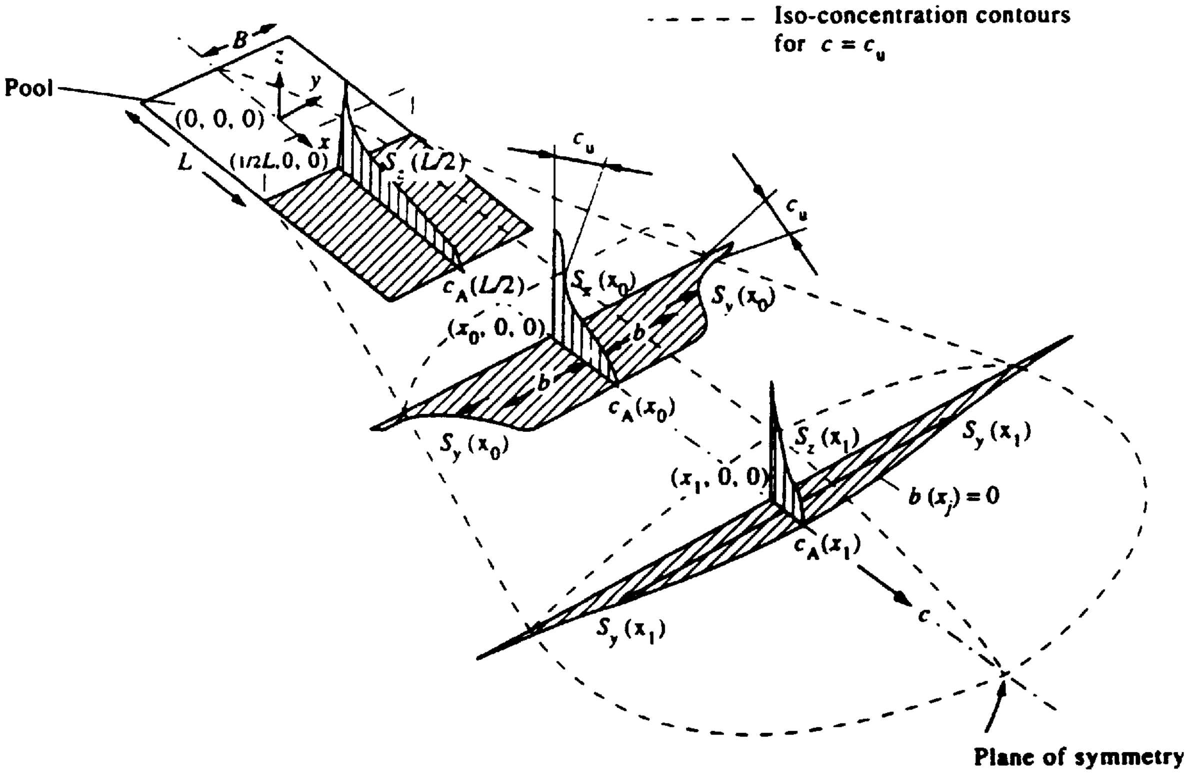

FIG. 1 - The HEGADAS similarity profile for the concentration c(x,y,z): c_A is the centre-line ground-level concentration, b the crosswind half-width along which the ground-level concentration equals c_A. S_y the crosswind dispersion coefficient defining the Gaussian decay in concentration at larger crosswind distances, and S_z the vertical dispersion coefficient defining the vertical decay; B is the half-width and L is the length of the ground-level pool. The figure includes also iso-concentration contours (dashed lines) in the planes y=0, z=0, x=1/2L, $x=x_0$ and $x=x_1$

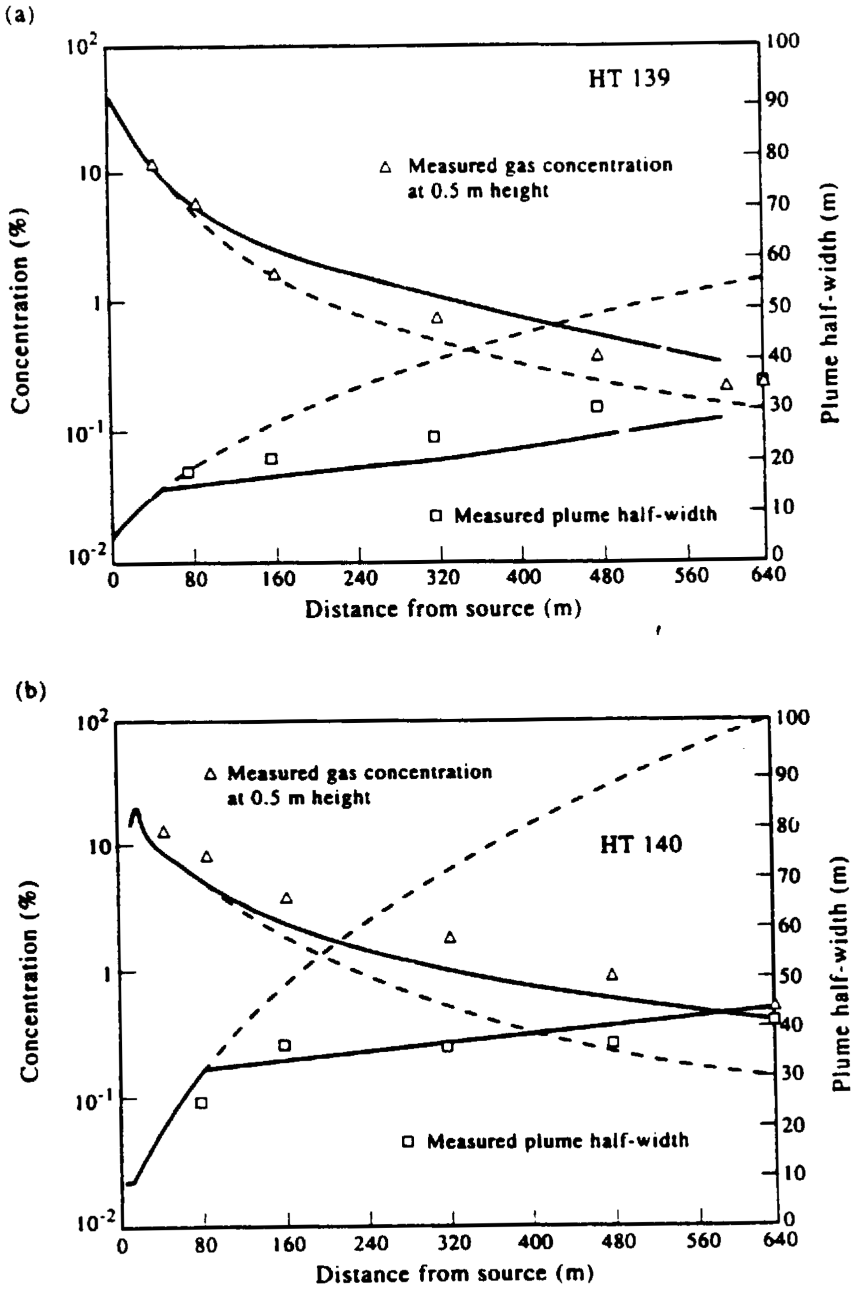

FIG. 2 - Effect of changing the gravity-spreading formulation in HEGADAS to describe the plume spread observed in the HTAG dispersion experiments (see McFarlane et al. (1990)). The dashed lines show the plume widths and centre-line concentrations predicted by the HEGADAS-4 model. The HTAG data (squares) shows a sharp reduction in the plume spread at about 80 m. The solid lines show the revised HEGADAS-5 model predictions that take this into account;
(a) surface roughness = 0.03 m, gas/air density ratio = 1.4,
(b) surface roughness = 0.03 m, gas/air density ratio = 3.9.

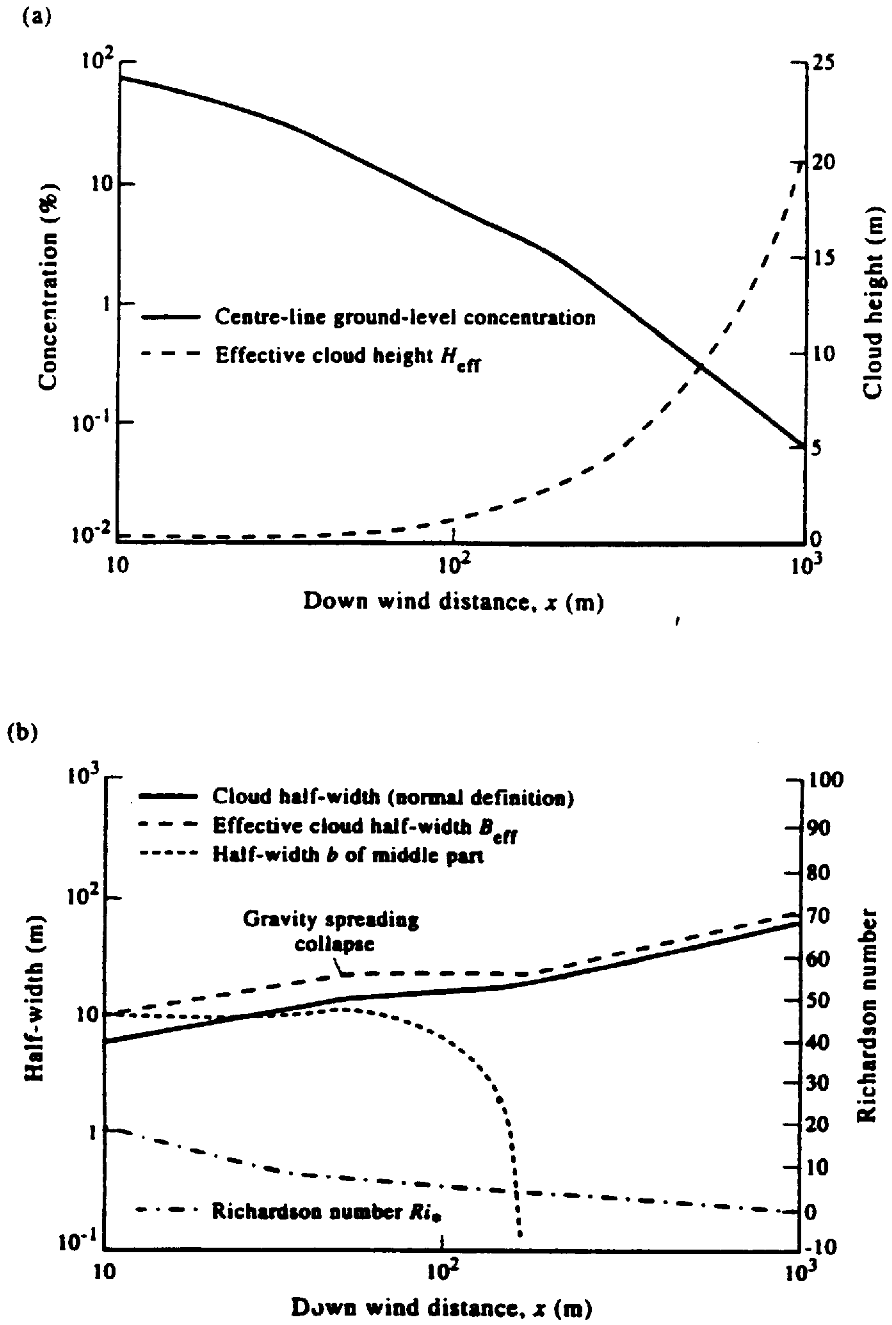

FIG. 3 - HEGADAS-S dispersion predictions from ground-level pool of propane located at x=0 (evaporation rate E = 32 kg/s):
(a) centre-line ground-level concentration (molar fraction),
(b) cloud half-width, effective half-width B_{eff}, and half-width b of uniform section of concentration profile

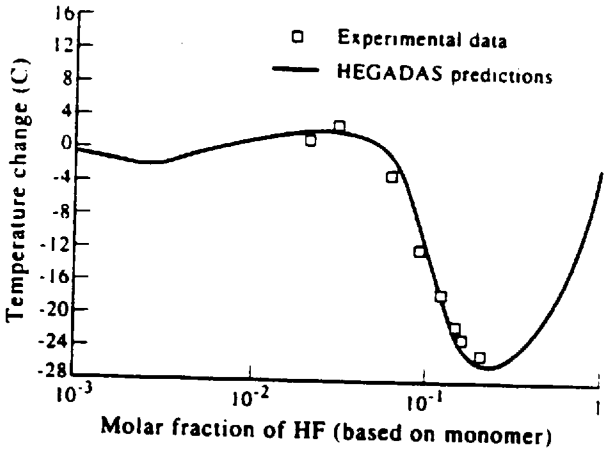

FIG. 4 - Mixing of anhydrous HF with moist air (relative humidity = 50%) at 26°C: experimental data from Schotte (1987) and HEGADAS-5 predictions of change in temperature $\Delta T = T - 26$ as a function of the molar fraction y_{pol} of HF

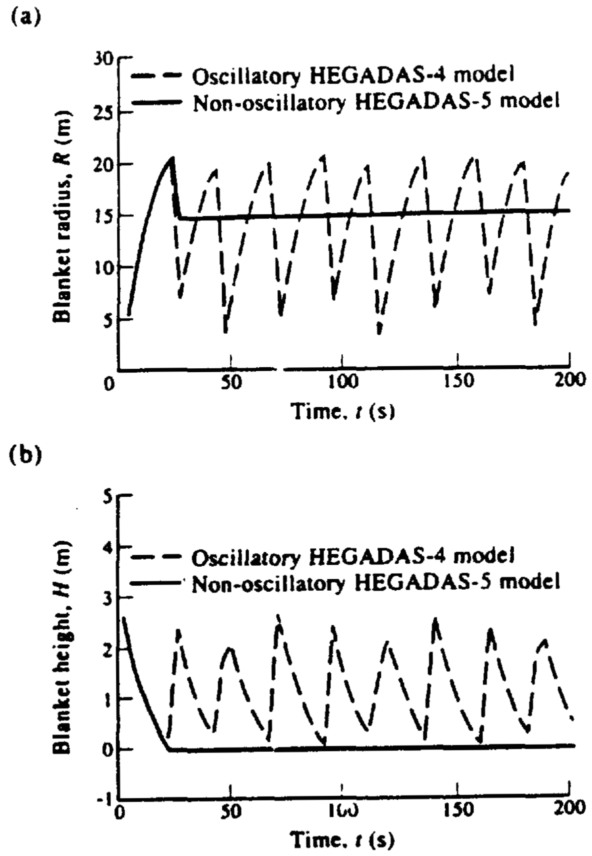

FIG. 5 - Vapour source from a boiling propane pool of radius $R_p = 3$ m. evaporation rate $E = 30$ kg/s and spill duration = 200 seconds; gas-blanket predictions by HEGADAS-4 and HEGADAS-5 models;

(a) blanket radius R_g (t)

(b) blanket height H_g (t)

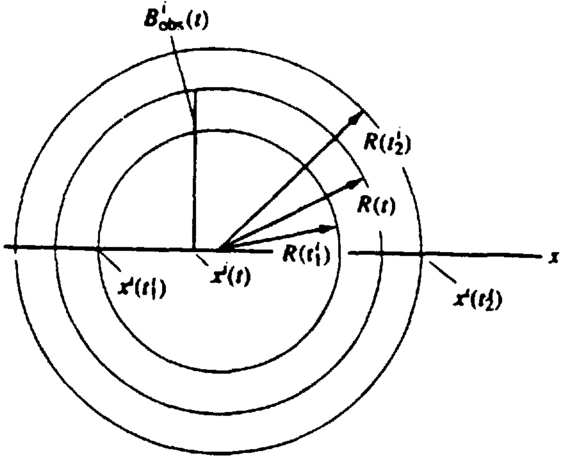

FIG. 6 - Movement of observer i over time-dependent secondary source. Observer i passes over the upwind and downwind edges of the source at times $t=t^i_1$ and $t=t^i_2$. At time t ($t^i_1<t<t^i_2$), observer i is located at $x^i(t)$, and sees a source width $B^i_{obs}(t) = [R^2(t) - x^i(t)x^i(t)]^{1/2}$, and a source flux Q(t)

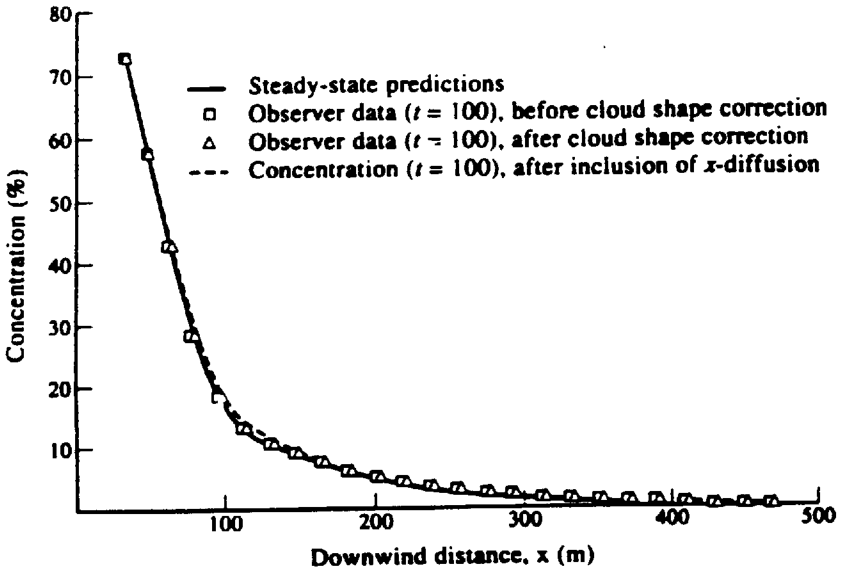

FIG. 7 - HEGADAS-T predictions of centre-line ground-level concentration (% molar fraction) at time t = 100 s for finite-duration steady flow of propane through the transition plane x_{tr} = 30 m . (propane flow E(t) = 32 kg/s, 0<t<100) and HEGADAS-S predictions for corresponding steady flow (E = 32 kg/s)

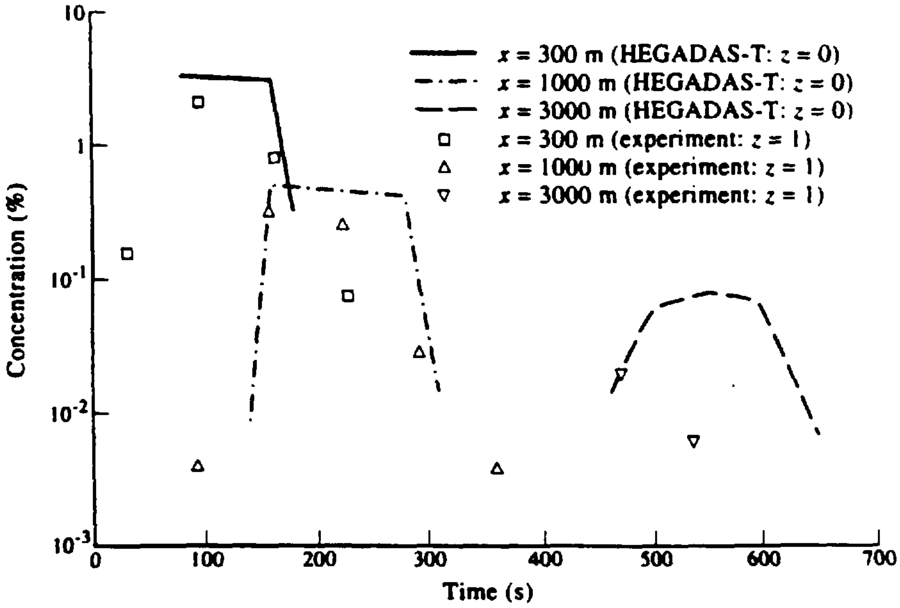

FIG. 8 - HEGADAS-T simulation of Goldfish 1 experiment (steady pressurised release of anhydrous HF for 125 seconds); HEGADAS-T simulation is started from transition plane at 188 m with transition data derived from the near-source model HFPLUME. Experimental data at 3000 m are too low, since the centre-line of the plume was not aligned with the line on which the concentration measurements were made

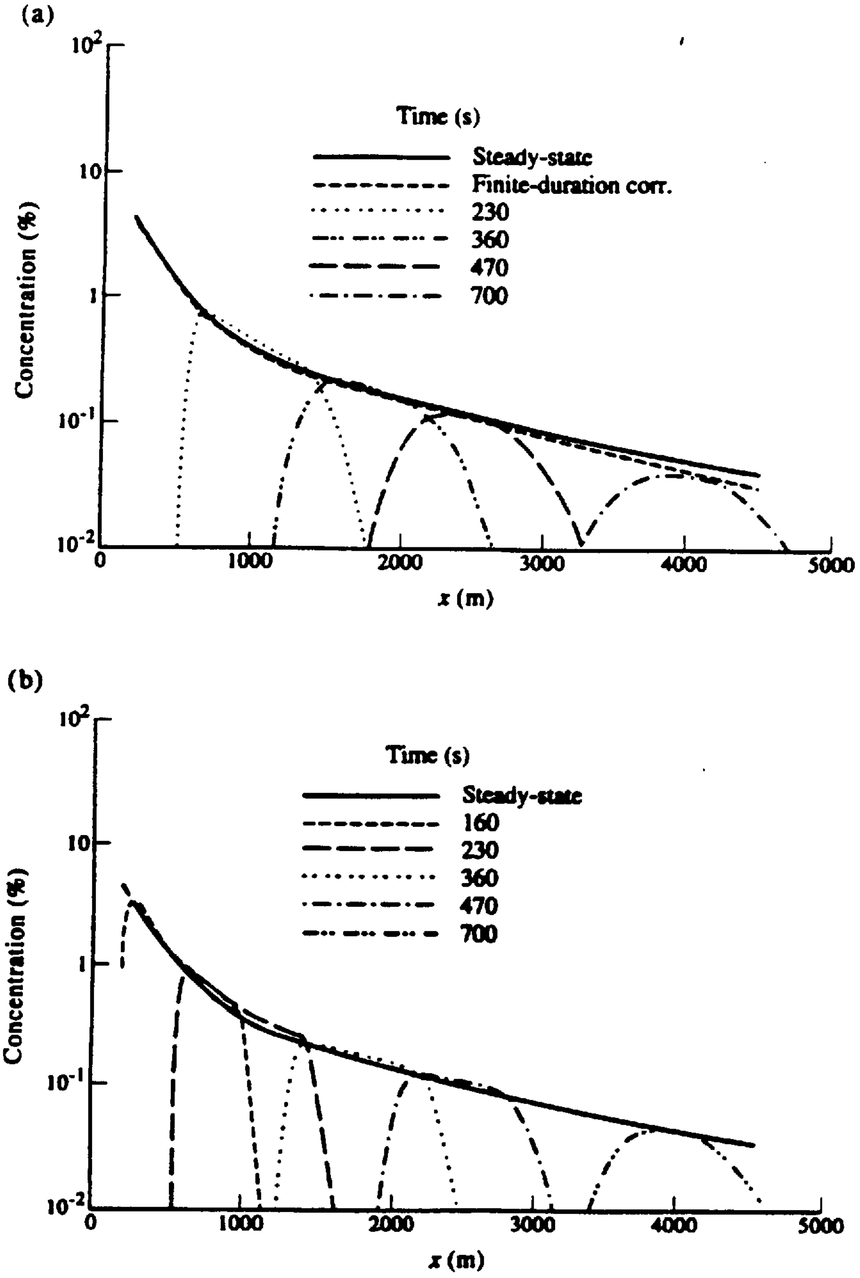

FIG. 9 - HEGADAS simulation of Goldfish 1 experiment (HF-release rate of E = 27 kg/s for 125 seconds; HFPLUME/HEGADAS transition data at 188 m). Comparison of HEGADAS-S steady-state predictions, HEGADAS-S/HSPOST steady-state predictions with finite-duration error-function correction and HEGADAS-T time-dependent predictions:
(a) use of adapted Ermak's σ_x - formulation in HEGADAS-T
(b) use of adapted Chatwin's σ_x - formulation in HEGADAS-T

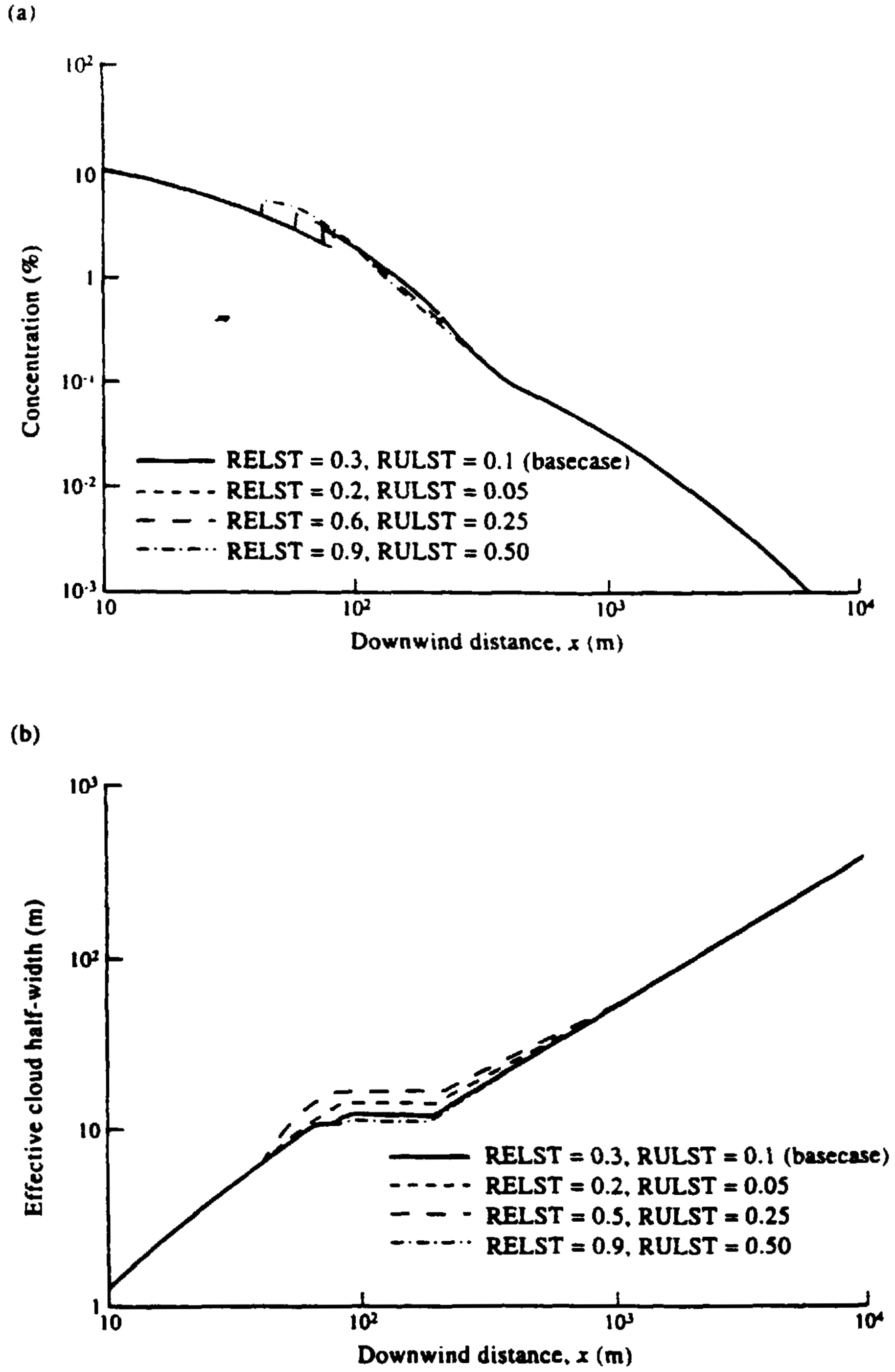

FIG. 10 - Steady pressurised release of HF under typical rural conditions: effect of variation of HFPLUME/HEGADAS-S transition criteria: transition from HFPLUME to HEGADAS-S is made if the proportion of heavy-gas entrainment in the total entrainment is larger than (1-RELST)*100% and the difference in plume speed and ambient speed is less than RULST*100%: recommended values are RELST = 0.03 and RULST = 0.1:

(a) centre-line concentration (% molar fraction: HFPLUME sectional-mean value and HEGADAS value at ground-level)

(b) effective half-width B_{eff} of cloud

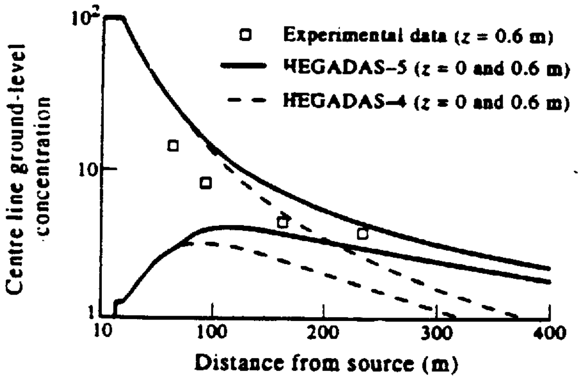

FIG. 11 - Steady dispersion of propane over water (Maplin Spill 54). HEGADAS-4 and HEGADAS-5 predictions of centre-line ground-level concentration (% molar fraction)

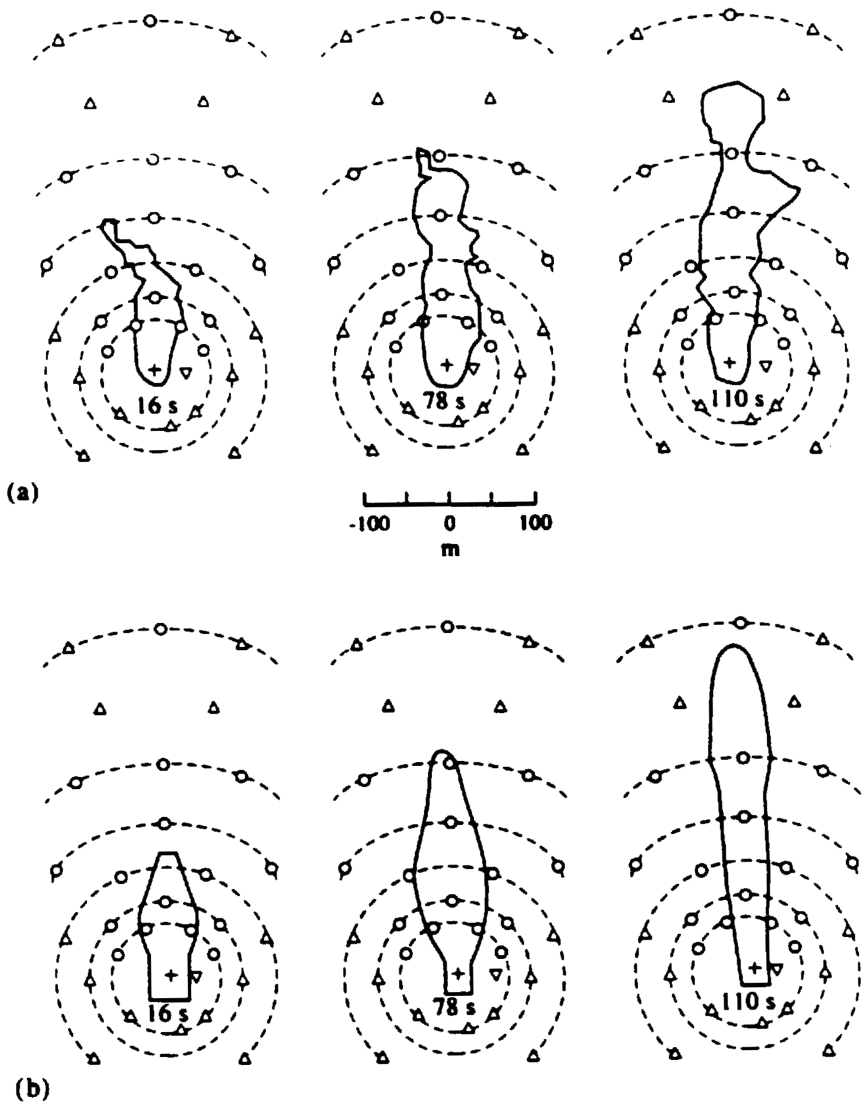

FIG. 12 - Time-dependent dispersion of LNG over water (Maplin Spill 22; relase of 10 m^3): 3% concentration contours
(a) experimental data at times t = 16, 78 and 110 s
(b) HEGADAS-4-T predictions at times t = 16, 78 and 110 s

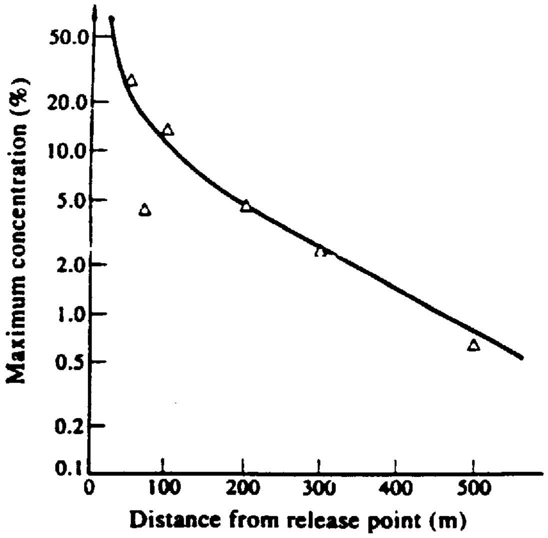

FIG. 13 - Instantaneous release of Freon (Thorney Island trial 15): observed peak concentrations at 0.4 m height versus HEGABOX/HEGADAS centre-line ground-level predictions

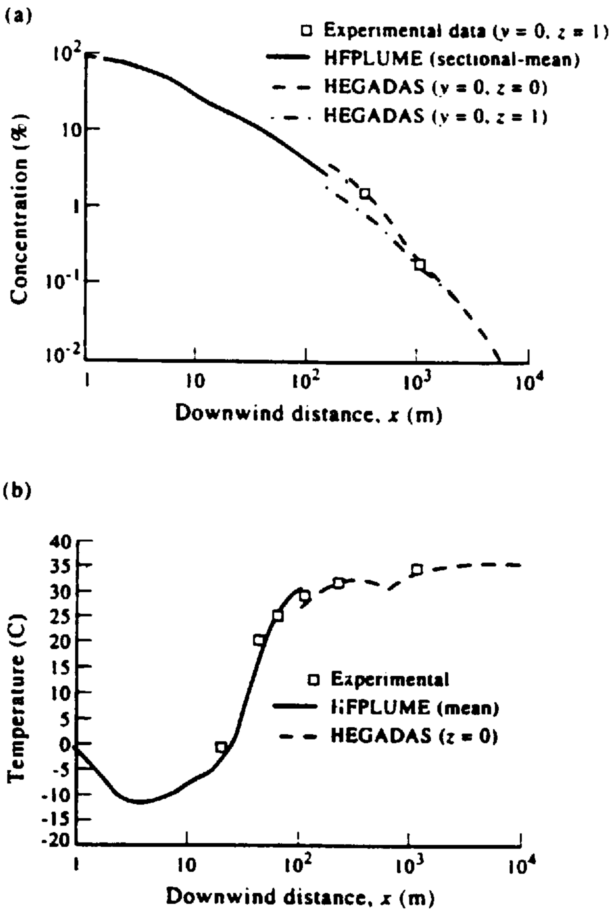

FIG. 14 - Simulation of Goldfish 3 experiment (steady pressurised release of anhydrous HF) by the near-source model HFPLUME and the heavy-gas-dispersion model HEGADAS-S;
(a) centre-line concentration
(b) temperature

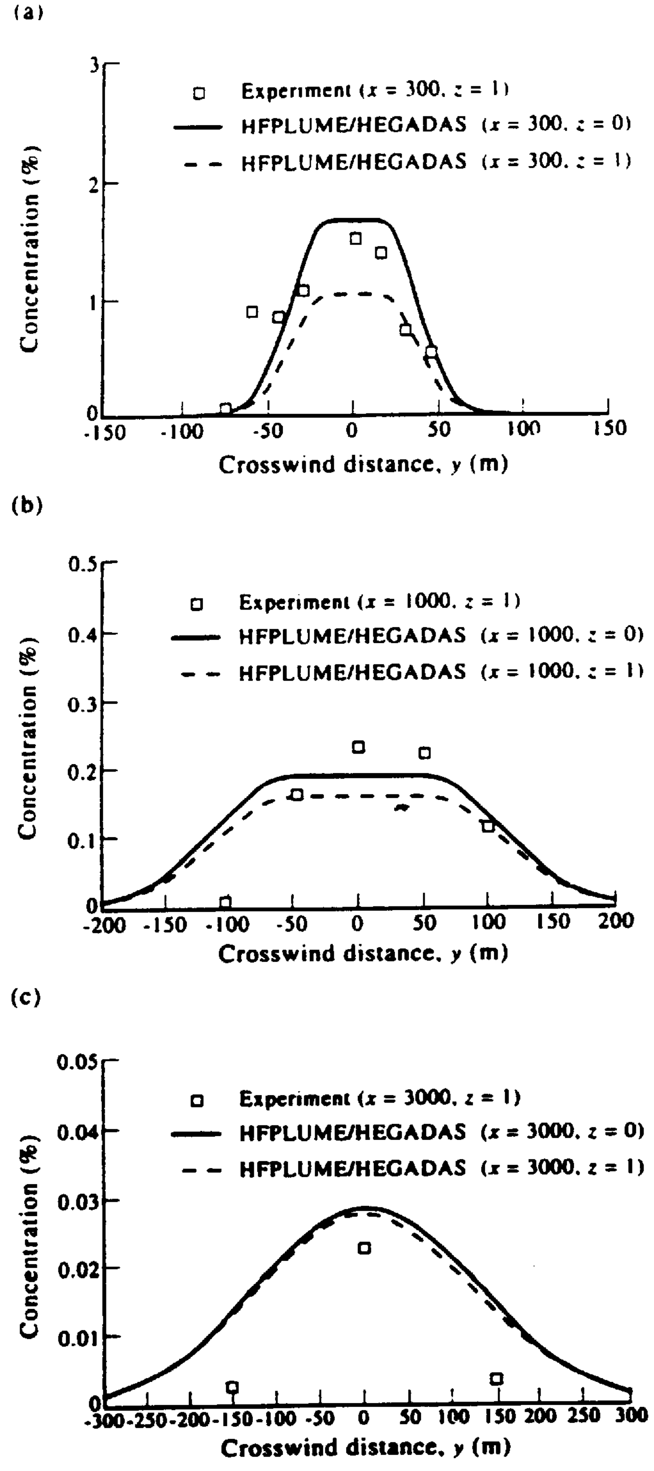

FIG. 15- HEGADAS predictions of crosswind ground-level concentration profile for Goldfish 3 experiment 3 at downwind distances of (a) 300 m, (b) 1000 m and (c) 3000 m

Appendix 7.A.A - Evaluation of ambient data

This Appendix describes the evaluation of the ambient data which are required in the dispersion calculations in HEGADAS.

WIND-SPEED PROFILE

The wind velocity in the atmospheric surface layer as a function of height z is taken from the following formula given by Businger (1973) and revised by Wieringa (1980),

$$u_a(z) = \frac{u_*}{\kappa} \cdot \left[\ln\left(\frac{z + z_R}{z_R} \right) - \Psi_m\left(\frac{z}{\lambda} \right) \right] \tag{A.1}$$

where u_* is the ambient friction velocity, z_R the surface roughness, $\kappa = 0.41$ the Von Kármán constant and λ the Monin-Obukhov length; $\Psi_m(z/\lambda)$ is given by the following formulas for stable ($\lambda > 0$) and unstable ($\lambda < 0$) conditions:

$$\Psi_m\left(\frac{z}{\lambda} \right) = \begin{cases} -6.9 \cdot \dfrac{z}{\lambda} & (\lambda > 0) \\ 2 \cdot \ln[\tfrac{1}{2}(1+a)] + \ln[\tfrac{1}{2}(1+a^2)] - 2 \cdot \tan^{-1}(a) + \tfrac{1}{2}\pi & (\lambda < 0) \end{cases} \tag{A.2}$$

with $a=(1 - 22 \cdot z/\lambda)^{1/4}$. Expression (A.1) is used directly in calculating u_* for given $u(z = z_0) = u_0$. Subsequently the exponent α in the HEGADAS power-law (2.1) is determined from the best fit with the ambient wind velocity (A.1). This matching is performed by means of least square fitting with a weighting function $w(z)=[1 + 10 \cdot z/z_0]^{-1}$, i.e. by minimising the functional

$$f(\alpha) = \int_0^{2z_0} w(z) \cdot \left[u_0 \cdot (z/z_0)^{\alpha} - u_a(z) \right]^2 dz \tag{A.3}$$

over α.

TEMPERATURE AND DENSITY PROFILES

The potential temperature Θ (Kelvin) in the atmospheric surface layer as a function of height z is taken from the following formula given by Paulson (1970) and revised by Wieringa (1980),

$$\Theta - \Theta(z=0) = \frac{\Theta_*}{\kappa}\cdot\left[\ln\left(\frac{z+z_R}{z_R}\right) - \Psi_h\left(\frac{z}{\lambda}\right)\right] \qquad \text{(A.4)}$$

with

$$\Psi_h\left(\frac{z}{\lambda}\right) = \begin{cases} -9.2\cdot\dfrac{z}{\lambda} & (\lambda > 0) \\ 2\ln[\tfrac{1}{2}+\tfrac{1}{2}\cdot\left(1-13\cdot\dfrac{z}{\lambda}\right)^{\frac{1}{2}}] & (\lambda < 0) \end{cases} \qquad \text{(A.5)}$$

$$\Theta_* = -\overline{u_z T'} / u_* = u_*^2 T / [g\kappa\lambda] \qquad \text{(A.6)}$$

In the above formula T (Kelvin) is the ambient temperature at height z, T' is the turbulent fluctuation of T, u' is the turbulent fluctuation of u and the over-bar signifies an average over the turbulent fluctuations.

The potential temperature Θ is the temperature of the ambient air if it was brought adiabatically from the ambient pressure P to the pressure P_0 = 1 bar; Θ is related to the ambient temperature T by

$$\Theta = T\cdot(P_0/P)^{R/C_p^a} = T\cdot(P_0/P)^{0.2852} \qquad \text{(A.7)}$$

where R = 8314.3 J/K/kmole is the gas constant and C_p^a = 29120 J/K/kmole the specific heat of air. [Note. In HEGADAS the pressure P always equals 1 atmosphere, implying that $P_0 \approx P$ and $\Theta \approx T$].

Using equations (A.7) and (A.6) into (A.4) the following expression is obtained for the temperature profile in the atmospheric surface layer

$$T = T(z=0) / \left[1 - \frac{u_*^2}{\kappa^2\cdot g\cdot\lambda\cdot(P_0/P)^{0.2852}}\cdot\left[\ln\left(\frac{z+z_R}{z_R}\right) - \Psi_h\left(\frac{z}{\lambda}\right)\right]\right] \qquad \text{(A.8)}$$

Using the ideal-gas law $\rho_{amb}\cdot T = \rho_{amb}(z=0)\cdot T(z=0)$ leads to the following air-density profile,

$$\rho_{amb} = \rho_{amb}(z=0)\cdot\left[1 - \frac{u_*^2}{\kappa^2\cdot g\cdot\lambda\cdot(P_0/P)^{0.2852}}\cdot\left[\ln\left(\frac{z+z_R}{z_R}\right) - \Psi_h\left(\frac{z}{\lambda}\right)\right]\right] \qquad \text{(A.9)}$$

where the ground-level ambient density $\rho_{amb}(z = 0)$ is found from the ideal-gas law,

$$\rho_{amb}(z=0) = P \cdot m_{amb} / (R \cdot (T_a + 273.15)) \tag{A.10}$$

with T_a (°C) the ambient temperature at ground level and m_{amb} the molecular weight of the humid air (kg/kmole).

MOLECULAR WEIGHT, WATER-VAPOUR PRESSURE AND ENTHALPY

The mole fraction of water in the ambient air is the ratio of the partial water-vapour pressure P_w^{amb} and the total ambient pressure P. Thus the molecular weight in equation (A.10) is defined by

$$m_{amb} = m_a \cdot \left[1 - P_w^{amb} / P\right] + m_w \cdot \left[P_w^{amb} / P\right] \tag{A.11}$$

The partial water-vapour pressure P_w^{amb} is given by

$$P_w^{amb} = r_H \cdot P_v^w(T_a) \tag{A.12}$$

with r_H the ambient humidity ($0 < r_H < 1$) and $P_v^w(T)$ the vapour pressure of water (atm) in 100% humid air at temperature T (°C).

In HEGADAS the formula $P_v(T)$ is taken from Lowe and Ficke (1974) for temperature T between 0 °C and 50 °C, and from an exponential formula for the vapour pressure of ice for T<0,

$$P_v^w(T) = \begin{cases} a_0 + a_1 T + a_2 T^2 + a_3 T^3 + a_4 T^4 + a_5 T^5 + a_6 T^6 & (0 < T < 50) \\ b_1 \exp(-b_2 / (T + 273.15)) & (T < 0) \end{cases} \tag{A.13}$$

where the constants are given by a_0=6.0279, $a_1=4.3785 \cdot 10^{-1}$, $a_2=1.4102 \cdot 10^{-2}$, $a_3=2.6159 \cdot 10^{-4}$, $a_4=2.9916 \cdot 10^{-6}$, $a_5=2.0075 \cdot 10^{-8}$, $a_6=6.0566 \cdot 10^{-11}$, $b_1=3.452 \cdot 10^{7}$ and b_2=6134.

The enthalpy of the moist air (Joule/kmole of moist air) is given by

$$H_{air}^{wet} = \left\{C_p^a \cdot \left(1 - P_w^{amb} / P\right) + C_p^{wv} \cdot \left(P_w^{amb} / P\right)\right\} \cdot (T_a - T^*)$$

where T^* is the reference temperature at which the enthalpy is taken to be zero; T^*=25 °C for the HF thermodynamics model (described in Chapter 2.B) and T^*=0 °C for the ideal-gas thermodynamics model (described in Chapter 2.A).

Appendix 7.A.B - Cross-wind diffusion effects

The derivation of the differential equation for the crosswind dispersion coefficient S_y is based on an empirical formula for the non-dense crosswind dispersion coefficient σ_y.
In HEGADAS-4 this formula is restricted to a power-law dependence of σ_y on the downwind distance x. Thus it does not allow for, for example, Briggs formula, which is more physically reasonable in the far field.

In this Appendix a generalised theoretical formulation for the evaluation of S_y is introduced. This formulation allows for any arbitrary empirical function $\sigma_y = \sigma_y(x)$, provided this function can be inverted to $x = x(\sigma_y)$.
In this section first the general formulation is given. Secondly the formulation is applied to Briggs formula.

BASIC EQUATIONS AND ASSUMPTIONS

The following basic equations and assumptions are adopted.

1. The crosswind concentration distribution used to describe passive dispersion is considered,

$$c = c_A \cdot \exp\left\{-\frac{1}{2}\cdot\left(\frac{y}{\sigma_y}\right)^2\right\} \tag{B.1}$$

   in which c_A is the centre-line concentration and σ_y is the crosswind dispersion coefficient.

2. The crosswind dispersion coefficient σ_y is assumed to be known as an invertible, empirical function of the downwind distance x,

$$\sigma_y = \sigma_y^e(x) \tag{B.2}$$

   with the inverse

$$x = x^e(\sigma_y) \tag{B.3}$$

3. The concentration profile (B.1) satisfies the simple two-dimensional diffusion equation

$$u_x \frac{\partial c}{\partial x} = \frac{\partial}{\partial y}\left(K_y \cdot \frac{\partial c}{\partial y}\right) \tag{B.4}$$

in which u_x is the horizontal wind speed (independent of x and y) and K_y the crosswind diffusion coefficient. K_y is assumed to be proportional to u_x, with the proportional factor k_y being a (to be determined) function of the cloud half-width $W = (\pi/2)^{1/2}\cdot\sigma_y$,

$$K_y = u_x \cdot k_y = u_x \cdot k_y^e(W) \tag{B.5}$$

REDUCED DIFFUSION EQUATION

Upon insertion of equations (B.1) and (B.5) the diffusion equation (B.4) reduces to

$$\frac{1}{c_A}\cdot\frac{\partial c_A}{\partial x}+\frac{y^2}{\sigma_y^3}\cdot\frac{\partial \sigma_y}{\partial x}=k_y^e(W)\cdot\left\{\frac{y^2}{\sigma_y^4}-\frac{1}{\sigma_y^2}\right\} \tag{B.6}$$

Since the above equation should apply for all y, we deduce the following two equations by equating powers of y,

$$\frac{1}{c_A}\cdot\frac{\partial c_A}{\partial x}=-k_y^e(W)\cdot\frac{1}{\sigma_y^2} \tag{B.7}$$

$$\sigma_y\cdot\frac{\partial \sigma_y}{\partial x}=k_y^e(W) \tag{B.8}$$

The continuity equation,

$$\int_0^\infty u\,c\,dy = \text{constant} \tag{B.9}$$

is by use of equation (B.1) easily seen to lead to $c_A\cdot\sigma_y\cdot u$ = constant. Thus it can be shown that the system of equations (B.7), (B.8) is equivalent to the set of equations (B.9), (B.8). Hence equation (B.7) is not considered further, but attention is restricted to the differential equation (B.8) for σ_y.

By inserting equation (B.2) into equation (B.8), the dependence of k_y on the cloud half-width W can be determined,

$$k_y = k_y^e(W) = \sigma_y\cdot\frac{\partial \sigma_y^e}{\partial x}[x = x^e(\sigma_y)] \qquad \text{with } \sigma_y = \sqrt{2/\pi}\cdot W \tag{B.10}$$

EQUATIONS FOR THE CROSSWIND DISPERSION COEFFICIENT S_y

The derivation of equation (B.8) for the non-dense crosswind dispersion coefficient σ_y is based on the 'pure Gaussian' crosswind concentration profile (B.1).

In the HEGADAS concentration profile (2.2) the crosswind dispersion coefficient S_y corresponds to $2^{1/2}\cdot\sigma_y$; the concentration c is uniform in a middle part of half-width b and it exhibits Gaussian decay for $|y| > b$ only. Therefore in the calculation of S_y in HEGADAS-5 a generalisation of equation (B.8) is adopted for b>0,

$$S_y \cdot \frac{\partial S_y}{\partial x} = 2 \cdot k_y^e(B_{eff}) \tag{B.11}$$

with $B_{eff} = b + W = b + \frac{1}{2}\sqrt{\pi}\cdot S_y$ being the effective half-width of the cloud.

The differential equation (B.11) is applied in HEGADAS for distances downwind of the pool with the middle part of the concentration profile b > 0. Let $x = x_t$ be the downwind distance at which b becomes 0. The following equation is adopted to evaluate S_y for $x > x_t$,

$$S_y(x) = 2^{1/2} \cdot \sigma_y^e(x + x_v) \qquad (b = 0) \tag{B.12}$$

in which x_v is determined from

$$x_t + x_v = x^e\left(\sigma_y = 2^{-1/2} \cdot S_y(x_t)\right) \tag{B.13}$$

EXAMPLE: BRIGGS FORMULA FOR σ_y

Briggs formula and its inverse are given by

$$\begin{gathered} \sigma_y = \sigma_y^e(x) = \frac{\delta \cdot x}{\sqrt{1 + \gamma \cdot x}} \\ x = x^e(\sigma_y) = \frac{\sigma_y^2 \cdot \gamma}{2 \cdot \delta^2} \cdot \left\{ 1 + \sqrt{1 + \left(\frac{2 \cdot \delta}{\gamma \cdot \sigma_y} \right)^2} \right\} \end{gathered} \tag{B.14}$$

Insertion of equation (B.14) into equation (B.8) leads to

$$k_y^e(W) = \frac{2\cdot\delta^2}{\gamma}\cdot\left\{S^{-1} - S^{-2}\right\} \qquad \text{with } S = S^e(W) = 1 + \sqrt{1 + 2\cdot\pi\cdot\left(\frac{\delta}{\gamma\cdot W}\right)^2} \qquad \text{(B.15)}$$

For the option of Briggs formula, the equations for S_y now follow by insertion of equations (B.14), (B.15) into equations (B.11) and (B.12).

Appendix 7.A.C - Inclusion of heat and water-vapour transfer from substrate

This Appendix describes the inclusion into the HEGADAS model of heat and water-vapour transfer from the substrate to the vapour cloud. The user is referred to Section 5 in Appendix 3 of the HGSYSTEM version 1.0 Technical Reference Manual (McFarlane, Prothero, Puttock, Roberts and Witlox, 1990) for further (historical) details and experimental validation.

Heat transfer from the substrate to the gas cloud can be caused by both *natural* convection and *forced* convection. Heat and water vapour effects are included by adding a surface-heat transfer equation and a water-vapour equation for the two additional unknown quantities, i.e. the heat H_e added from the surface (Joule/kmole of mixture) and the water-vapour y_{w3} added from the surface (kmole/kmole of mixture).

C.1. Heat transfer from substrate

The heat transfer equation

$$\frac{1}{2\cdot B_{eff}}\cdot\frac{d}{dx}\left[2\cdot H_e\cdot B_{eff}\cdot H_{eff}\cdot u_{eff}/V_m\right]=Q_H \qquad (C.1)$$

describes the heat flux Q_H transferred from the substrate into the gas cloud (Joule/sec per unit of cloud width and per unit of cloud length).
The term between brackets in equation (C.1) represents the cloud heat flow through the plane x = constant caused by pick-up of heat from the substrate (Joule/sec).

HEGADAS takes into account both the forced heat convection $Q_{H,f}$ and the natural heat convection $Q_{H,n}$.
For a substrate temperature T_s below the cloud temperature T_m the heat flux consists of only forced heat convection, while for $T_s > T_m$ the heat flux is chosen to be the maximum of forced and natural convection,

$$Q_H=\begin{cases}\max[Q_{H,n},Q_{H,f}] & T_s>T_m\\ Q_{H,f} & T_s<T_m\end{cases} \qquad (C.2)$$

FORCED CONVECTION

Holman (1981) formulated the following expression for forced convection flux from the substrate to the vapour cloud,

$$Q_{H,f} = \frac{1}{2}\cdot\left(\frac{\alpha_T}{\nu}\right)^{2/3}\cdot C_f\cdot\rho_m\cdot c_p^m\cdot u\cdot(T_s - T_m) \qquad \text{(C.3)}$$

where α_T is the thermal diffusivity (m^2/s), ν the kinematic viscosity (m^2/s), C_f the friction factor, ρ_m the mixture density (kg/m^3), c_p^m the specific heat of the mixture (J/kg/K), u the gas velocity (m/s), and T_s and T_m the temperatures of substrate and mixture (°C).
For methane $\alpha_T/\nu = 1.35$; for other gases this ratio is only slightly different.
The friction factor $C_f = 2\,(u_*/u)^2$, where u_* is the friction velocity (m/s).
For u we take the logarithmic wind velocity at 10 m height, u_{10}.
Thus expression (C.3) for forced convection heat flux can be rewritten as

$$Q_{H,f} = 1.22\cdot\left(\frac{u_*^2}{u_{10}}\right)^2\cdot\rho_m\cdot c_p^m\cdot(T_s - T_m) \qquad \text{(C.4)}$$

where ρ_m, c_p^m, T_m are mixture properties at centre-line and ground level; c_p^m (J/kg/K) is given by

$$c_p^m = \frac{y_{pol}\cdot\left[(1-\eta_w)\cdot C_p^{dp} + \eta_w\cdot C_p^{wv}\right] + (1-y_{pol})\cdot C_p^a}{y_{pol}\cdot\left[(1-\eta_w)\cdot m_{dp} + \eta_w\cdot m_w\right] + (1-y_{pol})\cdot m_a} \qquad \text{(C.5)}$$

with y_{pol} the ground-level centre-line mole fraction, C_p^{dp},C_p^{wv},C_p^a the molar specific heats (J/kmole/K) and m_{dp}, m_w, m_a (kg/kmole) the molecular weights of dry pollutant, water vapour and air, respectively.

NATURAL CONVECTION

McAdams (1954) formulated the following expression for natural convection flux from the substrate to the cold vapour cloud ($T_s > T_m$),

$$Q_{H,n} = 0.14\cdot\left[\alpha_T^2\cdot\zeta\cdot g\cdot(\rho\cdot c_p)^3/\nu\right]^{1/3}\cdot(T_s - T_m)^{4/3} \qquad \text{(C.6)}$$

where g is the gravitational acceleration (m/s^2), c_p the specific heat (J/kg/K), ρ the density (kg/m^3) and $\zeta = -\rho^{-1}\cdot(\partial\rho/\partial T)_p$.
Using the ideal gas law $P = R\cdot\rho\cdot T/m$ [P = pressure, T = temperature (K), R = gas constant, m = molecular weight], equation (C.6) can be rewritten as

$$Q_{H,n} = 0.14 \cdot g^{1/3} \cdot \frac{P}{R} \cdot \text{HEATGR} \cdot \left[\frac{(T_s - T_m)^2}{T} \right]^{1/3} \tag{C.7}$$

with HEATGR defined by

$$\text{HEATGR} = \left[\left(\frac{\alpha_T}{\nu} \right)^2 \cdot \left(\frac{\nu}{T^2} \right) \cdot \left(m \cdot c_p \right)^3 \right]^{1/3} \tag{C.8}$$

Strictly speaking the value of HEATGR in equation (C.8) should correspond to that of the mixture. Note that the natural convection heat flux given by equation (C.6) is only large if the substrate temperature is considerably lower than the mixture temperature, which can only occur if the concentration of the pollutant is very large. Therefore, for reasons of simplicity, the value of HEATGR is chosen to correspond to that for 100 % dry pollutant.

For methane, propane and air the value of the group equals 24, 29 and 20 $m^{-2/3}s^{-1/3}K^{-5/3}kmole^{-1}J$, respectively.

For T (Kelvin) in expression (C.6) we take the mean temperature 273.15 + $(T_s+T_m)/2$.

In HEGADAS the pressure P is taken to be the standard atmospheric pressure (1 atm = 760 mm Hg).

C.2. Water-vapour transfer from substrate

The water-vapour transfer equation

$$\frac{1}{2 \cdot B_{eff}} \cdot \frac{d}{dx} \left[2 \cdot y_{w3} \cdot B_{eff} \cdot H_{eff} \cdot u_{eff} / V_m \right] = Q_{wv} \tag{C.8}$$

describes the water-vapour flux Q_{wv} transferred from the substrate into the gas cloud (mole/sec per unit of cloud width and per unit of cloud length).

The term between brackets in equation (C.9) represents the molar flow of water through the plane x = constant caused by pick-up of water-vapour from the substrate (mole/sec).

The mechanism by which condensation within the thermal boundary layer can increase the rate of evaporation from a liquid surface has been described by Rosner (1967). Using the theoretical approach of Rosner (1967), Colenbrander and Puttock (1984) derived the following expression for Q_{wv}

$$Q_{wv} = \begin{cases} \dfrac{1}{\Delta} \cdot \dfrac{P_v^w(T_s) - P_v^w(T_m)}{c_p^m \cdot T_s \cdot P} \cdot Q_H & T_s > T_m \\ 0 & T_s < T_m \end{cases} \tag{C.10}$$

with $\Delta = 0.2$, P_v^w the vapour pressure of water given by equation (A.13) and c_p^m the specific heat of the mixture (Joule/kg/K) given by equation (C.5).

C.3. Effect of substrate water-vapour and heat transfer on entrainment

In the entrainment law (2.9),

$$\frac{1}{2 \cdot B_{eff}} \cdot \frac{d}{dx}\left[2 \cdot B_{eff} \cdot H_{eff} \cdot u_{eff} / V_m\right] = u_e(U_T) / V_0 + Q_{wv} \qquad (C.11)$$

the friction velocity u_* has been modified into u_T in order to take into account air entrainment caused by convective advents due to the temperature difference between the substrate and a cold vapour cloud.

Following Eidsvik (1980) u_T is taken to be

$$u_T = \sqrt{u_*^2 + (a \cdot w_*)^2} \qquad \text{with } a = 0.2 \qquad (C.12)$$

with the velocity scale w_* a velocity scale for characterising the turbulence in a free convection layer,

$$w_* = \left[\frac{g \cdot Q_H \cdot H_{eff}}{T_m \cdot \rho_m \cdot C_{pm}}\right]^{1/3} \qquad (C.13)$$

The value $a = 0.2$ was found by comparing HEGADAS against experimental data.

Appendix 7.A.D - Evaluation of pollutant enthalpy

This Appendix discusses the evaluation of the pollutant enthalpy H_{pol} (Joule/mole of pollutant); H_{pol} is required as input parameter to the hydrogen fluoride (HF) and multi-compound two-phase aerosol thermodynamic models as discussed in Chapter 2.A and 2.B.

The pollutant enthalpy is determined by the pollutant temperature, the pollutant composition and the pollutant pressure. HEGADAS assumes the total pressure P always be equal to the ambient pressure, and therefore the pollutant pressure is assumed to be equal to the ambient pressure. Therefore for pressurised releases the pollutant temperature and the pollutant composition should correspond to the thermodynamic state immediately following depressurisation or (in the case of flashing) the post-flash state.

AEROSOL THERMODYNAMICS MODEL

For the aerosol thermodynamics model (Chapter 2.A), the pollutant consists of dry pollutant and water. In addition, the model allows for the inclusion of liquid water initially picked up from the substrate by the pollutant at the source.

Thus the pollutant is defined by the following input parameters.

- pollutant temperature, T_{pol} (°C)
- mole fraction of water originally in pollutant (at temperature T_{pol}), η_{wp}
- mole fraction of liquid water pick-up (at substrate temperature T_s), η_{ws}

Thus the total mole fraction of water in the pollutant equals $\eta_w = \eta_{wp} + \eta_{ws}$.

The water originally present in the pollutant may consist of vapour, liquid and/or ice. Let η_{wpv}, η_{wpl}, η_{wpi} be the mole fractions of original water vapour, liquid and ice, respectively, then $\eta_{wp} = \eta_{wpv} + \eta_{wpl} + \eta_{wpi}$ and

$$\eta_{wpv} = \min\left\{\eta_{wp}, (1-\eta_{wp})\cdot P_v^w(T_{pol})/P\right\} \qquad \text{(D.1)}$$

$$\begin{aligned} &\eta_{wpl} = \eta_{wp} - \eta_{wpv}, \quad \eta_{wpi} = 0 \qquad (T_{pol} > 0) \\ &\eta_{wpi} = \eta_{wp} - \eta_{wpv}, \quad \eta_{wpl} = 0 \qquad (T_{pol} < 0) \end{aligned} \qquad \text{(D.2)}$$

where the partial vapour pressure of water $P_v^w(T_{pol})$ is defined by equation (A.13).

The pollutant enthalpy equals the sum of the enthalpies for the dry pollutant, the water vapour. liquid and ice original present in the pollutant, and the water liquid pick-up

$$\begin{aligned} H_{pol} = \; & (1 - \eta_w) \cdot C_p^{dp} \cdot T_{pol} + \eta_{wpv} \cdot C_p^{wv} \cdot T_{pol} + \eta_{wpl} \cdot (C_p^{wl} \cdot T_{pol} - H^w_{cond}) + \\ & \eta_{wpi} \cdot (C_p^{wi} \cdot T_{pol} - H^w_{fus}) + \eta_{ws} \cdot (C_p^{wl} \cdot T_s - H^w_{cond}) \end{aligned} \tag{D.3}$$

<u>Note.</u> The HGSYSTEM 1.0 (or NOV90) version of HEGADAS may include liquid water pick-up, but does not allow water to be originally present in the pollutant ($\eta_{wp} = 0$).

HYDROGEN FLUORIDE THERMODYNAMICS MODEL

For the HF thermodynamics model (Chapter 2.B), the released pollutant consists of hydrogen fluoride (HF), an ideal gas (denoted by N-gas) and water. The model does not allow for the inclusion of liquid water pick-up from the substrate. Thus the thermodynamic state of the released pollutant is described by the following input parameters

- pollutant temperature, T_{pol} (°C)
- equivalent mole fraction of water, η_w (based on all HF in monomer state)
- equivalent mole fraction of N-gas, η_N (based on all HF in monomer state)

By applying the thermodynamic equations to the 100 % pollutant ($y_a = 0$, $T_m = T_{pol}$) the composition of the pollutant can be determined; see Chapter 2.B for details.

Subsequently the pollutant enthalpy is determined from the following formula (which is equal to equation (17) from Chapter 2.B)

$$\begin{aligned} H_{pol} = \; & E_{pol}^{kin} + \\ & + \eta_{HFL} \cdot \{ C_p{}^{HFL} \cdot (T_{pol} - T^*) - H_{cond}^{HF} \} + \\ & + \{ \eta_N \cdot \{ C_p{}^{N} \cdot (T_{pol} - T^*) \} + \\ & + [\eta_w - (1 - x_{pol}) \cdot L_{pol}] \, C_p{}^{wv} \cdot (T_{pol} - T^*) + \\ & + [\eta_{HF} - \eta_{HFL} - x_{pol} \cdot L_{pol}] \cdot \{ H_{pol}^{\Delta HF} + C_p{}^{HFV} \cdot (T_{pol} - T^*) \} + \\ & - x_{pol} \cdot L_{pol} \cdot \{ H_{cond}^{HF} + H_{mix} \} + \\ & - (1 - x_{pol}) \cdot L_{pol} \cdot H_{cond}^{w} + \\ & + L_{pol} \cdot \{ C_p^{fog} (x_{pol}, T_{pol}) \cdot (T_{pol} - T^*) \} \end{aligned} \qquad (D.4)$$

<u>Note.</u> The HGSYSTEM 1.0 (or NOV90) version of HEGADAS does not allow for presence of N-gas and/or water in the pollutant, and η_w, η_N, L_{pol} are set equal to zero in equation (D.4).

Appendix 7.A.E - Observer position and observer speed

In order to express the observer dispersion data as a function of position and time, a formula needs to be provided for the position of each observer as a function of time. Ideally the observers should move with the average transport velocity u_{eff} of the vapour molecules (effective cloud speed) defined by equation (2.6).
At a given location x the value of S_z and accordingly u_{eff} differ from observer to observer and consequently some observers may overtake others. Therefore a simplified formula will be introduced which is a function of x only.

The simplified formula is assumed to be based on the two-dimensional case: no cross-wind spreading effects (B_{eff} = constant), a constant Richardson number Ri_*, neglect of heat and water vapour transfer from the substrate ($Q_{wv} = 0$, $Q_H = 0, u_T = u_*$) and a constant mixture volume V_m. For this case the entrainment equation (2.9) can be solved analytically for M_{eff}^{mol}, and subsequent use of equation (2.7) yields the following formula for S_z,

$$S_z = S_z(x) = z_0 \cdot \left\{ \frac{\kappa \cdot \beta \cdot u_* \cdot V_m \cdot (x - x_0)}{\Gamma((1+\alpha)/\beta) \cdot \Phi(Ri_*)\ u_0 \cdot V_0 \cdot z_0} \right\}^{1/(1+\alpha)} \tag{E.1}$$

with x_0 an integration constant.
Insertion of equation (E.1) into equation (2.6) for the effective cloud speed yields the following formula for the observer speed as a function of x,

$$u^{obs} = u^{obs}(x) = C_0 \cdot \left[\frac{(x - x_0)}{z_0} \right]^{\alpha/(1+\alpha)} \tag{E.2}$$

with

$$C_0 = \frac{\Gamma((1+\alpha)/\beta)}{\Gamma(1/\beta)} \cdot u_0 \cdot \left\{ \frac{\kappa \cdot \beta \cdot u_* \cdot V_m}{\Gamma((1+\alpha)/\beta) \cdot \Phi(Ri_*) \cdot u_0 \cdot V_0} \right\}^{\alpha/(1+\alpha)} \tag{E.3}$$

By integrating equation (E.2) to time the following formula for the observer position can be derived

$$x(t) = x_0 + z_0 \cdot \left\{ \left(\frac{x_{st}^{obs} - x_0}{z_0} \right)^{1/(1+\alpha)} + \frac{C_0}{z_0 \cdot (1+\alpha)} \cdot (t - t_{st}^{obs}) \right\}^{1+\alpha} \tag{E.4}$$

with x_{st}^{obs} the downwind distance and t_{st}^{obs} the time, at which the observer is released (where $x(t=t_{st}^{obs}) = x_{st}^{obs}$).

It now remains to evaluate the constants x_0 and C_0 in the above equations.

DISPERSION FROM GROUND-LEVEL POOL

The observers are released at $x = x_{st}^{obs} = -R_{max}$, where R_{max} is the maximum radius of the secondary source R(t). The following two assumptions are now made:

1. At the point of release the observer speed equals zero,

$$u^{obs}(x = x_{st}^{obs} = -R_{max}) = 0 \qquad \text{(E.5)}$$

2. Let R_m be the radius of the secondary source when the take-up rate $\pi R^2 Q$ is maximum, and let $S_z(x=\frac{1}{2}\pi^{\frac{1}{2}}R_m;\ E=\pi R^2 Q,\ B=\frac{1}{2}\pi^{\frac{1}{2}}R_m,\ L=\pi^{\frac{1}{2}}R_m)$ be the value of S_z at the downwind edge of a steady-state square source of strength $E = \pi R^2 Q$, half-width $B = \frac{1}{2}\pi^{\frac{1}{2}}R_m$ and length $L = \pi^{\frac{1}{2}}R_m$.
   The observer velocity at $x = \frac{1}{2}\pi^{\frac{1}{2}}R_m$ is then taken to be the effective cloud speed for this steady source at $x = \frac{1}{2}\pi^{\frac{1}{2}}R_m$.
   Using equation (2.6) it is found that

$$u^{obs}(x = \tfrac{1}{2}\sqrt{\pi}\cdot R_m) = u_0 \cdot \frac{\Gamma((1+\alpha)/\beta)}{\Gamma(1/\beta)} \cdot \left[\frac{S_z\left(x = \frac{1}{2}\sqrt{\pi}\cdot R_m\right)}{z_0}\right]^{\alpha} \qquad \text{(E.6)}$$

Imposing the assumptions (E.5) and (E.6) upon (E.2) leads to

$$x_0 = -R_{max} \qquad \text{(E.7)}$$

$$C_0 = u_0 \cdot \frac{\Gamma((1+\alpha)/\beta)}{\Gamma(1/\beta)} \cdot \left[\frac{S_z\left(x = \frac{1}{2}\sqrt{\pi}\cdot R_m\right)}{z_0}\right]^{\alpha} \cdot \left[\frac{\frac{1}{2}\sqrt{\pi}\cdot R_m + R_{max}}{z_0}\right]^{-\alpha/(1+\alpha)} \qquad \text{(E.8)}$$

DISPERSION FROM VERTICAL TRANSITION PLANE (BREAKPOINT)

The observers are released at the transition plane (breakpoint) $x = x_{st}^{obs} = x_{br}$. The constant x_0 is first determined by matching at $x = x_{br}$ equation (E.2) for the observer speed against a typical value of u_{eff} derived from the breakpoint data. Subsequently the constant C_0 is determined.

The effective cloud speed u_{eff} can be set from equation (2.6) and the value of S_z calculated at the breakpoint $x = x_{br}$. However the latter value for S_z varies from observer to observer. Therefore to arrive at a fixed value, the value of S_z is chosen to correspond to the breakpoint value $S_z^{br}(t_m)$ at the time t_m when the gas-flow rate $E_{br}(t)$ is maximum. The value for u_{eff} thus obtained from equation (2.6) is now assumed to be the value of the observer speed at x_{br}.

$$u^{obs}(x_{br}) = u_0 \cdot \frac{\Gamma((1+\alpha)/\beta)}{\Gamma(1/\beta)} \cdot \left\{ \frac{S_z^{br}(t_m)}{z_0} \right\}^{\alpha} \qquad \text{(E.9)}$$

Thus by inserting equation (E.9) into (E.12) it follows that

$$x_0 = x_{br} - z_0 \cdot \left\{ \frac{u_0 \cdot \Gamma((1+\alpha)/\beta)}{C_0 \cdot \Gamma(1/\beta)} \right\}^{(1+\alpha)/\alpha} \cdot \left\{ \frac{S_z^{br}(t_m)}{z_0} \right\}^{1+\alpha} \qquad \text{(E.10)}$$

The constant C_0 is assumed to be defined by equation (E.3) with $V_m = V_0$ and with Ri_* assumed to be value of the Richardson number at the breakpoint at time t_m, i.e. $Ri_* = Ri_*^{br}(t_m)$.

Appendix 7.A.F - Cloud shape correction for downwind gravity spreading

In low wind velocities HEGADAS simulations of time-dependent spills show considerable gravitational spreading of high density vapour clouds (e.g. propane) after the initial slumping of the vapour blanket.

Since the HEGADAS model allows for gravitational spreading in the crosswind direction only, the calculated crosswind dimensions are too large and the dimensions in wind direction too small.

As cloud shape becomes a parameter of increasing importance in more refined hazard assessment methods, a cloud-shape-correction routine has been designed for the time-dependent HEGADAS computer program. The basic consideration for this correction is that the gravitational spreading velocity should be the same in all directions. The HEGADAS model generates a cloud at a specified point of time consisting of elements (observer intervals) with calculated height, length, width and concentration. These elements retain their length while travelling downwind and spreading in the crosswind direction. Leaving height and concentration unchanged, as well as the product of length and width of each element, the width is reduced and the length increased in such a way that the amount of spreading in the downwind direction of the cloud as a whole equals the spreading in the crosswind direction. A subroutine of the HEGADAS time-dependent computer program contains the mathematical formulation of this correction which is described below.

Let L_c be the calculated cloud length and W_c the cloud width at a specified point at time t, and let W_0 be the initial cloud width.
The cloud width and length is now corrected in such a way that the spreading S in downwind direction equals the spreading in crosswind direction. This means, if L_c^{cor} and W_c^{cor} are defined to be the corrected length and width, that $L_c^{cor} = L_c + S$ and $W_c^{cor} = W_0 + S$.
Conservation of cloud surface area then requires

$$L_c^{cor} \cdot W_c^{cor} = L_c \cdot W_c \qquad \text{or} \qquad (L_c^* + S^*)\cdot(1+S^*) = L_c^* \cdot W_c^* \tag{F.1}$$

with $L_c^* = L_c/W_0$, $W_c^* = W_c/W_0$ and $S^* = S/W_0$.

Given L_c^* and W_c^*, equation (F.1) can be solved for S^*:

$$S^* = -\tfrac{1}{2}(1+L_c^*) + \tfrac{1}{2}\sqrt{(1+L_c^*)^2 + 4\cdot L_c^* \cdot (W_c^* - 1)} \tag{F.2}$$

so that

$$L_c^{corr} / L_c = (L_c^* + S^*) / L_c^* \qquad (F.3)$$

$$W_c^{cor} / W_c = (1 + S^*) / W_c^* \qquad (F.4)$$

Consider now an element i (observer interval) of the cloud with length Δx^i and half-width B^i_{eff}. The element i remains fixed at its location but its length and width are corrected in analogy to the above equations,

$$\Delta x^{cor,i} / \Delta x^i = (L_c^* + S^{*i}) / L_c^* \qquad (F.5)$$

$$B_{eff}^{cor,i} / B_{eff}^i = (1 + S^{*i}) / W_c^{*i} \qquad (F.6)$$

with

$$S^{*i} = -\tfrac{1}{2}(1 + L_c^*) + \tfrac{1}{2}\sqrt{(1 + L_c^*)^2 + 4 \cdot L_c^* \cdot (W_c^{*i} - 1)} \qquad (F.7)$$

$$W_c^{*i} = B_{eff}^i / B_{eff,0}^i \qquad (F.8)$$

with $B^i_{eff,0}$ the initial effective cloud half-width for element i.

Again, these correction formulae satisfy the essential condition of conservation of element surface area: $\Delta x^{cor,i} \cdot B_{eff}^{cor,i} = \Delta x^i \cdot B^i_{eff}$.

Let t_j be the j^{th} output time specified by the user. Let observer i be the observer released at time $t^i_{st} = t_{st} + i \cdot \Delta t_{obs}$ (i = 1,2,...), and let x_j^i be the downwind position of observer i at time t_j.

Let the observers i_j^L, i_j^R ($i_j^L > i_j^R$) be the observers which at time t_j see some gas ($y^i_{pol,j} > 0$) and which are located most upwind ('left') and downwind ('right'), respectively.

Let observer i_j^M be the observer with the maximum concentration (maximum value for $y^i_{pol,j}$; if the maximum is found in more than one element, the one located furthest from the source is chosen).

The corrected downwind positions and crosswind dispersion data at time k for observer i are denoted by $x_i^{cor,k}$, $b_i^{cor,k}$ and $S_{y,i}^{cor,k}$.

The algorithm for the cloud-shape correction adopted in HEGADAS is described below for the cases of a ground-level pool and a transition plane, consecutively.

DISPERSION FROM GROUND-LEVEL POOL

1. Set the initial cloud width W_0 equal to the maximum diameter of the gas blanket above the source. Set the initial half-width $B^i_{eff,0}$ for observer i (i = 1,2,....) equal to the half-width B_i of the source seen by the observer (see equation (3.12)).

2. Loop over the specified output times t_j (j = 1,2,....):
   a Determine observers IL = i_j^L, IR = i_j^R, IM = i_j^M (IL > IM > IR).
   Set cloud length $L_c = (x^k_{IR} - x^k_{IL})$. Set $L_c^* = L_c/W_0$.

   b Loop over the observers i = IL, IL-1, ..., IR+1, IR:

   - If $b_j^i > 0$ set $W_c^{*i} = B^i_{eff,j}/B^i_{eff,0}$ else $W_c^{*i} = 1$ (see equation (F.8)).
   - Set S^{*i} from equation (F.7).
   - Correct crosswind dispersion parameters for observer i by applying equation (F.6) to both the middle part and the Gaussian flanks of the crosswind concentration profile: $b_j^{cor,i}/b_j^i = S^{cor,i}_{y,j} / S^i_{y,j} = (1+S^{*i})/W_c^{*i}$.
     This implies that no correction is applied since $W_c^{*i} = 1$, $S^{*i} = 0$ if $b_j^i = 0$.

   c The cloud shape correction is started at observer IM:

   - Fix downwind location of observer IM: $x_j^{cor,IM} = x_j^{IM}$.
   - Apply cloud shape correction (F.5) consecutively for observers i = IM-1,IM-2,..,IL to set corrected observer positions downwind of x_j^{IM}:
     $$x_j^{cor,i} = x_j^{cor,i+1} + (x_j^i - x_j^{i+1})\cdot(L_c^* + S^{*i})/L_c^*$$
   - Apply cloud shape correction (F.5) consecutively for observers i = IM+1,IM+2,..,IR to set corrected observer positions upwind of x_j^{IM}:
     $$x_j^{cor,i} = x_j^{cor,i-1} - (x_j^{i-1} - x_j^i)(L_c^* + S^{*i})/L_c^*$$

DISPERSION FROM VERTICAL TRANSITION PLANE (BREAKPOINT)

1. Set the initial cloud width W_0 equal to the maximum cloud width specified at the breakpoint. Set the initial effective half-width $B^i_{eff,0}$ for observer i (i = 1,2,....) equal to the effective cloud half-width $B^{br}_{eff}(t^i_{st})$ seen by the observer at the transition plane.

2. Loop over the specified output times t_j (j = 1,2,....):

   a see point 2a for case of dispersion from ground-level pool b see point 2b for case of dispersion from ground-level pool

c The cloud shape correction is started at the most upwind observer IL:

- Fix downwind location of observer IL: $x_j^{cor,IL} = x_j^{IL}$.
- Apply cloud shape correction (F.5) consecutively for observers i = IL-1,IL-2,..,IR to set corrected observer positions downwind of x_j^{IL}:
  $$x_j^{cor,i} = x_j^{cor,i+1} + (x_j^{i} - x_j^{i+1})\cdot(L_c^{*}+S^{*i})/L_c^{*}$$

If the output time t_k equals the time $i\cdot\Delta t$ at which the present observer i is released at the breakpoint, it follows from the above that $W^{*i} = 1$, $S^{*i} = 0$, IL = i.
Thus the crosswind dispersion parameters b, S_y and the downwind position x remain unchanged. This implies that the conditions at the breakpoint x_{br} remain satisfied during the cloud shape correction.

7.B. PLUME SPREAD AND AIR ENTRAINMENT FORMULATION

7.B.1. Introduction

This chapter describes changes made to the HEGADAS model following a review of the treatment of lateral plume growth for dense clouds. The changes apply to the transition region where density effects become less important and turbulence increasingly determines the rate of plume spread. A concomitant change to the HEGADAS entrainment assumptions is described.

7.B.2. Plume spread and entrainment in HEGADAS

As described in section 7.A.2.3. the HEGADAS model assumes that a dense gas cloud passes through *three stages of lateral cloud growth.*

Initially the cloud spreads as a *gravity current* at a rate given by equation 7.A.2.12a (equation 2.12a in chapter 7.A.). The gravity current then *collapses* and the plume spreads slowly according to equation 7.A.2.12c which is developed assuming that flow is still driven by gravitational effects. Lastly, lateral plume growth is determined by *turbulent diffusion* and is described by empirical correlations based on field experiments, equation 7.A.2.13*.

The gravity current and slow spreading zones are sharply delineated by a phenomenon which is named *gravity current collapse*. The possibility of gravity current collapse was suggested by a comparison (Roberts (1990)) of HEGADAS predictions against some wind tunnel experiments carried out by Petersen and Ratcliff (1989). This comparison showed that the measured plume widths were much narrower than those predicted by HEGADAS. Petersen and Ratcliff (1989) themselves obtained similar results when comparing their data with other dense gas models (SLAB, DEGADIS). Conversely, the dense gas models *underpredicted* gas concentrations.

A semi-empirical correlation was developed for the onset of collapse using the wind tunnel data together with results from some lock-exchange experiments carried out by Linden and Simpson (1988) to investigate frontogenesis. Frontogenesis is one process by which gravity currents form in the atmosphere and ocean and is characterised by the sharpening of horizontal density gradients and increasing vertical density stratification. Linden and Simpson (1988) showed that mechanical stirring which destroyed the vertical density stratification in a gravity current caused the propagation speed to drop. It was hypothesised by us that this could be the cause of gravity current collapse in the wind tunnel when boundary layer turbulence provides the required vertical mixing. The correlation developed by us is given by equation 7.A.2.12b.

The mechanism that triggers the gravity current collapse is still not clearly understood. We hypothesised that some external event destroyed the leading edge of the current, converting the flow into one driven by a horizontal hydrostatic pressure gradient similar to that characterising the lock exchange experiments. This uncertainty is reflected in the empiricism of equation 7.A.2.12b, which also lacks a clear physical interpretation. We now recognise that this semi-empirical formula (7.A.2.12b) can be rewritten as:

$$\frac{u_e \cdot B_{eff}}{u_g \cdot H_{eff}} \geq \text{constant} \qquad (1)$$

where we have substituted the gravity spreading velocity, $u_g = \frac{dB_{eff}}{dt}$, (equation 7.A.2.12a) and entrainment velocity, u_e, (equation 7.A.2.10), in place of the explicit dependencies on the Richardson numbers (Ri and Ri_*).

The left hand side of equation (1) is a measure of the rate of volumetric addition of air (per unit downwind distance) into a cloud of height H_{eff} and width B_{eff} divided by the rate of volumetric growth of the cloud due to lateral gravity spread. When this ratio exceeds unity, the flow of air mixed into the top of the cloud exceeds the increase in cloud volume due to lateral expansion and the cloud height must increase, significantly changing the vertical distribution of dense gas. This process erodes the vertical density stratification within the body of the cloud that is needed to maintain the gravity current.

The criterion (1) is therefore a measure of the destruction of the internal vertical structure of the gravity current by mixing driven by the external turbulence. This is a much more robust and physically plausible interpretation of gravity current collapse than that made previously in which we required a "trigger" to destroy the leading edge.

We have since carried out a series of independent wind-tunnel experiments (Roberts and Hall, 1994), which have confirmed the measurements of Petersen and Ratcliff and established that equation 7.A.2.12b offers an adequate measure of the maximum cloud size attained by gravity spreading. This is therefore retained in the HEGADAS model.

The expression for the rate of cloud spread after gravity current collapse, equation 7.A.2.12c, derives from the analysis of flow due to a horizontal hydrostatic pressure gradient. It is numerically dependent on the wind-tunnel results of Petersen and Ratcliff through the constant C_D and, when applied to full scale problems the cloud spreading velocity (dB_{eff}/dt) appears overly small compared to characteristic turbulence velocities (u_*). Equation 7.A.2.12c assumes that the flow is due to gravitational influences, and while this is true to the original HEGADAS assumptions, it has the incorrect asymptotic behaviour in the far-field, tending to vanish as Ri → 0 whereas we should require that:

$$\frac{dB_{eff}}{dx} \rightarrow \frac{d\sigma_y}{dx} \quad \text{as Ri} \rightarrow 0 \tag{2}$$

On both of these grounds the formulation is unsatisfactory; equation 7.A.2.12c must have a limited range of applicability and should be replaced. The replacement must satisfy the initial conditions that dB_{eff}/dx be small after gravity current collapse, asymptote to $d\sigma_y/dx$ for large x and permit development of the HEGADAS concentration profile as discussed below. The formulation must give similar numerical results to 7.A.2.12c when used for wind-tunnel calculations.

We note that, for the wind-tunnel experiments used to set the value of C_D, dB_{eff}/dx was everywhere numerically similar to the values of $d\sigma_y/dx$ measured for neutrally buoyant (that is, Ri = 0) releases.

HEGADAS assumes that an initially top-hat concentration profile evolves into a Gaussian profile as set out in equations 7.A.2.2. The edges of the Gaussian plume are of width, S_y, and are assumed to grow according to equation 7.A.2.13. This equation is derived from the cross-wind diffusion equation and assumes a mixing-length eddy diffusivity based on plume width as described in section 7.A.2.3. The properties of this formulation are such that, when the edges join, the plume is entirely Gaussian, $S_y = \sqrt{2}\cdot\sigma_y$ and satisfies the input correlation for σ_y.

The development of the Gaussian edges in HEGADAS is assumed *not* to contribute to the overall plume width (B_{eff}). This is a reasonable assumption if the growth rate of the edges is very small compared to the overall lateral growth rate of the plume, but is inappropriate when turbulent diffusion is the faster process. This instance must arise if the plume is ever to reach a fully Gaussian cross-sectional profile. We therefore now assume that the overall plume width grows in sympathy with the thickness of the mixing layer which forms the Gaussian edge of the plume, and neglect the contribution of the lateral hydrostatic pressure gradient (equation 7A.2.12c).

We take

$$B_{eff} \cdot \frac{dB_{eff}}{dx} = 2 \cdot k_y^{\bullet}(S_y) \qquad (3)$$

by analogy with the model for S_y and with the function $k_y^{\bullet}$ chosen so that when $B_{eff} = \frac{1}{2}\sqrt{\pi} \cdot S_y$ equation (3) becomes identical to equation 7.A.2.13.

This formulation represents a solution to the diffusion equation with a diffusivity based on the mixing layer thickness S_y. It has the correct asymptotic behaviour and ensures that B_{eff} always increases more slowly than S_y so that the HEGADAS concentration profile always evolves to the Gaussian shape. When the input correlation for $\sigma_y(x)$ takes wind-tunnel values the numerical value of (3) is similar to that of equation 7.A.2.12c.

The changed assumptions about the mechanism of plume spread post gravity current collapse require some amendment of the HEGADAS entrainment model.

HEGADAS originally assumed that while the cloud width was prescribed by a gravity spreading equation the only active entrainment process is by mixing through the top of the cloud, equation 7.A.2.9.

This is an *exact* assumption for a gravity current in which there is no mixing across the leading edge and the cloud has a top-hat concentration profile. It is a *poor* assumption when turbulent diffusion acts to broaden the cloud and air is entrained by both lateral and vertical mixing. This was recognised in HEGADAS and was represented by a change in the entrainment equation from:

$$\frac{1}{2 \cdot B_{eff}} \cdot \frac{d}{dx}\left[2 \cdot B_{eff} \cdot H_{eff} \cdot u_{eff} / V_m\right] = u_e(u_T) / V_0 + Q_{wv} \qquad 7.A.2.9$$

which states that the total molar addition of air to the cloud takes place through the upper surface to:

$$\frac{d}{dx}\left[H_{eff} \cdot u_{eff} / V_m\right] = u_e(u_T) / V_0 + Q_{wv} \qquad 7.A.2.9^{*}$$

which represents the molar addition by entrainment per unit width of cloud.

It is implicitly assumed that the increase in the total molar flow due to the increase in plume width with distance arise through separate entrainment processes associated with lateral plume growth.

This change in equation formulation was imposed at the end of the 'gravity' regime which was marked by the attainment of a Gaussian concentration profile.

We previously discussed the evolution of the HEGADAS concentration profile, and identified that it was incorrect to neglect the contribution of lateral diffusion to plume width growth when lateral diffusion was faster than gravity spreading - as it must be for the HEGADAS profile to become Gaussian. In the same way it is incorrect to neglect the entrainment contribution from lateral diffusion. We therefore limit the applicability of equation 7.A.2.9 above to the region where the plume spreads as a gravity current and apply equation 7.A.2.9* everywhere downwind of the point of gravity current collapse.

We note that we could also implement this change by specifying the *additional entrainment* that arises through lateral mixing as a source term in equation 7.A.2.9. We could go further and develop a closure for the plume width B_{eff} based on the entrainment description as an alternative to equation (1).

7.B.3. Illustration of model changes

The effects of these changes to HEGADAS are have been illustrated using two examples which differ in the input correlation for $\sigma_y(x)$. The magnitude of $\sigma_y(x)$ has been doubled by changing the input averaging time. This changes the distance over which the cloud is 'gravity' dominated as well as the width of the cloud in the far-field.

Calculations have been carried out using the original HEGADAS-4 (no gravity current collapse) and HEGADAS-5 (as available in HGSYSTEM version 1.0) to illustrate the effect of the changes. The results shown in figure 1 use an instantaneous averaging time and in figure 2 a ten minute (600 s) averaging time.

Figure 1 compares predictions of plume width (1a) and of centreline concentration (1b) for the original HEGADAS-4 model, for HEGADAS-5 as supplied with HGSYSTEM 1.0 and for the revised model (as available in HGSYSTEM version 3.0) described here.

Figure 1 highlights the very large difference in plume width predictions arising from the assumption of gravity current collapse in HEGADAS-5. The model revisions give slightly greater plume width predictions than HEGADAS-5 near to the slope discontinuity that marks the start of the Gaussian profile, but matches smoothly both at the point of gravity current collapse and in the far-field. The concentration predictions show similar behaviour. The original model (HEGADAS-4) predicts significantly lower concentrations in the near field than HEGADAS-5. The new model gives intermediate concentrations and smoothes the slope discontinuity in the HEGADAS-5 predictions.

Figure 2 shows similar calculations, but now for an averaging time of 600 s. Here the input correlation for σ_y has a larger value so that the point at which the HEGADAS profile becomes Gaussian in the original HEGADAS-4 and HEGADAS-5 models moves upstream. Again the new model gives slightly greater plume-widths and slightly lower concentrations than HEGADAS-5. The difference between the new model and the original HEGADAS-4 predictions is also reduced.

We note that figure 2 shows quite clearly that the slope discontinuities in width and concentration existed in the formulation of the original HEGADAS model and were not artefacts of the HEGADAS-5 (HGSYSTEM version 1.0) version.

7.B.4. References

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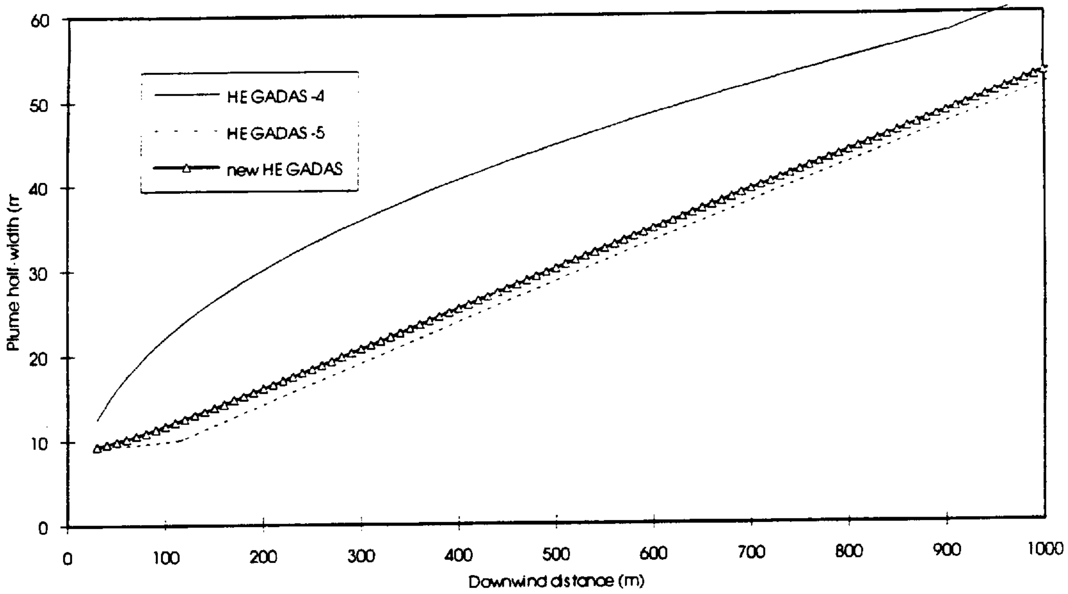

Figure 1a. Comparison of plume half-widths for an instantaneous release.

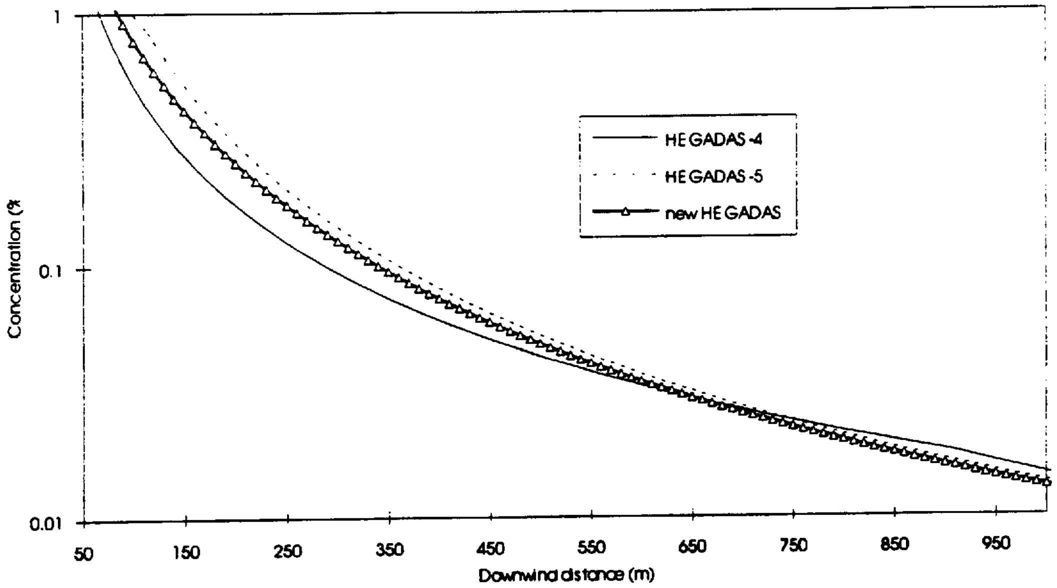

Figure 1b. Comparison of concentration profiles for an instantaneous release.

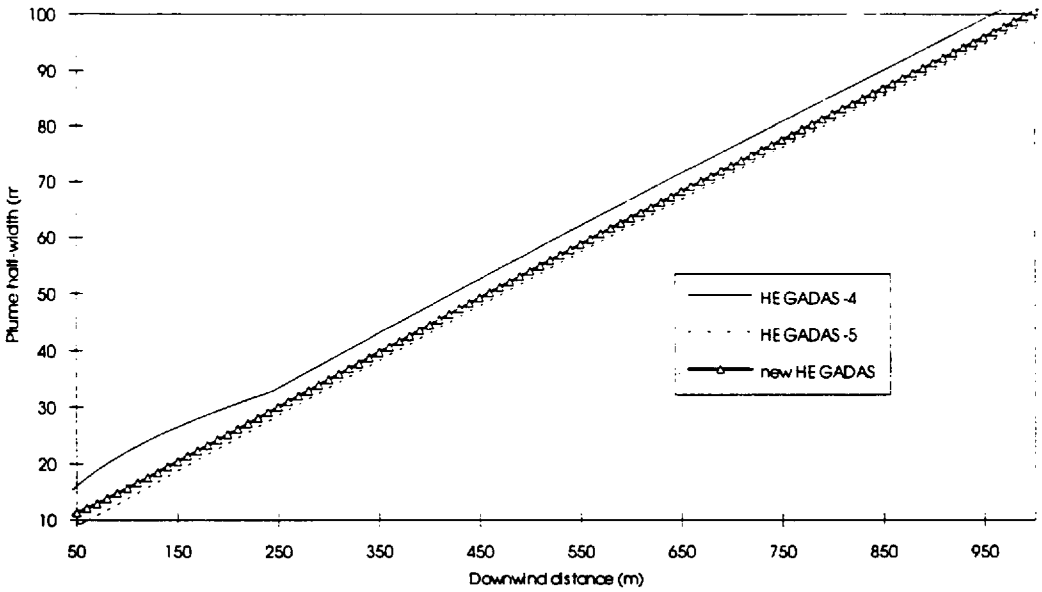

Figure 2a. Comparison of plume half-widths for a 600 s release.

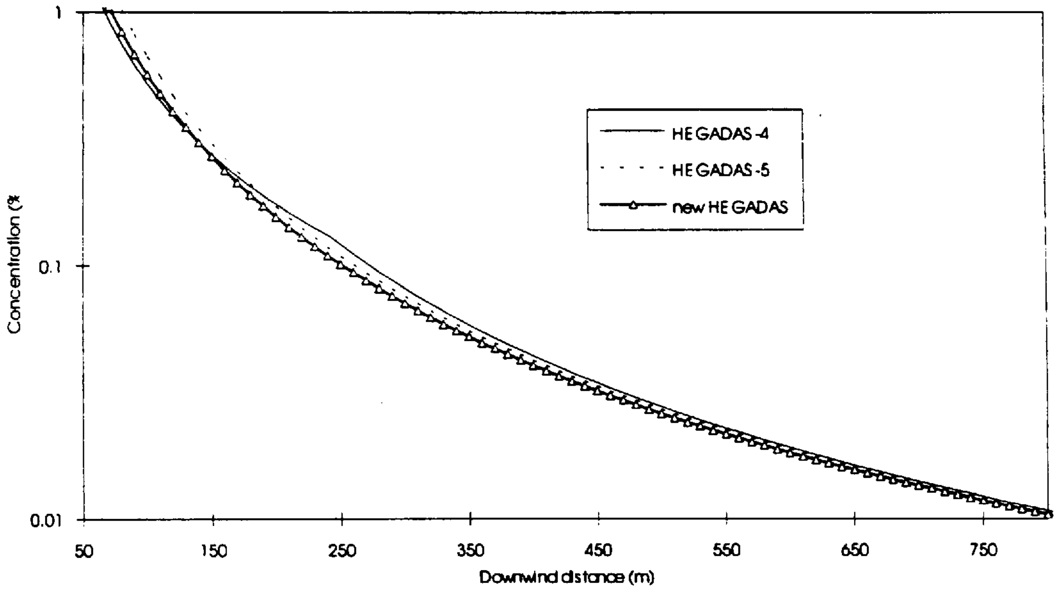

Figure 2b. Comparison of concentration profiles for a 600 s release.

7.C. NEW OPTIONS FOR THE HEGADAS MODEL

This Chapter discusses new options added to the HEGADAS model compared to the descriptions as given in Chapter 7.A. Most options apply to HEGADAS-T only and are intended to make the use of this complicated model more straightforward.

The options are only available in the HEGADAS model as supplied with *version 3.0* of HGSYSTEM and not in the 1.0 version.

7.C.1. Automated output times in HEGADAS-T

7.C.1.1. Introduction

When using the HEGADAS-T model to calculate transient dispersion phenomena, the user can study the results using a concentration versus downwind distance plot. This plot will contain separate concentration versus distance profiles for each requested output time.
These output times are chosen correctly if concentration values for intermediate output times can be calculated accurately enough using linear interpolation.

It usually takes considerable trial and error to find a proper set of output times for a given dispersion scenario. To avoid this time-consuming approach, an algorithm to calculate output times automatically has been developed. Using this algorithm will increase the total run-time per HEGADAS-T calculation, but the user will obtain useful extra information on the quality of the used set of output times. It is envisaged that the user spends a few runs to determine a proper set of output times using the algorithm. Once a suitable set of output times has been found, there is no need to use the algorithm again for similar scenarios.

For *every* run of HEGADAS-T (using the automatic output time algorithm or not), the program prints out information in the report file concerning the quality of the set of output times used. Based on this information, the user can decide to use the automatic generation of output times or not. Note that this information is calculated after taking the effects of along-wind diffusion and cloud shape correction into account.

The option to let HEGADAS-T calculate output times automatically, is available for all three HEGADAS-T scenarios: evaporating pool, post-AEROPLUME run and for a post-HEGABOX run. These cases had to be treated differently in the code.

Before the normal dispersion calculations are performed for all output times and for the required number of observers, the output time algorithm first performs dispersion calculations for a limited set of observers and for a set of three successive output times.
On the basis of the results thus obtained the algorithm decides whether the step between the output times can be increased or not. Then dispersion calculations for the next set of three output times are performed, again for the observer subset.
This process continues until a user-specified last output time has been reached.

The automatic output time algorithm is similar to the observer algorithm as discussed in section 3.2 of Chapter 7.A.

7.C.1.2. Algorithm

In the current implementation of the automatic output time algorithm, a subset of six (6) observers is taken.
For a post-HEGABOX run the total number of observers is always 21. The subset observer indices are 1, 5, 9, 13, 17 and 21. For the other two scenarios a maximum of 161 observers can be used. The subset indices are taken as 1, 33, 65, 97, 129 and 161.

For the selected observer subset, dispersion calculations are performed *only* for the current set of three (consecutive) output times, denoted by t_1, t_2 and t_3. These calculations do not take along-wind diffusion and a cloud shape correction into account.

The initial set of three output times is always taken as $t_1 = t_{first}$, $t_2 = t_{first} + \Delta t$ and $t_3 = t_{first} + 2 \cdot \Delta t$.
Here t_{first} is the user-specified first output time and Δt is the output time step.
As a result for every observer *i* in the subset a value of the ground level concentration for the output times t_1, t_2 and t_3 is found. Let these concentrations be denoted by $c(i,t)$.

To judge whether the time step between two consecutive output times can be increased, the 'exact' value of $c(i,t_2)$ is compared with a value based on *linear interpolation* between the t_1 value $c(i,t_1)$ and the t_3 value $c(i,t_3)$. This is done for all observers *i* in the subset.
Let $c_{inter}(i,t_2)$ denote this interpolated value then

$$c_{inter}(i,t_2) = c(i,t_1) + (t_2 - t_1) \cdot \frac{c(i,t_3) - c(i,t_1)}{t_3 - t_1} \qquad (1)$$

Per observer, an error $E(i)$ is being defined as the (absolute) difference between the value found using linear interpolation, $c_{inter}(i,t_2)$, and the 'exact' value, $c(i,t_2)$, normalised by the maximum concentration for that output time. In other words, $E(i)$ is defined as

$$E(i) = \frac{|c_{inter}(i,t_2) - c(i,t_2)|}{c_{max}(t_2)} \tag{2}$$

where $c_{max}(t_2)$ is defined as

$$c_{max}(t_2) = \max_{i \text{ in subset}} c(i,t_2) \tag{3}$$

Now a *mean error* MEANERR is defined as the average of the $E(i)$'s over all N observers in the subset, where the currently used value of N is 6.

$$\text{MEANERR} = \frac{1}{N} \cdot \sum_{i=1}^{N} E(i) \tag{4}$$

A *maximum* error MAXERR can also be defined as

$$\text{MAXERR} = \max_{i \text{ in subset}} E(i) \tag{5}$$

Using the same error measure as used in the (existing) algorithm for automated observer release, the mean absolute error MEANERR is taken to be the criterion for the automatic output time calculation. This reflects the idea that the *overall curve* should be represented accurately enough.

If MEANERR is *greater* than a pre-set tolerance ε, then the algorithm proceeds with a new set of three output times, where new t_1 value is the old t_2 value and the new t_2 value is the old t_3 value. The new value for t_3 is simply $t_3 + \Delta t$. The dispersion calculations are then repeated for these new output times and a new value for MEANERR is calculated.

If MEANERR is *less* than the tolerance ε, then the output time step Δt is increased by multiplying it with a pre-set factor α. Thus effectively the distance between all output times coming *after* the current ones, is increased. The next set of three output times is found as above. The new value for t_3 is again $t_3 + \Delta t$, but now the *new* (increased) value for Δt is used.

If MEANERR is greater than $3 \cdot \varepsilon$, then a warning message is printed by the program. In this case the user might consider choosing a smaller (initial) value for Δt, a smaller value for α or a larger value for t_{first} (the latter implies that the first cloud print output location will be further away from the source).

For a post-HEGABOX run the number of observers is fixed (21). Therefore with increasing t_{last}, the distance between observers will increase, leading to larger errors. In this case choosing a smaller value for t_{last} will decrease the value of MEANERR.

If the value of MAXERR is too large (larger than $(N-1)\cdot\varepsilon$), then a warning message is printed. Thus the algorithm cycles through sets of three output times, each time judging whether it is possible to increase the time step to be used in the *next* set of output times..
This process stops when either a maximum number of output times has been found (currently this maximum is 20) or when a new output time t_3 exceeds a user-specified last output time t_{last}. The last output time is always taken to be exactly equal to t_{last}, if the maximum number of output times has not been reached yet.

Because of the way the algorithm works, the value of t_{last} must always at least be equal to $t_{first} + 2\cdot\Delta t$. The HEGADAS-T program checks for this and modifies t_{last} if necessary.
For a post-AEROPLUME run or a post-HEGABOX run, t_{first} must always exceed the time at which the transition takes place. The code again checks for this.
After all calculation have been completed by HEGADAS-T, a final check is made where per output time the values of MEANERR and MAXERR are recalculated but now for *all* observers used. The largest value of MEANERR and MAXERR for all used output times are then printed in the report file to serve as a check for the user on the quality of the output time choice.
This information is *always* printed, also when the automatic output times algorithm was not used. Thus the user can decide to use the algorithm in subsequent runs.

7.C.1.3. Implementation

In the HEGADAS-T input file the user can either specify explicit output times using the CALC input block or he can use the option of automatic output times generation using the new input block AUTOTIM .
The user must always specify either the CALC or the AUTOTIM input block, but not both. The HEGADAS-T program will check that precisely one of these two input blocks has been specified.

The AUTOTIM input block has two *mandatory* input parameters, TFIRST and TLAST. TFIRST is the first output time and TLAST the last one.
The value of TLAST should be at least equal to TFIRST + 2·DTMIN, where DTMIN is the initial step Δt between output times.

The user can optionally specify DTMIN. The default value for DTMIN is 20.0 seconds.

It is also optional to specify OTEPS, the tolerance ε used in the algorithm, or OTFACT, the multiplication factor α used in the algorithm. The default value for OTEPS is 0.05 (or 5 %) and the default value for OTFACT is 1.50.

Monitoring and warning messages are printed both to the screen and the report file.
On the basis of this information the user should check whether his current set of parameters for the Δt algorithm is satisfactory or not.

7.C.2. Automatic downwind stepsize in HEGADAS-T

7.C.2.1. Introduction

When using the HEGADAS-T program, dispersion data is reported per output time for a series of equidistant downwind distances. Let Δx be the stepsize between the downwind reporting distances. For small output times, the value of Δx should be small enough to represent the concentration profile correctly. For larger output times, the downwind distances will be larger and larger values for Δx will be sufficient to give an accurate plot of concentration as a function of downwind distance.

In the steady-state program HEGADAS-S it is possible to let the value of Δx become larger with increasing values of downwind distance x. In the transient program HEGADAS-T the value of Δx used to be constant per program run.

A new algorithm implemented in HEGADAS-T to increase the value of Δx for larger output times, while still maintaining a reliable representation of the concentration profile, will be discussed now.

The option to let HEGADAS-T increase the value of Δx automatically is available for all three HEGADAS-T scenarios: evaporating pool, post-AEROPLUME run and for a post-HEGABOX run.

The general idea behind the Δx algorithm is that the value of Δx can be increased if the use of linear interpolation between given ground level concentrations at given downwind distances gives a reliable estimate of the concentration values at intermediate downwind distances.

7.C.2.2. Algorithm

For a given output time, the ground level concentrations are given at a series of N equidistant downwind distances x_{first}, $x_{first} + \Delta x$, $x_{first} + 2\cdot\Delta x$, ... , $x_{last} = x_{first} + (N-1)\cdot\Delta x$, where N is an integer number.
The values of x_{first} and x_{last} are determined by the HEGADAS-T program and are chosen in such a way that concentrations outside the interval $[x_{first}, x_{last}]$ are negligible for the current output time.

Consider all N-2 sets of three consecutive equidistant downwind distances x_1, x_2 and x_3, with $x_1 = x_{first} + (i-1)\cdot\Delta x$, $x_2 = x_{first} + i\cdot\Delta x$ and $x_3 = x_{first} + (i+1)\cdot\Delta x$, for $i = 1, 2, .. N-2$.

Let the ground level concentration at downwind distance x be denoted by c(x). To check whether the stepsize Δx can be increased for the *next* output time, the values of c(x) for all the sets of three values of x are being considered. A given set of three consecutive x values is indexed by $i = 1, 2, .. N-2$, the three concentrations per set are denoted by $c(i,x_1)$, $c(i,x_2)$ and $c(i,x_3)$.

The 'exact' value of $c(i,x_2)$ is compared with a value based on *linear interpolation* between the value at distances x_1 and x_3. Let $c_{inter}(i,x_2)$ denote this interpolated value then

$$c_{inter}(i,x_2) = c(i,x_1) + (x_2 - x_1)\cdot\frac{c(i,x_3) - c(i,x_1)}{x_3 - x_1} \tag{6}$$

Per set of three x values, an error E(*i*) is defined as the absolute difference between the interpolated value $c_{inter}(i,x_2)$ and the 'exact' value $c(i,x_2)$, normalised by the maximum concentration occurring at x_2. The expression for E(*i*) is thus

$$E(i) = \frac{\left|c_{inter}(i,x_2) - c(i,x_2)\right|}{c_{max}(x_2)} \tag{7}$$

with $c_{max}(x_2)$ defined as

$$c_{max}(x_2) = \max_{i=1,\ldots,N-2} c(i,x_2) \tag{8}$$

After calculating the values of E(*i*) for all $i = 1, 2, ..., N-2$, several error measures can be calculated. The *maximum error* MAXERR for the current output time is defined as

$$MAXERR = \max_{i=1,\ldots,N-2} E(i) \tag{9}$$

The *mean error* MEANERR is defined as

$$\mathrm{MEANERR} = \frac{1}{\mathrm{N}-2} \cdot \sum_{i=1}^{\mathrm{N}-2} \mathrm{E}(i) \tag{10}$$

Using the same error measure as in the automatic output time algorithm and as in the automated observer release algorithm, the mean absolute error MEANERR is taken as the criterion for the automatic downwind stepsize algorithm.

Calculations with HEGADAS-T have shown that even for quite smooth concentration curves, with a low MEANERR value, it can happen that E(i) is quite large for a very few i-values. Usually points with a high value for E(i) are at the front and at the end of the gas cloud, where large relative changes in concentration occur because of the steep 'flanks'.

An illustration of this is given in Figure 1, where an example c(i,x) curve has been plotted and relative errors have been given for some i-values. In Figure 1, the mean relative error is 0.015, which is quite low, but the maximum relative error is 0.165, which is 11 times higher. The value for Δx in this example is 0.10 m and N is 48. The maximum concentration used to normalise the errors is 0.0709 kg/m^3 in this example.

This example supports the choice to base the criterion to increase the value of Δx on the value of MEANERR. The value of MAXERR is printed out in the report file to enable the user to monitor the development of the gas cloud profile.

If MEANERR is *greater* than a pre-set tolerance ε, then for the next output time the value of the stepsize Δx is *not* changed.

If MEANERR is *less* than the tolerance ε, then the value of Δx is multiplied by a pre-set factor α. This new value of Δx will be used in the printout of dispersion data for the *next* output time.

If MEANERR is greater than 3·ε, then a warning message is printed by the program. In this case the user might consider choosing a smaller initial value for Δx, a smaller value for α or a larger value for the first output time (the latter implies that the first cloud print output location will be further away from the source).

If the value of MAXERR is found to be very large (larger than (N-1)·ε), then a warning message is printed in the report file.

The HEGADAS-T code will only use the Δx algorithm if, for the current output time, there are at least five consecutive downwind distances where dispersion data is being reported.

7.C.2.3. Implementation

The HEGADAS-T input parameters involved in the Δx algorithm have been added to the already available CLOUD input block.

The parameter XSTEP, default value 10 metre, should now be interpreted as the *initial* value of Δx. The new parameters XSEPS and XSFACT are the tolerance ε and the multiplication factor α respectively. The default value for XSEPS is 0.05.

The default value for XSFACT is 1.0, which indicates to HEGADAS-T that the Δx algorithm is *not* to be used. Thus if the user wants to use the Δx algorithm it is *mandatory* to specify a value for XSFACT not equal to 1.0. A reasonable value for XSFACT when using the algorithm is 1.5.

Monitoring and warning messages are printed to the report file only. On the basis of this information the user should check whether his current set of parameters for the Δx algorithm is satisfactory or not.

Per output time, HEGADAS-T saves the series of reported downwind distances x and ground level concentrations c(x) in two arrays with size ALLMAX. The current value of ALLMAX is 100. For very small (initial) values of Δx, this array size might be too small. Only the first ALLMAX values of x and c(x) are then used in the Δx algorithm. The HEGADAS-T program will print out a warning when ALLMAX is too small and the user can then consider increasing the size of ALLMAX in the HEGADAS-T Fortran code (routine CLOUDC).

7.C.3. Surface roughness breakpoints in HEGADAS-T

7.C.3.1. Introduction

The steady-state heavy gas dispersion program HEGADAS-S allows the user to specify several so-called *breakpoints* using the TRANSIT input block.

A *full* breakpoint occurs when a transition from AEROPLUME to HEGADAS-S is being made. Data from AEROPLUME is made available to HEGADAS-S using the TRANSIT and TIMEDATA input blocks as written to the link file.

The user can also specify a *partial* breakpoint using the TRANSIT block, if at a certain downwind distance he wants to change the value of some variable. The description in the User's Manual of the TRANSIT input block, lists the variables that can currently be reset at a partial breakpoint.

One of these variables is the surface roughness z_r. Thus currently in HEGADAS-S the user can specify a change in surface roughness at a specified downwind distance. This can be done for up to 20 downwind distances; in other words the TRANSIT block can be specified up to 20 times to define a partial breakpoint.

In the transient heavy gas program HEGADAS-T a full breakpoint formulation is available, which is identical to the HEGADAS-S full breakpoint option.

Also for HEGADAS-T, an out-of-date (HEGADAS-4) partial breakpoint formulation was available in HGSYSTEM 1.0, which was not advocated to be used. However, this formulation did not allow the user to change the surface roughness.

To facilitate users wanting to change the surface roughness at downwind locations, a new surface roughness breakpoint formulation has been implemented and at the same time the out-of-date HEGADAS-4 breakpoint formulation has been removed from the HEGADAS code.

HEGADAS-T now allows the user to set multiple breakpoints (up to 20) where the surface roughness can be reset. *Only* the surface roughness can be changed at these breakpoints.

Please note that the provision of this facility is *not* expected to give a simple means of performing accurate simulations of dispersion over a change in surface roughness. See section 7.6.2. in the HGSYSTEM 1.0 Technical Reference Manual for comments on the original HEGADAS-S implementation of surface roughness breakpoints.

The actual implementation of this new roughness breakpoint is not a straightforward task due to the complexity of the transient HEGADAS version.

Although different implementations are necessary for the different HEGADAS-T scenarios, the surface roughness breakpoint option is available for all three HEGADAS-T scenarios: the standard evaporating pool case , a post-AEROPLUME run and a post-HEGABOX run.

7.C.3.2. Algorithm

For every observer used in the HEGADAS-T calculations, a HEGADAS-S dispersion calculation is needed to obtain the total transient dispersion behaviour. Within the steady-state calculation per observer, the change in surface roughness z_r is taken into account in the same way as in HEGADAS-S.

To avoid serious complications, the distances travelled by each observer are calculated using constants based on the *initial* value of z_r.

For values of z_r less than about 0.5 m and for all atmospheric stability classes, a sensitivity study has shown that this simplification has little effect on the calculated observer distances. It is recommended only to use z_r values less than 0.5 m, when specifying a surface roughness breakpoint in HEGADAS-T.

When the surface roughness changes, a large number of other parameters have to be updated. One of these is the Monin-Obukhov length which is a function of surface roughness and stability class.

Normally the HEGADAS code will calculate the Monin-Obukhov length itself and in this case it will be updated automatically when a surface roughness change occurs. Note however, that if the user has *explicitly specified* a certain value for the Monin-Obukhov length, by using he MONIN keyword in the DISP input block, then this value will *not* be updated when the surface roughness changes.

The implementation of the surface roughness breakpoint option in HEGADAS-T has been tested by comparing HEGADAS-T individual observer results with HEGADAS-S results. In these comparisons the cloud correction algorithm was not used.

It should be noted that the post-processor POSTHT in HGSYSTEM version 3.0 uses a constant ALPHA to calculate off-centre, above-ground level concentrations. ALPHA depends on z_r. Although in the dispersion calculations in HEGADAS-T the value of ALPHA is updated when z_r changes, in POSTHT the *initial* value of ALPHA is used. Centre-line, ground level concentrations are computed correctly in POSTHT even when z_r changes.

7.C.3.3. Implementation

To use the new surface roughness breakpoint, the user can specify the TRANSIT input block up to 20 times. In this block the DISTS parameter is mandatory; this parameter specifies the downwind distance at which the breakpoint occurs.

If the user *only* specifies the DISTS parameter, then HEGADAS-T will treat the breakpoint as a *full* breakpoint and additional information must be specified in the TIMEDATA input block. A full breakpoint can only be specified *once*. See the User's Manual for details.

To define a *surface roughness* (partial) breakpoint, in addition to the DISTS parameter, the ZRS parameter must also be given in the TRANSIT block. The ZRS parameter specifies the new value of the surface roughness.

As an example, assume that the user has specified an initial surface roughness of 0.01 m. In other words, the DISP input block contains the line

```
        ZR      = 0.01
```

Now assume that the user wants to change the value of the surface roughness to 0.1 m at a downwind distance of 100 m. The following lines should then be added to the input file

```
TRANSIT

        DISTS = 100

        ZRS   = 0.1
```

Thus in the HEGADAS-T dispersion calculations, for downwind distances less than 100 m, the used value for z_r is 0.01 m and for downwind distances greater than 100 m, the used value of z_r is 0.1 m.

7.C.4. Other new options

7.C.4.1. Volumetric concentrations in CLOUD input block

In the CLOUD input block, three concentrations could be specified. CAMIN is the ground-level centre-line concentration (in kg/m^3) at which calculations will stop. CU and CL are upper and lower concentration limits (in kg/m^3) used in contouring and cumulative cloud data.

Three new parameters, COMIN, CUV and CLV, have been added to the CLOUD block, these being the volumetric counterparts of the existing parameters CAMIN, CU and CL.

COMIN (in vol-%) has the same function as CAMIN.

CUV and **CLV** (both in vol-%) have the same function as CU and CL.

Normally the user should either specify CAMIN or COMIN. If CAMIN and COMIN are both specified, COMIN will be used. If neither CAMIN nor COMIN is specified, then COMIN will be used with a default value. Normally the user should specify either CU or CUV. If CU and CUV are both specified then CUV will be used. If neither CU nor CUV is specified, then CUV will be used with a default value.

Whenever CUV (vol-%) has a value, a value of CU (kg/m^3) is calculated for use in contouring and cloud contents calculations. The calculated value of CU is

$$CU = \frac{CUV}{100} \cdot \frac{MM}{22.4} \cdot \frac{273.15}{273.15+TAP} \tag{11}$$

where MM is the molar mass of the dry pollutant and TAP is the ambient temperature at reference height. Note that this method only gives an *approximate* conversion of the vol-% value CUV to a kg/m^3 value CU but in the far field it will be quite appropriate.

Also note that the only situation where this conversion will be *not* be used, is if CU, *but not* CUV, has been specified by the user.

The CL and CLV parameters are treated analogously to the CU and CUV parameters.

It is not necessary to specify only vol-% or only kg/m^3 values. All combinations of three out of the six parameters are allowed.

The default value for CUV is 2.0 vol-%, for COMIN and CLV the default is 0.1 vol-%. Defaults for CAMIN, CU and CL are no longer relevant: if they are not user-specified, the vol-% counterpart will be used.

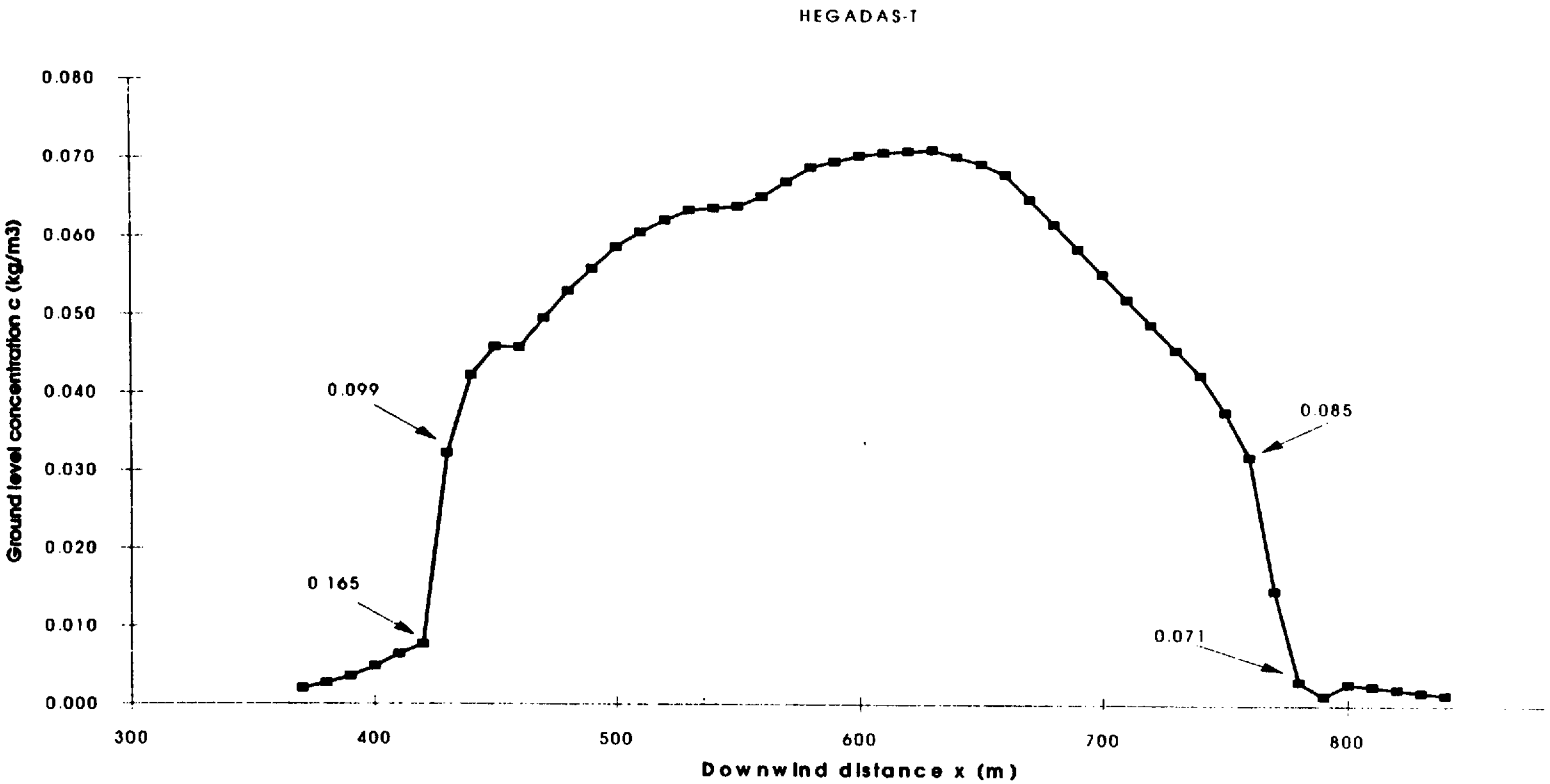

Figure 7.C.1. Example of HEGADAS-T concentration profile. Mean error is 0.015, maximum error is 0.165. Labels indicate individual errors. Maximum concentration 0.0709 kg/m³. Step size Δx is 0.10 m.

8. THE HEGABOX MODEL

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8. THE HEGABOX MODEL

8.1. Introduction

The first public domain release of HGSYSTEM (version 1.0 or NOV90), contained a range of models to simulate the different aspects of an hazardous release. However, a model to describe the initial phase in the spreading of an initially stagnant, dense cloud was not yet available within this first HGSYSTEM version. The second public domain release, HGSYSTEM version 3.0, does now contain such a model, called HEGABOX, and in this chapter some background information for this new HGSYSTEM model will be given.

The HEGABOX box model was available as a stand alone model since it was developed [1,2], but has been incorporated into HGSYSTEM version 3.0, completely analogous to and compatible with the other HGSYSTEM models. HEGABOX is linked with the database program DATAPROP and the far-field time-dependent heavy gas dispersion model HEGADAS-T, both available within HGSYSTEM.

The two standard HGSYSTEM thermodynamical descriptions are available in HEGABOX: a multi-compound, two-phase, non-reactive model and a model containing the full reactive hydrogen fluoride (HF) chemistry and thermodynamics.

In this chapter a global description of the HEGABOX model is given as well as a discussion on its implementation into HGSYSTEM.

8.2. Model description

The HEGABOX model was developed by Puttock to describe the transient dispersion behaviour of instantaneous 'box' releases of heavy gases. Details of model assumptions are given in [1,2], here only a global description is given.

HEGABOX describes the gravity-dominated phase of the dispersion of a suddenly released amount of heavy gas which initially has no momentum of its own. In this phase *slumping* caused by gravity and the (strongly time-dependent) mixing associated with this phenomenon, are dominant. The scenarios which can be simulated using HEGABOX are dense gas releases at low wind speeds or the sudden release of a large quantity of a dense gas

For an instantaneous release or a release at low ambient wind speeds, not only the *gravity-driven lateral spreading* of the cloud is important, but also the *gravity spreading* and *slumping* along the wind direction. The model takes both these effects into account.

HEGABOX assumes the cloud to have a cylindrical shape and the pollutant concentration is assumed to be uniform within the cylinder.

After the release, the cloud radius R will start growing due to the gravity-driven slumping of the dense cloud. The cloud height H will initially decrease (R increases), but eventually H will increase due to *entrainment* of ambient air. Entrainment is caused by the slumping of the cloud (principally at the cloud edge), but there is also entrainment through the top of the cylindrical cloud.

The cloud (bulk) velocity, which is initially zero, will start to increase as momentum from the ambient air is imparted to the cloud. For longer times the cloud will move with the ambient wind speed.

After this initial phase, the influence of ambient turbulence on the pollutant dispersion becomes more and more important with increasing time. Spreading in the wind direction by gravity slumping becomes much less important than the spreading caused by the cloud's own speed, which for longer times will be equal to the ambient wind speed. HEGABOX does not take these effects into account and therefore we should make a transition from HEGABOX to a far-field model to adequately simulate the cloud behaviour for longer times. In HGSYSTEM this model is the transient version of far-field heavy gas model HEGADAS-T.

8.3. Implementation in HGSYSTEM

8.3.1. Thermodynamics

In line with the other major HGSYSTEM modules the pollutant in HEGABOX can be either a non-reactive two-phase mixture consisting of several compounds or a reacting aerosol of HF, water and an inert gas. Pure ideal gas calculations are a special case of the non-reactive aerosol thermodynamical model. It is thought that this flexibility will make it possible to apply HEGABOX simulations to a wide range of pollutant releases.

To facilitate the use of HEGABOX with more complicated pollutant compositions (with or without HF), the HGSYSTEM database program DATAPROP can be used prior to a HEGABOX calculation. DATAPROP produces a link file with HEGABOX input parameters (GASDATA block) in a similar way as it does for other HGSYSTEM modules.

8.3.2. Initial conditions

The initial cloud size for any HEGABOX simulation is determined from fluid properties (using the relevant thermodynamical model), the user-specified spill size and a user-specified initial radius. In calculating the initial cloud size, HEGABOX assumes that all liquid (if any) is dispersed as a fine mist (aerosol) throughout the cloud.

Problems with significant liquid pools on the ground cannot be dealt with, liquid dropout from the cloud to the ground is not being modelled. If the initial cloud composition as found by HEGABOX results in a cloud with a very high liquid fraction then increasing the user-specified initial entrainment (see discussion on input parameters) might be helpful.

In the report file the user can check whether the liquid mole fraction in the cloud exceeds reasonable values. It is the user's responsibility that aerosol liquid fractions are not too high as to violate model assumptions (no dropout, liquid finely dispersed).

The initial cloud temperature has to be specified by the user and it will in general be different from ambient temperature. It could be the result of a flash calculation. The cloud pressure is taken to be equal to the ambient pressure and in HEGABOX (just as in HEGADAS) this is always taken to be 1.0 atm (760 mm Hg).

Heat transfer and convective entrainment are included in a similar way as in HEGADAS.

8.3.3. Transition to far-field model

After calculation of the early stages of the cloud dispersion, HEGABOX has to make a smooth transition to the far-field heavy gas dispersion model available within the HGSYSTEM environment to allow a more accurate and detailed description of the dispersion process for longer times. As the HEGABOX release scenario is strongly time dependent, a transition is made to the transient variant of the HEGADAS model, HEGADAS-T, rather than to the steady state version.

A transition can be made if the influence of gravity-spreading no longer dominates as strongly as in the initial phase compared with the spreading due to the cloud's own velocity. The relevant dimensionless group, comparing the gravity forces with the inertia forces, is the Richardson number (Ri). In general it is defined as

$$\mathrm{Ri} = \frac{g \cdot \Delta\rho \cdot L}{\rho \cdot (\Delta u)^2} \qquad (1)$$

where g is the acceleration of gravity (m/s^2), ρ a density (kg/m^3), Δρ a density difference (kg/m^3), L a length scale (m) and Δu a velocity difference (m/s).

The transition from HEGABOX to HEGADAS-T occurs when the Richardson number based on an internal cloud velocity, drops to a specified value (default value is 10, can be changed by the user). This 'critical' Richardson number Ri* is defined as

$$Ri^* = \frac{g' \cdot H}{(u^*)^2} \tag{2}$$

where g' is the reduced gravity defined by

$$g' = g \cdot \frac{\rho - \rho_a}{\rho_a} \tag{3}$$

where ρ is the cloud density (kg/m^3), ρ_a the ambient density (kg/m^3) and g the acceleration of gravity (m/s^2).
Further in (2), H is the cloud height and u* is an internal velocity scale defined as

$$u^* = \frac{\kappa \cdot U_b}{\log(H/z_r) - 1} \tag{4}$$

where κ is the von Kármán constant (value 0.41), z_r the surface roughness length and U_b the cloud bulk velocity. For more details see [1,2].

Thus the HEGABOX simulation ends when the value of Ri* falls below the pre-set transition value which has a default value of 10. This is the normal way of ending a HEGABOX run.

At the end of each run, HEGABOX prepares a link file which contains input parameters used by HEGADAS-T, completely in line with the normal HGSYSTEM approach. Apart from this link file, HEGABOX also prepares a file containing observer data, which HEGADAS-T needs to continue the dispersion simulation. Details on how the observer data are being calculated and on assumptions made when linking to HEGADAS-T, can be found in [1,2].

A complete simulation, involving consecutive runs of DATAPROP, HEGABOX and HEGADAS-T, can be made using either the interactive environment HGINTER or using HGSYSTEM in the batch mode (for more experienced users) and this can be done for pollutants with or without HF.

8.4. Model validation

When preparing the HGSYSTEM version of HEGABOX, the results of several HEGABOX runs using the original HEGABOX thermodynamic routine were compared with the older mainframe run results and they were found to be close, as they should be. Results are not identical because of updates in HEGADAS-T and the thermodynamical routines. Differences are generally less than 2 %.

Puttock in [1] made a detailed comparison between HEGABOX/HEGADAS-T and the experimental results obtained at Thorney Island. He found a quite good agreement between predictions and experiments.

As the HGSYSTEM implementation for these cases (ideal gas thermodynamics) is principally the same as the model used by Puttock, it is concluded that the current HGSYSTEM models HEGABOX and HEGADAS-T are in very good agreement with the Thorney Island data.

To demonstrate this we take as an example trial number 16, which is a typical Thorney Island run. We only consider HEGABOX results here. Observed data and results of previous HEGABOX runs are taken from [1]. The predicted average cloud speed 8-16 seconds after the release is 1.84 m/s (old mainframe version) or 1.97 m/s for the HGSYSTEM model. The observed value is 1.80 m/s.

We can also look at the distances required for a certain decay of peak pollutant concentration. To reach a concentration of 5 %, the observed distance is 120 m, the old model predicts 157 m and the current HGSYSTEM model predicts 156 m. For a decay to 2.5 %, the experimental distance is 205 m, the old model predicts 243 m and the HGSYSTEM version 242 m. To reach 1 % the observed distance is 370 m, the old model gives a distance of 380 m and the new version predicts a value of 386 m.

For a complete overview of the HEGABOX model performance we refer to [1].

It can be concluded that HGSYSTEM version 3.0 contains a model to simulate near-field dispersion of instantaneous releases, HEGABOX, which has a link to the far-field model HEGADAS-T. The results obtained with these models are in good agreement with experimental observations obtained at Thorney Island.

8.5. References

1. Puttock, J.S., '*Comparison of Thorney Island data with predictions of HEGABOX / HEGADAS*', J. of Hazardous Materials, **16**, 439-455, 1987.
2. Puttock, J.S., '*A model for gravity-dominated dispersion of dense-gas clouds*', Stably stratified flow and dense gas dispersion, Conf. Proceedings, ed. J.S. Puttock, Clarendon Press, Oxford, 1988.

9. TECHNICAL DESCRIPTION OF 'MMES' OPTIONS

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9. TECHNICAL DESCRIPTION OF 'MMES' OPTIONS

This chapter contains a description of five special options for HGSYSTEM that were developed by The Earth Technology Corporation, USA, as part of their work on HGSYSTEM for Martin Marietta Energy Systems Inc and the U.S. Department of Energy.

These options are included in HGSYSTEM because they might be useful to some other users, and are referred to as HGSYSTEM-MMES in the following text.

The five added options are:

1. Removal by dry and wet deposition
2. Plume lift-off
3. Meteorological pre-processor
4. Concentration fluctuations and variations with averaging time
5. Effects of buildings and terrain obstacles

The full technical documentation of the work done by The Earth Technology Corporation is in the report by Hanna, Chang and Zhang (1994). This Chapter is broadly the same as Chapter 6 of the full Earth Technology report (plus relevant references).

For further information and technical support on the options described in this Chapter, the user should consult Earth Technology Corporation, 196 Baker Avenue, Concord, Massachusetts 01742-2167, U.S.A., telephone 508.371.4200, fax 508.371.4280.

9.1. Removal By Dry And Wet Deposition

9.1.1. Overview of Removal Processes

The plume will consist of a mixture of gases, solid particles, and aerosols. Larger particles and aerosols will fall to the ground due to gravitational settling. Smaller particles and aerosols and gases will deposit on the surface due to a process called dry deposition, which is caused by a combination of phenomena such as chemical reactions and physical interception by the ground and vegetation. In the presence of rain, fog, or snow, the pollutant may be removed from the plume and deposited on the ground either by absorption or collection by the water drops or snow flakes. These processes are illustrated in Figure 9-1. Thorough reviews of the topics of dry deposition and wet scavenging are given by Sehmel (1984) and Slinn (1984), respectively.

Models for hazardous gas dispersion (e.g., SLAB, DEGADIS, or HGSYSTEM) generally do not account for dry or wet deposition, since, at distances within a few hundred meters of the source, these processes are significant only for large particles (diameter $D_p > 1000$ μm). Most of the research on dry and wet deposition has been connected with much larger time and space scales (e.g., acid deposition over the North-eastern U.S. over time periods of several days). In addition, there has been concern about deposition of toxic substances such as dioxin which are produced at solid waste incinerators. Consequently, comprehensive wet and dry deposition modules have been built into the EPA's Regional Acid Deposition Model (RADM) and Industrial Source Complex-Version 2 (ISC-2) model.

The original research on wet and dry deposition in the 1950's was spurred by the U.S. Atomic Energy Commission's concern with fallout from nuclear weapons tests and with deposition from fuel production and reprocessing facilities (see Sehmel 1984 and Slinn 1984). The results of this work formed the basis for the models in use today.

9.1.2. Desired Complexity Level in Deposition Algorithms

Martin Marietta's PLM89A model (Bloom et al., 1989) contains some simplified dry and wet deposition formulas. These formulas have been reviewed and some formulas have been added for gravitational settling and wet removal. It is recognized that deposition is a minor component of the conservation equation for most chemicals in the plume, and it is not necessary to account for all the various details of the removal processes. Furthermore, there are large uncertainties in the required input information, such as the size spectrum for the particles formed after a flashing liquid release. Consequently, simplified default methods are suggested. If, in the future, field experiments suggest that certain details must be included, revised formulas can be developed.

The dry deposition formulas are applied as a post-processor in HGSYSTEM-MMES, given the ground level distribution of calculated concentrations. At the moment, it is assumed that there is no feedback between dry deposition and the plume chemistry and thermodynamics.

9.1.3. Removal by Gravitational Settling and Dry Deposition

<u>Gravitational Settling of Large Particles or Aerosols</u>

Large particles or aerosols, with diameter, D_p, greater than about 50 μm (where 1 μm = 10^{-6} m), will have a gravitational settling speed, v_s, of greater than 10 cm/s. In this case, removal is dominated by simple gravitational settling. Stoke's law can be used with a slip correction factor:

$$v_s = \frac{(\rho_p - \rho_{air}) \cdot g \cdot D_p \cdot c_2}{18 \cdot \mu} \cdot S_{CF} \tag{9-1}$$

where,

ρ_p (g/m^3) = particle density
ρ_{air} = air density
g (9.81 m/s^2) = acceleration of gravity
D_p (μm) = particle diameter
μ = 1.81 x 10^{-4} g/cm·s = air viscosity
c_2 = 1 x 10^{-8} cm^2/μm^2 = conversion factor

and S_{CF} is the slip correction factor for larger particles:

$$S_{CF} = 1 + \frac{0.13\cdot\left(1.257+0.4\cdot e^{-8.5\cdot D_p}\right)}{D_p} \tag{9-2}$$

It is implied that a plume of large particles with a given diameter, D_p will fall away from the gaseous part of the plume with a speed of v_s, as illustrated in Figure 9-2. The vertical distance 'fallen' by the particle plume relative to the remainder of the gas plume at downwind distance, x, is given by $v_s x/u$. This is called the 'tilted plume' model in the literature. It is assumed that the tilted plume has the same shape as the remainder of the gas plume, but is displaced downward due to the settling of the particles.

The large particles are modelled in HGSYSTEM-MMES by the following steps:

1) Assume that the large particles can be divided into a few size classes, where each size class is characterized by a diameter, D_p, and a concentration, $C(D_p)$. The particle plume is assumed not to affect the remainder of the plume.

2) The local particle deposition flux to the ground is given by

$$F_{D_p} = v_s\, C(D_p,x,y,0) \tag{9-3}$$

where $C(D_p,x,y,0)$ refers to the ground level concentration of that size class of particles at position (x,y) of the tilted plume.

Dry Deposition of Small Particles and Gases

Aside from the large particles, the remaining components of the plume (gas, small particles, and aerosol) do not have appreciable settling velocities. For example, in an HF plume the HF·H_2O compound is assumed by the current version of the model to be in the gas phase. But even if this compound were in the liquid phase, the $HF \cdot H_2O$ aerosol drops would have diameters typical of natural fogs (about 1 to 10 μm). Consequently, standard dry deposition formulas can be used to calculate the deposition to the ground surface. Also, because we are primarily interested in distances within a few hundred meters of the source, and because it is desirable in the plume thermodynamics algorithms that no mass be removed from the plume, it is assumed that the mass removal due to dry deposition is insignificant when compared to the total mass flux in the plume.

The dry deposition formula that is proposed is based on that in the EPA's revised ISC2 model, and is similar to that used in the PLM89A model by Bloom et al. (1989). Most state-of-the-art deposition models now use the resistance analogy, where the deposition velocity is assumed to be inversely proportional to the sum of a set of resistances, as expressed below:

$$v_d = \frac{1}{r_a + r_s + r_t} + v_s \tag{9-4}$$

where v_s is the gravitational settling speed, which is non-zero for particles (see equations 9-1 and 9-2) and is zero for gases.

The resistances have the following definitions:

r_a (s/m) - aerodynamic resistance
r_s (s/m) - surface or laminar layer resistance
r_t (s/m) - transfer resistance dependent on surface characteristics.

The aerodynamic resistance term is the same for both gases and small particles:

$$r_a = \frac{1}{0.4\, u_*}\left(\left(\ln\left(\frac{z_d}{z_o}\right) - \Psi_H\left(\frac{z_d}{L}\right)\right)\right) \tag{9-5}$$

where u_* is friction velocity, L is Monin-Obukhov length, z_d is reference height (assumed to equal 10 m) and the function ψ_H is given by:

$$\Psi_H\left(\frac{z}{L}\right) = -5 \cdot z / L \qquad 0 < z/L \tag{9-6a}$$

$$\Psi_H\left(\frac{z}{L}\right) = 0 \qquad z/L = 0 \tag{9-6b}$$

$$\Psi_H\left(\frac{z}{L}\right) = 2 \cdot \ln\left(\frac{1+(1-16 \cdot z/L)^{1/2}}{2}\right) \qquad z/L < 0 \qquad (9\text{-}6c)$$

The HGSYSTEM-MMES model will automatically provide values of u_* and L based on observations of wind speed and stability. The code will also provide estimates of stability class based on the surface roughness length and the estimated value of L. As a default, the following parameterizations can be made:

$$u_* = u(10\ \mathrm{m})/15. \qquad (9\text{-}7)$$

$$L = \begin{cases} -20\ \mathrm{m} & \text{Class A} \\ -50\ \mathrm{m} & \text{Class B} \\ -100\ \mathrm{m} & \text{Class C} \\ \infty & \text{Class D} \\ 50\ \mathrm{m} & \text{Class E} \\ 20\ \mathrm{m}. & \text{Class F} \end{cases} \qquad (9\text{-}8)$$

The surface or laminar layer resistance, r_s, is dependent on the molecular diffusivity of gases or the Brownian diffusivity of particles, and can be estimated from the formula:

$$r_s = \left[Sc^n + \frac{St}{(1 + St^2)} \right]^{-1} u_*^{-1} \qquad (9\text{-}9)$$

where Sc is the Schmidt number, St is the Stokes number, and

$$n = -0.5 \text{ for } z_o < 0.1\ \mathrm{m}$$

$$n = -0.7 \text{ for } z_o > 0.1\ \mathrm{m} \qquad (9\text{-}10)$$

The Schmidt number is given by:

$$Sc = v/D_B \qquad \text{for particles} \qquad (9\text{-}11a)$$

$$Sc = v/D \qquad \text{for gases} \qquad (9\text{-}11b)$$

where ν is the molecular viscosity of air ($\nu = \mu/\rho = 0.15\ \mathrm{cm^2/s}$), D_B is the Brownian diffusivity of the particles in air, and D is the molecular diffusivity of the pollutant gas in air. For many gases, Sc is on the order of unity. For particles, the Brownian diffusivity, D_B, is a strong function of particle size, ranging from $D_B \sim 10^{-7}\ \mathrm{cm^2/s}$ for $D_p \sim 1\ \mu m$ to $D_B \sim 0.1\ \mathrm{cm^2/s}$ for $D_p \sim 10^{-4}\ \mu m$. The ISC2 model uses the following formula to calculate Brownian diffusion D_B for particles:

$$D_B = 0.81 \cdot 10^{-9} \frac{T\, S_{CF}}{D_p} \tag{9-12}$$

where T is air temperature in K and S_{CF} is the slip correction factor (see equation 9-2). The units of D_B are cm²/sec and the units of particle size D_p are μm.

The Stokes number is non-zero only for particles and is given by:

$$St = \left(\frac{v_s}{g}\right)\left(\frac{u_*^2}{n}\right) \tag{9-13}$$

It is evident that r_s is an important term only for gases or very small particles (diameters of 10^{-3} μm or less). r_s can be ignored for particles with sizes of about 1 μm or greater.

The third resistance term, the transfer resistance r_t, has been the subject of extensive research studies and is generally parameterized by the following formulas:

For particles,

$$r_t = r_a\, r_s\, v_s \tag{9-14a}$$

For gases,

$$r_t = \frac{1}{\dfrac{LAI}{r_f} + \dfrac{LAI}{r_{cut}} + \dfrac{1}{r_g}} \tag{9-14b}$$

where LAI is the leaf area index (area of leaves over a unit area of ground surface), r_f is the stomate resistance, r_{cut} is the cuticle resistance, and r_g is the resistance to transfer across the non-vegetated ground or water surface. The first two terms are significant only when vegetation is actively growing and the pollutant is sufficiently reactive to be absorbed by the vegetation. The last term is also significant only if the pollutant is reactive with the surface. For non-reactive gases, the surface transfer resistance, r_t, is infinity and the deposition velocity is therefore zero (see equation 9-4).

The terms r_f, r_{cut}, and r_g are well-known only for gases involved in acid deposition processes, such as SO_2, NO_2, HNO_3, PAN, and O_3. For these gases, Pleim et al. (1984) suggest that r_t is on the order of 10 s/cm, with variations of ± factor of 3 depending on the particular gas.

For more highly reactive materials, set $r_t = 0.02$ s/cm in the HGSYSTEM-MMES model. If future field and laboratory studies permit r_f, r_{cut}, and r_g to be estimated, then this new information can be used to update r_t by means of equation (9-14b).

9.1.4. Removal of Particles and Gases by Precipitation and Clouds

Particles and gases can be removed from the plume by rain, snow, clouds, or fog by two mechanisms - 1) in-cloud scavenging by small cloud or fog water drops, and 2) below-cloud scavenging as large precipitation drops or snowflakes fall through a polluted plume. The first mechanism, in-cloud scavenging, is important only for reactive gases and particles, since the water drops are assumed to be not moving through the pollutant cloud, and therefore the only way the gases or particles can mix with the drops is by means of an absorption process. As Slinn (1984) explains, if the pollutant and the drops are exposed to each other for a long time, the concentration of chemicals such as SO_2 and NO_2 in the liquid reach an equilibrium determined by Henry's law. This process is clearly different from mechanism 2) above, where the liquid drops fall through the pollutant cloud in a relatively short time (a few seconds, at most) and the primary removal mechanism is via capture of pollutant particles or aerosols by the droplets.

Both in-cloud and below-cloud scavenging mechanisms can be parameterized in models using a scavenging scale, Λ, with units $(\text{sec})^{-1}$, which is approximately proportional to the precipitation rate, P, with units (mm/hour). The local concentration, C, is assumed to decrease exponentially with time:

$$C(t) = C(0)\, e^{-\Lambda t} \tag{9-15}$$

where t is the time the plume has been exposed to the liquid water drops. The precipitation-induced flux of material to the ground, F_{wet}, is given by:

$$F_{wet} = \int_0^{z_w} \Lambda \cdot C(z)\, dz \tag{9-16}$$

where z_w is the depth of the wetted plume layer.

Bloom et al. (1989) include a wet removal time factor in their PLM89A model and assume that it equals 10^{-3} sec^{-1} for HF, ClF_3, and ClO_2; 2 x $10^{-3}sec^{-1}$ for UF_6 and UO_2F_2; and 0.0 for HCl, F_2 and inert substances. Ramsdell et al. (1993) use the following parameterizations for Λ for iodine gas and aerosol compounds as a function of precipitation rate in their RATCHET model:

Rain $$\Lambda = 4 \cdot 10^{-4}\ Pr^{3/4} \tag{9-17a}$$

Snow $$\Lambda = 6 \cdot 10^{-5}\ Pr \tag{9-17b}$$

where the precipitation rate, Pr, is in mm/hr, and the following rates are suggested.

	Pr (mm/hr liquid equivalent)		
	Light	Moderate	Heavy
Rain	0.1	3	5
Snow	0.03	1.5	3.3

For example, equation (9-17a) gives $\Lambda \approx 10^{-3}sec^{-1}$ or about $(15\ minutes)^{-1}$ for moderate rain. This means that most of the pollutant would be removed after being subjected to 15 minutes of moderate rain.

It is seen that the Λ values in the PLM89A and RATCHET models are consistent. It is suggested that a default value of $(1000\ sec)^{-1}$ be used in the HGSYSTEM-MMES code if the precipitation rate is not known. Equations (9-17a) and (9-17b) can be used if the precipitation rate is known. In the future, as experimental data become available, revised Λ values can be prescribed for specific chemicals such as HF-H_2O. Equation (9-16) can be used, knowing Λ and C(z), to calculate the wet flux to the ground.

Because travel times to receptors of interest would be on the order of 10 to 100 sec for accidental releases, it is possible to neglect the reduction in total mass flux due to wet deposition of chemicals in the plume. The plume chemistry and thermodynamics calculations are assumed not be affected by the wet removal at these times and distances. Of course, for larger travel times of 1000 sec or more and for distances of a few kilometers, the wet removal may be significant and may affect the plume thermodynamics.

The present version of HGSYSTEM neglects the in-cloud scavenging by fog drops, since that term is insignificant for travel times of 10 to 100 sec.

9.2. Plume Lift-Off Module

A buoyant plume blowing along the ground may 'lift off' the ground if the buoyancy forces exceed the turbulent forces within the ambient boundary layer. The few previous analyses of this problem (Briggs 1973, Meroney 1979, Poreh and Cermak 1986, Hall and Waters 1986, and Slawson et al. 1990) all dealt with plumes which tend to conserve their initial buoyancy flux, $F_o = w_o R_o^2 g(\rho_a - \rho_o)/\rho_a$, where subscript o refers to the initial plume, subscript a refers to the ambient environment, and w is plume vertical velocity, R is plume radius, g is acceleration, and ρ is density. However, a reactive plume and its subsequent products may not conserve its initial buoyancy flux, and in fact the relative plume density $(\rho_a - \rho)/\rho_a$ may change from positive to negative, depending on the influence of 1) the molecular weights of the gases that exist, 2) the enhanced effective density due to small liquid droplets and small particles carried by the plume, 3) the addition of heat due to exothermic reactions and condensation of liquids, and 4) the removal of heat due to endothermic reactions, depolymerization, and evaporation of liquids.

For example, consider a simple system where HF is released at ambient temperature and then reacts with ambient water vapor. The plume will first be very dense $((\rho_a - \rho)/\rho_a < 0)$ and may eventually be buoyant $((\rho_a - \rho)/(\rho_a > 0)$. All during this process, the plume will be growing in the vertical (depth H) and the horizontal (width W) and will be characterized by a local buoyancy flux.

$$F = (V/\pi)\, g(\rho_a - \rho)/\rho_a \tag{9-18}$$

where V is the plume volume flux (m³/s). For a plume of dimensions H and W which is traveling at speed u, the volume flux, V, equals uHW. Figure 9-3 shows typical time series of these variables. Also shown is the time series for the Briggs (1973) lift-off parameter, L_p, which is defined by the following expression:

$$L_p = \frac{gH(\rho_a - \rho)/\rho_a}{u_*^2} \tag{9-19}$$

where u_* is the friction velocity (approximately given by $u_* \approx u(10\ \mathrm{m})/15$). The parameter L_p is proportional to the ratio of the internal plume turbulent energy due to buoyancy forces to the ambient atmospheric turbulent energy. Observations of plume lift-off in laboratory studies by the researchers mentioned above suggest that the ground-based plume will lift off the ground when $L_p \approx 20$ (there is an uncertainty of about a factor of two in this number). Prior to that point the plume may stretch vertically without lifting completely from the ground.

Note that the criterion in equation (9-19) implies that, once a plume is buoyant ($(\rho_a - \rho) > 0$), a wind speed always exists that will give $L > 20$. Assuming that $u_* = u/15$, we can use equation (9-19) to calculate that lift-off will occur when

$$u < 3.4\left(gH((\rho_a - \rho)/\rho_a\right)^{1/2} \tag{9-20}$$

For example, if $H = 10$ m and $(\rho_a - \rho)/\rho_a = 0.01$, then lift-off will occur if $u < 3.4$ m/s. If $H = 1$ m and $(\rho_a - \rho)/\rho_a = 0.001$, then lift-off will occur only if $u < 0.34$ m/s.

Briggs and the others employ criterion (9-19) along with assumptions for the growth of volume flux, V, with time to derive formulas for calculating the distance at which $L_p = 20$ for plumes where buoyancy flux F is conserved. These formulas are not given here because F is not conserved in some reactive plumes.

The default procedure for calculating plume lift-off in HGSYSTEM is the following:

(1) Once the plume is on the ground, either because it was initially released at the ground or because it sank to the ground due to excess density, it will remain on the ground (i.e., plume base at the ground) as long as the local $L_p < 20$. Note that H and ρ are the local plume depth and density as calculated by the AEROPLUME or HEGADAS algorithms in HGSYSTEM-MMES.

(2) Once the plume depth and buoyancy increase so that the local $L_p = 20$, the plume centerline (or point of maximum concentration) is allowed to begin lifting off the ground at the rate determined by the buoyant plume vertical equation of motion in AEROPLUME or by the Briggs 'two-thirds' law' in HEGADAS.

After plume lift-off is triggered in HEGADAS, the code carries out its calculations as if the plume were still touching the ground, but the code 'remembers' that lift off is to be accounted for later. In a postprocessor, the rise of the plume centerline is calculated using the differential form of the plume rise formulas suggested by Briggs (1975) and Weil (1988):

$$\Delta z = \left(\frac{3\,\ell_b}{2\,\beta^2}\right)^{1/3} \frac{2}{3}\, x^{-1/3}\, \Delta x \tag{9-21}$$

where Δx is the integration step size, and Δz is the amount of plume rise within a downwind distance increment, Δx. The buoyancy length scale, ℓ_b, is defined by

$$\ell_b = \frac{H^2 \, g \, \Delta\rho}{u^2 \, \rho_a} \tag{9-22}$$

In the lift-off algorithm applied to HEGADAS, the height z refers to the 'bottom' of the HEGADAS plume, since that model assumes that the maximum concentration occurs at the bottom of the plume. x is the downwind distance from the point where L_p first equals 20, β is an empirical constant = 0.6, and u is the ambient wind speed (taken to be measured at 10 m). Note that ℓ_b defined in Equation (9-21) is based on the plume parameters at the point when L_p first equals 20, and is treated as a conserved quantity in subsequent calculations.

The so-called 'break-up' formula is used to determine the final buoyant plume rise. The plume will stop rising when the plume vertical velocity becomes less than the ambient turbulent velocity. The following criterion is used:

$$\frac{\frac{dz}{dt}}{1.1\,u_*} = \frac{\textit{plume vertical velocity}}{\textit{ambient}\ \sigma_w} \sim 1 \tag{9-23}$$

This criterion is satisfied when $x = \ell_b (u/u_*)^3$. It can be shown that x ~ 100 H for HEGADAS, assuming that $L_p = 20$ and H equals the plume depth at the point of lift-off.

9.3. Meteorological Preprocessor

9 3.1. Background

The original (NOV90 or 1.0) version of the HGSYSTEM model (McFarlane et al., 1990) had a very brief and limited meteorological processor. A few basic meteorological parameters (wind speed, stability class, surface roughness, relative humidity, temperature) are input to the model. The model uses a simple power law formula to calculate the Monin-Obukhov length, L, as a function of surface roughness and stability class, and then uses standard Monin-Obukhov similarity formulas to calculate the variation of the wind speed with height.

The cross-wind passive dispersion parameters σ_y and σ_z in the HGSYSTEM model are functions of stability class, downwind distance, surface roughness, and averaging time. The along-wind passive dispersion parameter is, in addition, a function of vertical wind shear.

The methods in the HGSYSTEM model are standard, robust procedures that have been used by modelers for over 40 years. Similar procedures are used in the PLM89A model (Bloom et al., 1989). However, as recommended by Sykes and Lewellen (1992), advanced procedures now exist for calculating boundary layer turbulence and dispersion that could be incorporated in the HGSYSTEM-MMES model. These advanced procedures can be divided into three categories of formulas:

1) Meteorological Surface Flux Formulas
2) Meteorological Profile Formulas
3) Dispersion Algorithms

Hanna et al. (1982) propose some simple formulas for each of the categories of new algorithms. For example, observations of wind speed and cloudiness could be used to estimate surface fluxes of heat and momentum. These flux estimates could then be used to generate vertical profiles of wind speed and turbulence. Finally, dispersion (σ_y and σ_z) could be calculated based on this knowledge of turbulent energy and time scales.

9 3.2. Approach to Revised Meteorological Preprocessor

State-of-the-art formulas for surface fluxes, vertical profiles, and turbulent dispersion are proposed by Hanna and Chang (1992, 1993) for their SIGPRO meteorological preprocessor and HPDM dispersion model. These are closely related to the formulas suggested by Sykes and Lewellen (1992) and to the algorithms in recent models developed by Weil (1992) and Carruthers et al. (1992).

If one were to adapt the entire set of formulas in SIGPRO and HPDM, major changes would be required to the passive dispersion algorithms in HGSYSTEM. Because the HGSYSTEM dispersion algorithms produce σ_y and σ_z estimates that are not much different from those in HPDM, it is preferable to retain the HGSYSTEM dispersion algorithms for the time being. In the future it may be appropriate to revise those passive dispersion algorithms.

As a first step, the SIGPRO and HPDM meteorological surface flux and profile preprocessors are adapted for use in HGSYSTEM. With this approach, no major revisions to HGSYSTEM are needed because that model does not currently include a major meteorological preprocessor algorithm. The codes from SIGPRO and HPDM have been directly used in the new HGSYSTEM-MMES model.

9 3.3. Description of Revised Meteorological Preprocessor

Because the two articles by Hanna and Chang (1992, 1993), describe the SIGPRO and HPDM meteorological preprocessor in great detail, the derivations are not repeated here. The reader is referred to these articles for a full discussion. For example, Section 3 of Hanna and Chang (1993) lists the assumptions and the formulas for surface heat flux Q_H, friction velocity u_*, Monin-Obukhov length L, mixing depth h, and vertical profiles of wind speed u, turbulence components (σ_v and σ_w), and temperature T.

The following input parameters are required:

z_o	surface roughness
α	surface moisture availability
L_{min}	minimum stable Monin-Obukhov length
u	wind speed at some reference height, z_{ref}
ν	solar elevation angle
N	cloud cover

The references give tables of z_o, α, and L_{min} as a function of land-use type. The reference height for the wind speed observation is usually about 10 m. The solar elevation angle (used for calculating the solar energy flux) is known from astronomical tables (e.g., the ISC2 model contains methods for determining ν from a knowledge of latitude, longitude, and time of day). The cloud cover N (ranges from 0.0 to 1.0) is observed routinely at National Weather Service stations.

To be consistent with EPA and NRC regulatory models, this revised method is designed so that it permits estimation of the Pasquill-Gifford-Turner stability class. In the new HGSYSTEM-MMES meteorological processors, the Golder (1972) nomogram (see Figure 9-4) is used, in which stability class is given as a function of z_o (in the range from 0.1 cm to 50 cm) and 1/L (in the range from -0.13 m^{-1} to 0.09 m^{-1}). The HGSYSTEM model employs this nomogram in reverse, calculating L as a function of z_o and stability class. Depending on the requirements of the regulatory agency or the project sponsors, the meteorological processor can be applied using a range of types of input parameters.

9 4. Concentration Fluctuations And Variations With Averaging Time

The effects of concentration fluctuations and averaging time are discussed in Sections 9.4.1 and 9.4.2 below for two types of receptor definitions: 1) a receptor on the plume centerline, and 2) a receptor at a fixed geometric position. Because HGSYSTEM is intended for application to the first type of receptor, the model has been modified following the suggested formulas in the first section, 9.4.1.

9.4.1. Plume Centerline Concentrations at a Given Downwind Distance

Hazardous gas models such as HGSYSTEM can predict the crosswind concentration distribution at distance x from the source for a certain averaging time, T_a. The basic model predictions of the dense gas modules are appropriate for averaging times of about two minutes, which correspond to the field data on which the dense gas algorithms are based. The predictions of the passive gas models generally refer to an averaging time of about 10 or 20 minutes, which is the averaging time for the passive gas field data used in deriving the Pasquill-Gifford-Turner σ_y and σ_z curves. Also, the HGSYSTEM prediction is for an ensemble average--that is, the average of millions of independent realizations of that particular experiment for those specific initial and boundary conditions and other input parameters. Those millions of individual realizations would themselves have a distribution about the ensemble average.

The model predictions of the ensemble average plume centerline concentration, $C_{cl}(x,T_a)$, are not keyed to any particular geographic point--the only restriction is that the downwind distance must be x. But because natural plumes meander or swing back and forth, the ensemble average centerline concentration will drop as averaging time increases, and the position of the centerline may also shift as T_a varies. The effects of averaging time on plumes are thoroughly discussed in the review report by Wilson and Simms (1985).

Consider an ensemble of concentration observations under certain initial and boundary conditions. Then the variation of the distribution of C_{cl} with T_a at a fixed x would be as shown in Figure 9-5. The box plots indicate key points on the distribution function at each T_a. The dashed line on the figure passes through the mean or median (whichever you prefer) of the distributions. If the model predictions are corrected for averaging time, T_a, the corrected ensemble average concentrations should fall along this dashed line. As averaging time, T_a, approaches 0.0 (i.e. an instantaneous snapshot of the plume), the concentration C_{cl} should approach a value representative of the instantaneous plume.

It should be mentioned that some models such as TRACE are designed to be conservative--i.e., to predict concentrations, C_{cl}, higher than the mean. The descriptions of these models do not specify the quantitative percentile (e.g. the 99th percentile) of the distribution that they are aiming for. However, if a model were designed to predict the 99th percentile at each T_a, the concentration predictions would follow the dotted line in Figure 9-5. If a model were designed to give the maximum at a given T_a for a given total sampling time (60 min, in this case) the concentration predictions would follow the dash-dot line. In this latter example, the percentile associated with the single maximum concentration would increase as T_a decreases, since the total number of concentration values equals (60 min/T_a).

Parameterizations

Most hazardous gas models that correct for averaging time are attempting to follow the dashed line in Figure 1, even though they do not articulate these conditions. In addition, most models accomplish this correction by applying a $T_a^{1/5}$ power law to the lateral dispersion coefficient, σ_y, due to ambient turbulence.

$$\frac{\sigma_y(T_{a2})}{\sigma_y(T_{a1})} = \left(\frac{T_{a2}}{T_{a1}}\right)^{1/5} \tag{9-24}$$

In order to prevent σ_y from dropping below its known value for instantaneous conditions, which would inevitably happen with equation (9-24) as $T_{a2} \rightarrow 0$, a 'minimum T_{a2}' criterion is usually applied. This is the T_{a2} which would result in σ_y equalling the following values given by Slade (1968) for instantaneous plumes or puffs:

Unstable $\sigma_{yI} = 0.14 \cdot x^{0.92}$ (9-25)
Neutral $\sigma_{yI} = 0.06 \cdot x^{0.92}$ (9-26)
Very Stable $\sigma_{yI} = 0.02 \cdot x^{0.89}$ (9-27)

For neutral conditions, this criterion is satisfied at T_{a2} equal to about 20 seconds, where it is assumed that σ_y for continuous plumes is given by the Briggs-EPA formulas. However this minimum T_{a2} is dependent on what is assumed for (1) distance x, and (2) representative averaging time for the Briggs-EPA formulas. Furthermore, equations (9-25)-(9-27) themselves are based on limited data and would have significant uncertainties (say ± 50%).

As a default parameterization, the existing formulas in HGSYSTEM for accounting for averaging time are used, with the following assumptions:

- The σ_y Briggs-EPA formulas for continuous plumes are valid for an averaging time of 10 minutes.
- The 'minimum T_a' criterion is 20 seconds.
- Equation (9-24) is valid for σ_y corrections for T_a.

The HEGADAS model above assumes that the lateral distribution in a dense gas plume is made up of a dense gas core of width W and Gaussian edges with standard deviation, σ_y. The averaging time correction is then applied only to the Gaussian edges. We depart from this approach by assuming that the averaging time correlation applies to the entire plume width:

$$\frac{C_{cl}(T_{a1})}{C_{cl}(T_{a2})} = \left(\frac{T_{a2}}{T_{a1}}\right)^{1/5} \tag{9-28}$$

If we are interested in the centerline concentration at a given averaging time at a given percentile as the distribution (see the dotted line on Figure 9-5), an assumption is needed for the form of the distribution. For in-plume fluctuations, a log-normal distribution is applicable (see Hanna, 1984):

$$P(\ln C) = \int_{-\infty}^{\ln C} p(\ln C')\, d(\ln C') \tag{9-29}$$

$$p(\ln C') = \frac{1}{\sqrt{2\pi}\,\sigma_{\ln C'}}\, e^{-(\ln C' - \overline{\ln C'})^2/2\sigma^2_{\ln C'}} \tag{9-30}$$

where P is the cumulative distribution function (ranges from 0.0 to 1.0) and p is the probability distribution function.

At small averaging times ($T_a \sim 20$ seconds or less), atmospheric data show that

$$\frac{\sigma_{\ln C}}{\left|\overline{\ln C}\right|} \approx 1.0 \tag{9-31}$$

We assume that this relation is valid and that $\sigma_{\ln C}$ decreases as averaging time increases according to the following approximation to Taylor's formula:

$$\frac{\sigma^2_{\ln C}(T_a)}{\sigma^2_{\ln C}(20\text{ sec})} = \frac{1}{1+\dfrac{T_a}{2T_I}} \tag{9-32}$$

where T_I is the integral scale for turbulent fluctuations in concentration. For plumes in the atmospheric boundary layer, a default assumption would be

$$\text{Default} \qquad T_I \approx 300 \text{ seconds.} \tag{9-33}$$

With this value of T_I, equations (9-31) and (9-32) give

$$\sigma_{\ln C}(\text{one hour}) = 0.4 \cdot \sigma_{\ln C}(20 \text{ sec})$$

The formulas given above have been implemented in HGSYSTEM.

9.4.2. Concentrations at a given Receptor Position

The discussions in the previous subsection were concerned with predicted concentrations on the plume centerline or axis, which can shift position with time. For that type of model application, the analyst is concerned only with the maximum plume impact independent of location. The HGSYSTEM model takes that approach. Another type of model application would be concerned with the plume impact at a given receptor position, as defined by for example a monitoring site or a critical subset of the surrounding population (say a school or a hospital). The HGSYSTEM model does not currently treat this type of receptor. Nevertheless, the equations are derived below with the thought that they can be used in future modifications.

Consider an ensemble of concentration observations from a given monitoring site. The data are taken from many independent field studies, all with nearly the same ambient conditions (i.e. release rate, wind speed and direction, stability). These observations would show a variation of distribution functions with averaging time as suggested in Figure 9-6. Note that there are three major differences between Figures 9-5 and 9-6:

Figure 9-5 **Centerline C**	**Figure 9-6** **Fixed Receptor C**
Median C decreases as T_a increases	Median C is constant with T_a
There are no zeros in C	There are many zeros in C
σ_c is relatively small	σ_c is relatively large

All of these differences are due to the fact that, in the case of Figure 9-6, the plume can meander away from the receptor, leading to many C = 0 observations at that receptor. In contrast, by definition C_{cl} is always greater than zero in Figure 9-5, which is appropriate for HGSYSTEM.

Often the variation of C_{max} with T_a is calculated from data at fixed receptors. A time series C(t) is searched in order to identify the various $C_{max}(T_a)$; for example this was done by us using the field data from the Burro, Coyote, and Desert Tortoise experiments. The resulting C_{max} values would follow the dot-dashed-curve in Figure 9-6. In that example, the total length of the time series is 60 min (the sampling time T_s). The percentile of C_{max} for each T_a is given by:

$$\text{Percentile} / 100 = 1 - (T_a / 60 \text{ min}) \tag{9-34}$$

Note that the variation of C_{max} with T_a is greater than the variation of C (fixed percentile) with T_a. From a theoretical point of view, C (fixed percentile) is preferable, but from a practical point of view researchers always seem to work with C_{max}. It is clearly important to at least recognize the difference.

The distribution function that is proposed for the data in Figure 9-6 must account for the possibility of many zeros. The exponential cumulative distribution function is recommended by Hanna (1984):

$$P(C) = 1 - I \exp(-IC/\overline{C}) \tag{9-35}$$

$$\sigma_c/\overline{C} = ((2/I) - 1)^{1/2} \tag{9-36}$$

where I is the so-called intermittency, or fraction of non-zero observations in the total record (I = 1.0 if the plume is always impacting the receptor). A typical value of I in the atmosphere is about 0.2, giving $\sigma_c/\overline{C} = 3$. In the absence of other information, it is recommended that a default value of I = 0.2 be used for very small averaging times, T_a:

$$\left.\begin{array}{l} P(C) = 1 - 0.2 \exp(-0.2\, C/\overline{C}) \\ \sigma_c/\overline{C} = ((2/I) - 1)^{1/2} = 3 \end{array}\right\} \text{as } T_a \rightarrow 0 \tag{9-37}$$

As averaging time increases to 60 minutes, equation (9-31) can be used to calculate $\sigma_c^2(T_a)/\sigma_c^2(0)$, again assuming that the integral time scale is 300 seconds and that $\sigma_c/\overline{C} = 3$ at $T_a \rightarrow 0$. 'I' can be calculated by inverting equation (9-36):

$$I = 2/\left(1 + (\sigma_c/\overline{C})^2\right) \tag{9-38}$$

The sequence to be followed is given below

Step 1: Calculate $\dfrac{\sigma_c^2(T_a)}{\sigma_c^2(0)} = \dfrac{1}{1 + T_a/600\text{ sec}}$

Step 2: Calculate $I(T_a) = \dfrac{2}{\left(1 + (\sigma_c/\overline{C})^2\right)}$

Step 3: Calculate $P(C) = 1 - I \exp\left(-IC/\overline{C}\right)$

It is assumed that $\overline{C}$ is known and that $\sigma_c / \overline{C}$ $(T_a \rightarrow 0) = 3$ and hence that I $(T_a \rightarrow 0) = 0.2$.

Note: These formulas should not be used at $T_a > 3600$ sec, since the intermittency, I, would be calculated to exceed 1.0, which is impossible. Instead, use $I = 1.0$ and $\sigma_c / \overline{C} = 1.0$ at $T_a > 3600$ sec.

As mentioned above, the formulas in Section 9.4.2 for the fixed receptor position are not implemented in HGSYSTEM since the model is used to calculate concentrations for receptors on the plume centerline. Future modifications may make use of Section 9.4.2.

9.5. Effects Of Buildings And Terrain Obstacles

9.5.1. Introduction

Releases can occur in the vicinity of buildings and may be influenced by nearby terrain obstacles. These obstacles may alter the boundary layer wind flow patterns so that the trajectory and rate of dilution of the plume may be altered. In the past, hazardous gas models have ignored the influence of buildings and other obstacles because the model developers believed that these obstacles generally lead to enhanced dilution and lower concentrations.

There are several reasons why it is best to include methods for accounting for the effects of obstacles:

1. The buildings at gaseous diffusion plants, for example, are large, with relatively narrow 'canyons' between them. The plume would be constrained by the walls of the buildings.

2. Releases could occur from storage tanks and pipes within buildings, with emissions to the outside through exhaust vents on the roofs of the buildings.

3. Releases from short stacks could be mixed to the ground in the wakes of buildings, leading to increased ground level concentrations.

Simplified algorithms have been added in the HGSYSTEM-MMES code to account for these three phenomena. Later, other algorithms can be added to account for the myriad of other possible scenarios involving the effects of buildings and terrain obstacles.

9.5.2. Background

The algorithms suggested below are based on the results of a review of the effects of structures on toxic vapor dispersion carried out by Schulman, Hanna, and Britter (1990). That document drew heavily on previous reviews of the effects of structures on passive and dense gas plumes by Britter (1989) and Brighton (1989). The USAF research had the objectives of reviewing the literature on the effects of structures on toxic vapor dispersion, assessing the feasibility of producing a viable quantitative model, and determining whether the building effects were significant relative to overall model uncertainty. The literature survey followed a framework defined by a matrix based on source location and receptor location relative to the structure:

Source location?	Upwind of structure On structure Downwind of structure
Receptor location:	On face of structure In wake or cavity of structure Downwind of wake of structure

The literature was also stratified into dense gases and passive gases, and into puff and continuous plume sources. The research attempted to answer the following questions:

- Do sufficient data and mathematical models exist for developing quantitative models for the effects of structures that can be used as subroutines in existing toxic vapor dispersion models?
- Are the expected changes in concentrations due to the effects of structures significant relative to overall model uncertainties?
- Do models and data exist for trapping of toxic clouds inside large open structures?
- What is the relative accuracy of the subroutines for various source scenarios and various structure geometries?
- At what level of structure complexity do the models become inaccurate?

The results of the review suggested that sufficient information existed to develop models for a few of the source-receptor combinations listed above. In those cases, simplified formulas were suggested which are given below. In other cases, there was no information to permit even simple models to be suggested, and it would be necessary to carry out further wind tunnel or field studies to fill in the matrix. Fortunately, experimental data and empirical formulas have been developed for the three topics of interest in the current study (i.e., lateral confinement in building canyons, concentration patterns on building faces due to vent releases, and downwash into building wakes).

Most of the literature dealt with neutral or passive gases. Dense gases have not been studied as much, although it is recognized that dense gases tend to spread more laterally and less vertically.

9.5.3. Plume Confinement by Canyons

Consider the scenario shown in Figure 9-7, where the hazardous gas source is near or within a canyon between large buildings. The building height is H_B and the canyon width is W_C. Laboratory experiments by Konig (1987) and Marotske (1988) suggest that maximum concentrations are increased by a factor of as much as three due to the confinement by the canyon. This effect can be decreased if the plume height grows so that leakage occurs above the buildings.

The following simple model is proposed:

If (1) the source is between the buildings or if (2) the source is upwind of the buildings and $\sigma_y < W_C/2$ when the plume enters the canyon, and if (3) $H/H_B < 1$, then do not allow σ_y to exceed the limit:

$$\sigma_y \text{ (maximum)} = W_C / \sqrt{12} \qquad (9\text{-}39)$$

This value of σ_y corresponds to a uniform lateral distribution across W_C. (Note: σ_y as used here is assumed to apply to the <u>total</u> plume width, not just to the plume edge.)

If $H/H_B > 1$, then only the lower part of the plume is confined by the canyon, and the upper part of the plume is free to disperse laterally as if the canyon were not there. In this case, use the following interpolation formula:

$$\text{Effective } \sigma_y \text{ (maximum)} = \left(\frac{H_B}{H}\right)\left(\frac{W_C}{\sqrt{12}}\right) + \left(\frac{H-H_B}{H}\right)\cdot\left(\sigma_y \text{ (without canyon effect)}\right) \qquad (9\text{-}40)$$

where σ_y (without canyon effect) refers to the lateral dispersion as ordinarily calculated by the model in the absence of obstacles. When the plume reaches the end of the canyon, lateral diffusion resumes, and a virtual source procedure should be applied to calculate concentrations further downwind.

9.5.4. Concentrations on Building Faces due to Releases from Vents

If pollutant is released accidentally within a building, it will be exhausted by vents that typically take the form of very short stacks on the roof of the building. The concentration in the plume in the exhaust vent will have been reduced by dilution through the volume of the building and most chemical reactions will have taken place (i.e., the plume will consist of small particles, gas, and aerosol). Because there will be little buoyancy to the plumes being vented, the gas can be modeled as if it were neutral or passive.

There have been many wind tunnel studies of distributions of dimensionless concentration,

$$K = \frac{CuA}{Q} \tag{9-41}$$

on the faces of buildings of various shapes due to releases from vents on various positions on the buildings. 'A' is a representative area of the building. The source and receptors are assumed to be on the same or adjacent faces. Meroney (1982) and Wilson and Britter (1982) provide reviews of some of this work. Using the definitions in Figure 9-8, the maximum concentrations on the building at a distance, r, from the source, are given by the formulas:

$$C = 9\,Q/u_H r^2 \quad \text{for } r/A^{1/2} < 1.73 \quad \text{source receptor on upper 2/3 of building} \tag{9-42}$$
$$C = 30\,Q/u_H r^2 \quad \text{for } r/A^{1/2} < 1.73 \quad \text{source receptor on lower 1/3 of building} \tag{9-43}$$

where u_H is the wind speed at the height of the building in the flow upwind of the building, and A is the building area, assumed to equal $H_B W_B$.

As distance, r (the shortest distance along the surface between the source and receptor), decreases, the concentration does not increase indefinitely but should be capped by the concentration in the vent exhaust (C_{max} = Q/(volume flux from vent)).

Note that if there is a significant air flow from the vent, the vent plume may be transported up and away from the roof. In this case, the concentrations given by equations (9-42) and (9-43) would be conservative.

These formulas say nothing about the lateral or vertical extent of the plumes from the vents. Equations (9-42) and (9-43) are most useful for estimating maximum concentrations with the condition that the plume is being blown directly from the source vent to the receptor position on the building face.

The restriction that $r/A^{1/2} < 1.73$ in equations (9-42) and (9-43) is applied so that concentrations smoothly transition to the formula in the next section for the near wake (i.e., $C = 3Q/u_H A$).

9.5.5. Concentrations on the Building Downwind Face (the Near-Wake) due to Releases from Sources on the Building

This algorithm is concerned with a continuation of the vent scenario covered in the previous section. The source emissions are again assumed to be neutral or passive, and we are now concerned with the concentration in the near-wake or the recirculating cavity. This is a turbulent well-mixed zone that extends about two to five building dimensions downwind, and it is assumed that concentrations are uniform across this zone. Wilson and Britter (1982) find that the concentrations in the near wake are given by

$$C = \frac{3Q}{u_H A} \qquad \left(r / A^{1/2} \geq 1.73\right) \tag{9-44}$$

where $A = W_B H_B$ for blockish buildings and $A = H_{B^{4/3}} W_{B^{2/3}}$ for wide buildings. Figure 9-9 provides a schematic depiction of this scenario. Note that the condition $r/A^{1/2} \geq 1.73$ is applied to equation (9-44), where r is the distance from the source to the receptor.

9.5.6. Other Effects of Buildings

The three building effects covered in Sections 9.5.3, 9.5.4, and 9.6.5 are all easily handled through simple empirical formulas and all tend to increase concentration impacts. In the future, other types of effects can be included in the model as new information comes from wind tunnel and field experiments.

Some building effects have been ignored here because they tend to significantly decrease concentrations. Therefore the 'flat-terrain' solution is conservative. For example, if a source is upwind of a building, fence, or other obstacle, the increased turbulence due to the obstacle will tend to dilute the hazardous gas plume. Fences have been investigated because of their potential for mitigating the plume, and enhanced dilutions of a factor of three or more have been observed. Also, shallow dense gas plumes approaching taller obstacles are seen to be caught in the horseshoe vortices formed around the obstacle, and are therefore transported laterally away from the obstacle.

Generally, chemical reactions have been assumed to be insignificant in the simple models in the previous sections. If one were to include chemical reactions, the entrainment rate of ambient air would have to be estimated, so that the reactions of HF with water vapor could be included. Unfortunately, these entrainment rates are not well known for plumes under the influence of obstacles. Future wind tunnel studies should emphasize observations of entrainment into plumes being influenced by obstacles.

We suggest that the next algorithm that could be included in the model could be the EPA's downwash algorithm for the far wake as implemented in their Industrial Source Complex (ISC) model. This algorithm applies to the scenario when there is a stack of significant height (h_s equal to about 1 to 2 H_B) near the building and ground-level concentrations are to be calculated at a distance of about 10 H_B or greater from the stack (see Figure 9-10). The algorithm allows for enhancement of σ_y and σ_z, depending on the ratio h_s/H_B. This algorithm is not implemented in the HGSYSTEM-MMES model at the present time because (1) most sources are at the ground or at vents on the roofs of buildings, and (2) maximum impacts would occur in the near wake during the scenarios described in Sections 9.5.4 and 9.5.5.

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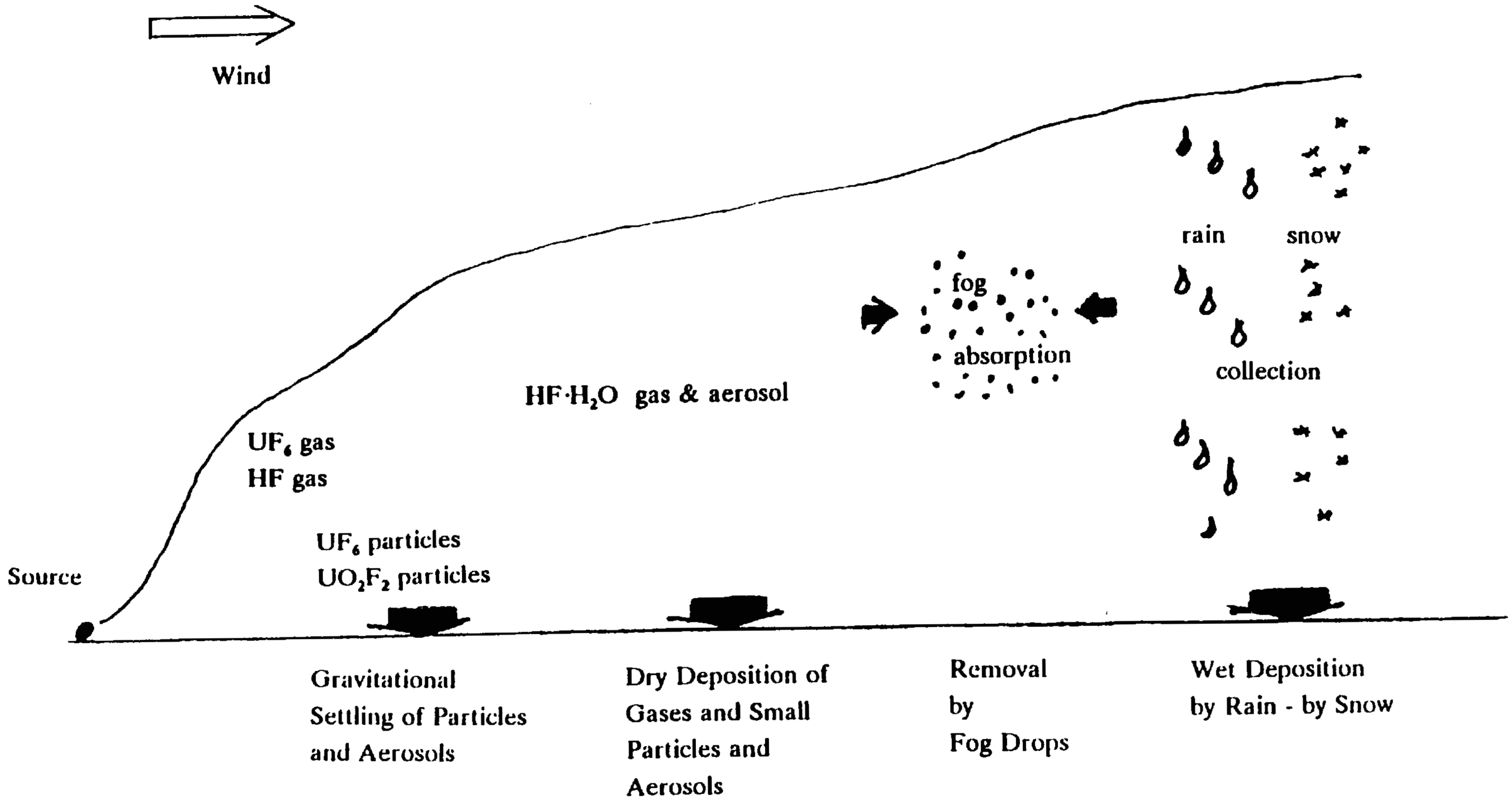

Figure 9-1. Schematic diagram of processes leading to removal of plume material by deposition to the ground.

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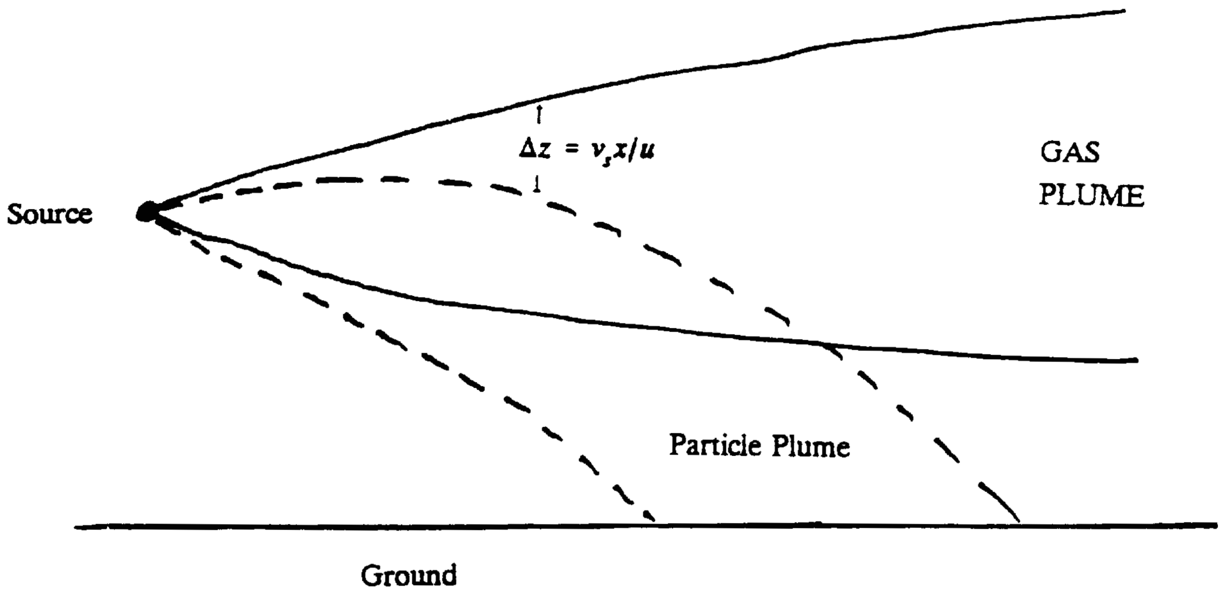


Figure 9-2. Illustration of how a large particle plume will fall away from the rest of the gas plume.

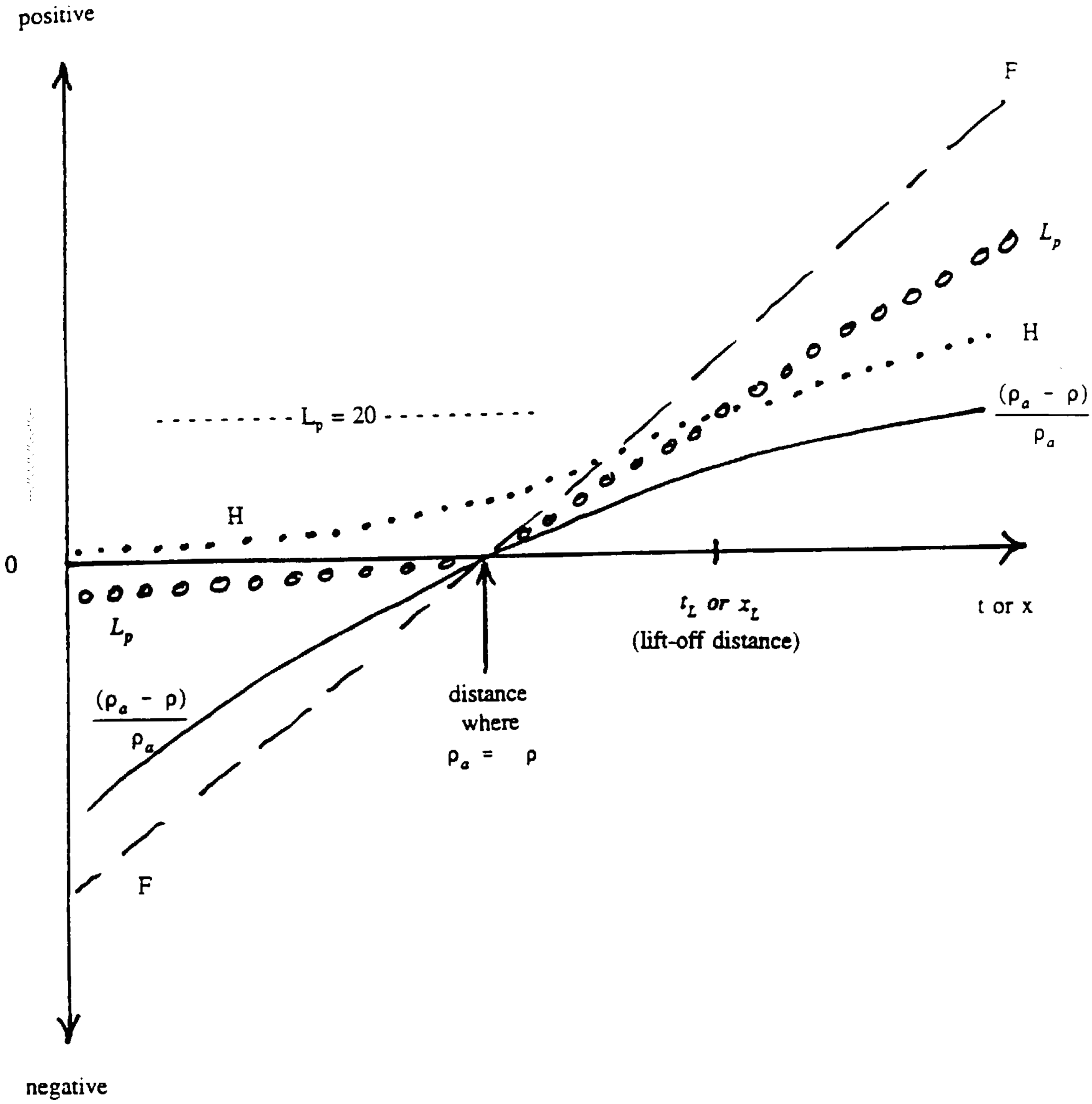


Figure 9-3. Typical time series of $(\rho_a-\rho)/\rho_a$, buoyancy force F, plume depth H, and lift-off parameter L_p for a UF_6 plume.

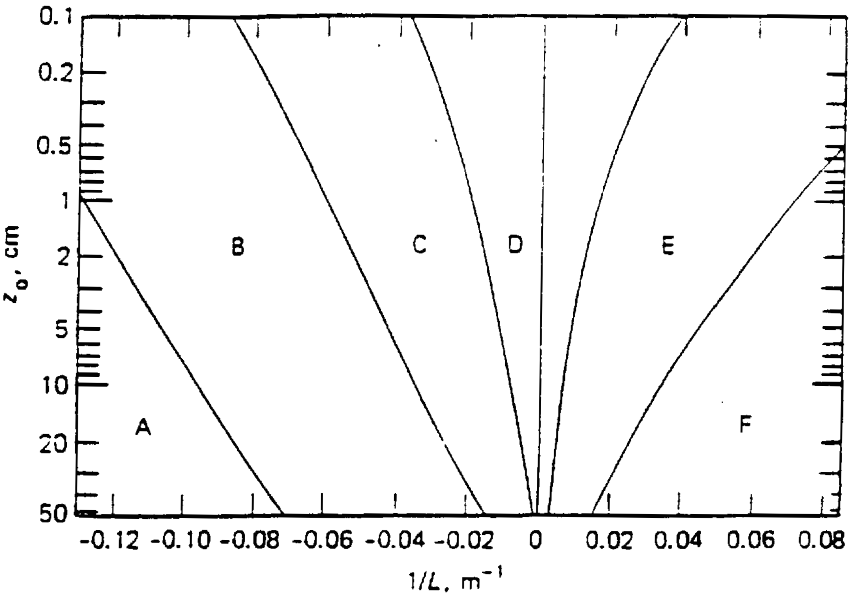


Figure 9-4. Curves showing Pasquill-Gifford-Turner turbulence types as a function of the Monin-Obukhov length and the aerodynamic roughness length. A, extremely stable conditions; B, moderately stable conditions, C, slightly unstable conditions; D, neutral conditions (applicable to heavy overcast day or night); E, slightly stable conditions; F, moderately stable conditions. [From D. Golder, Relations among stability parameters in the surface layer, *Bound. Layer Meteorol.*, **3**, 56 (1972)].

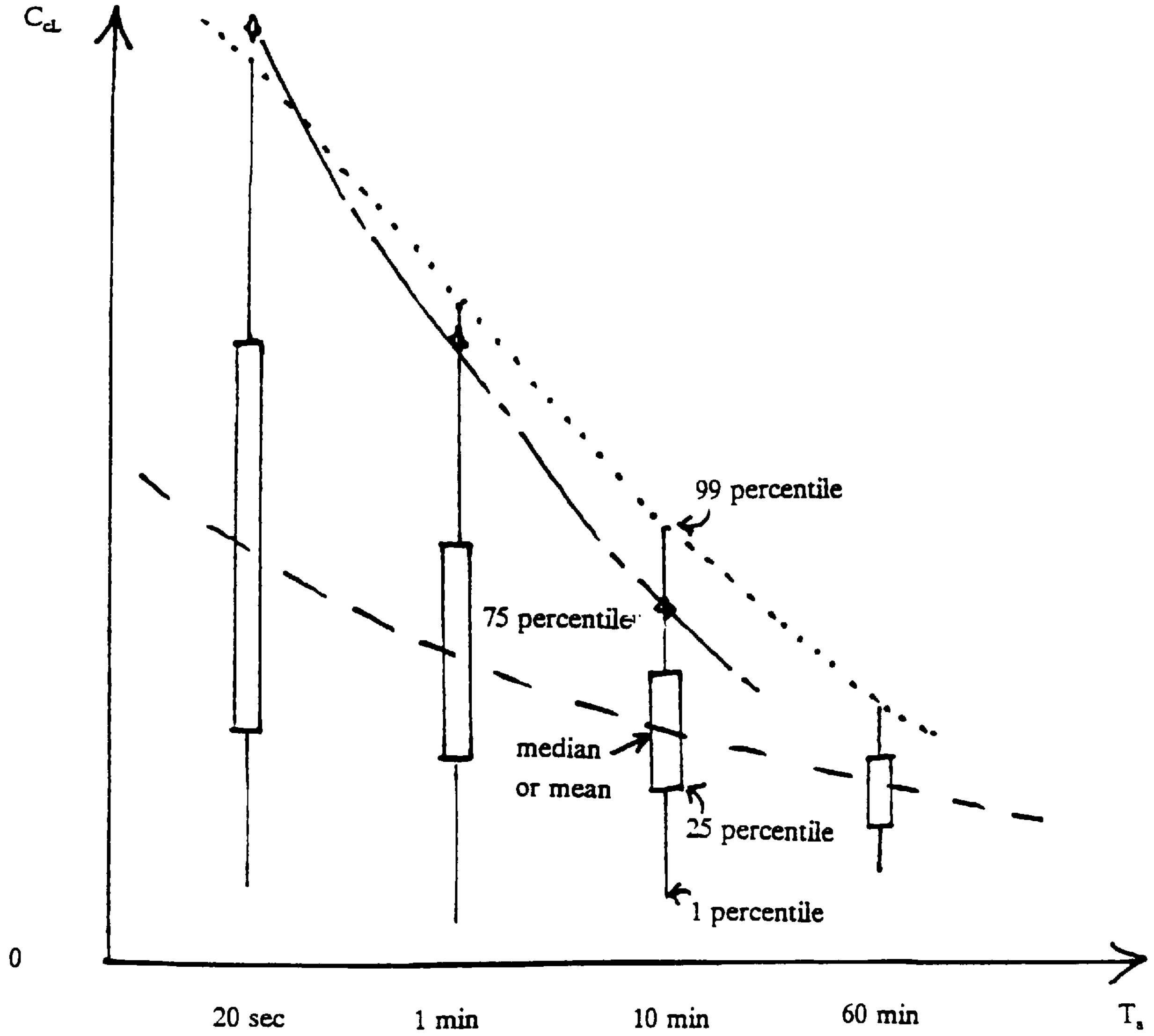


Figure 9-5. Typical distributions of centerline concentration, C_{cL}, observed at a given x, for various averaging times, T_a. The dashed line goes through the means at each T_a, and the dotted line goes through the 99th percentile of each distribution. The dashed-dotted line goes through the maximum at that T_a assuming the sampling time is 60 min.

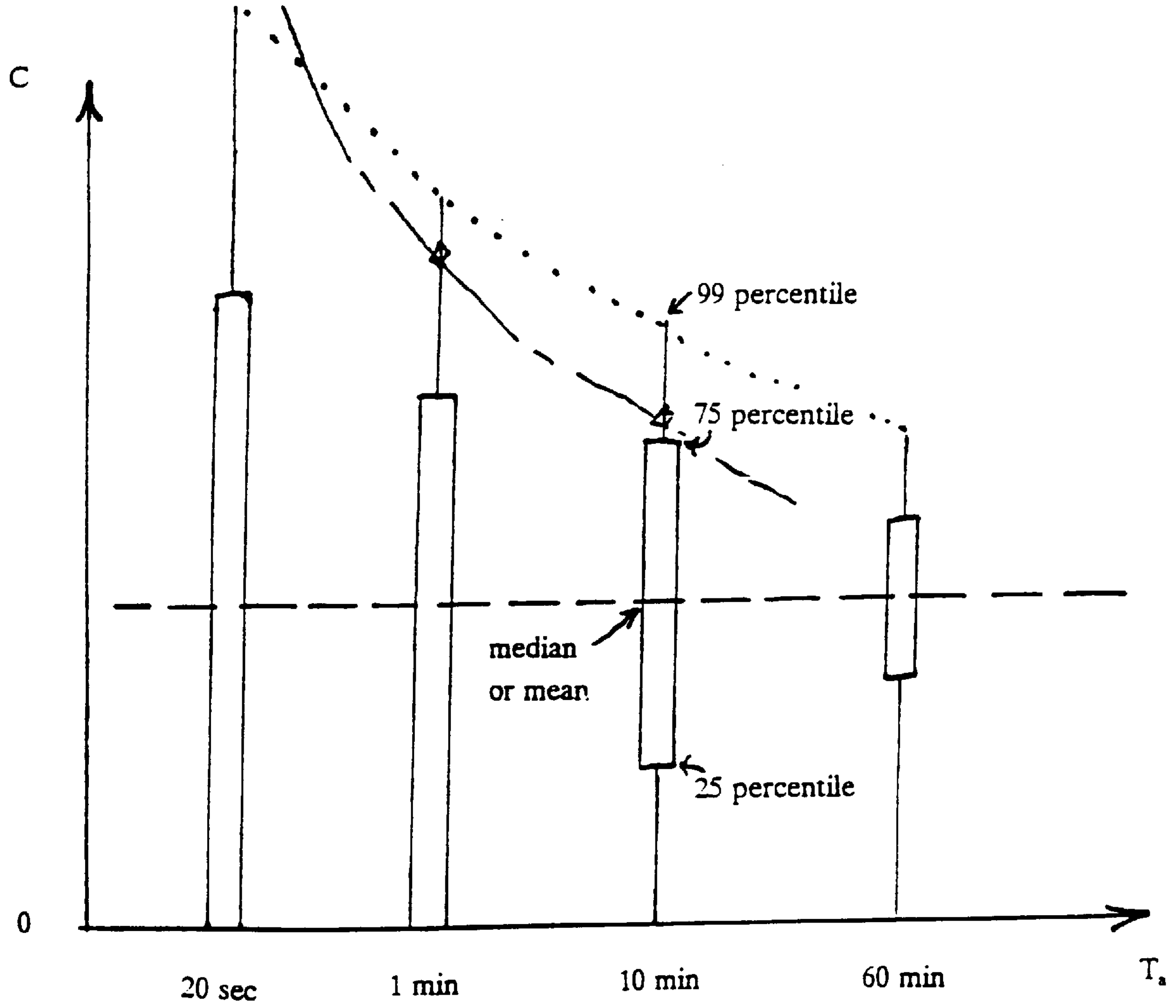
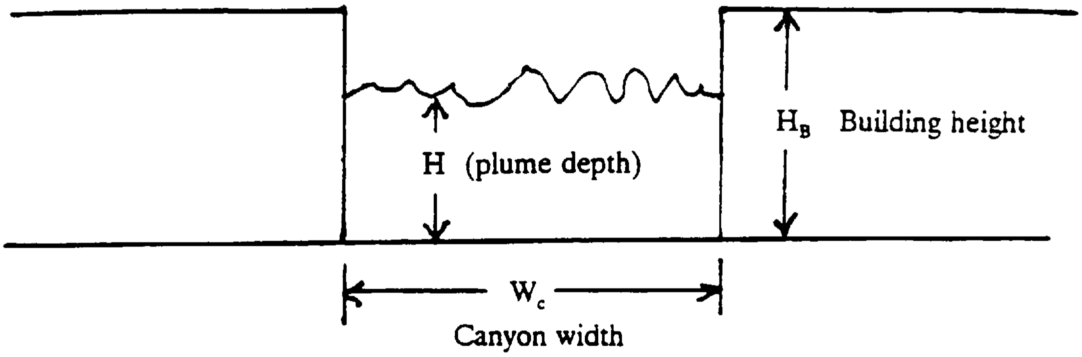
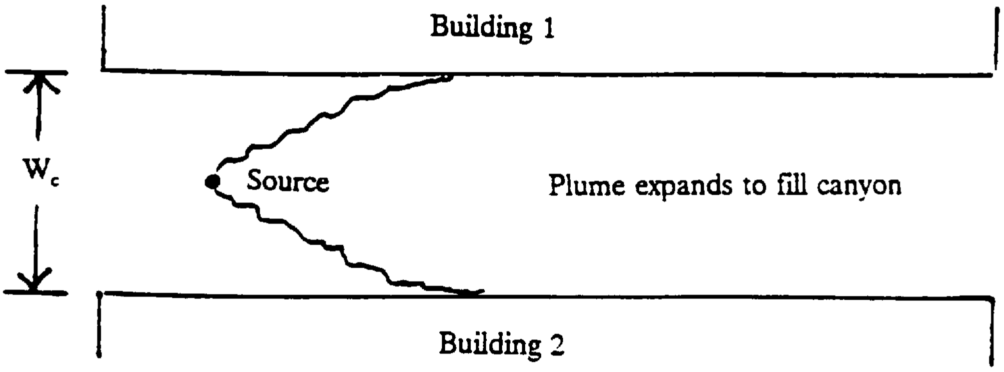


Figure 9-6. Typical distributions of concentration observed at a given monitor location, for various averaging times, T_a. The dashed line goes through the means at each T_a, and the dotted line goes through the 99th percentile of each distribution. The dashed-dotted line goes through the maximum at that T_a assuming the sampling time is 60 min.



a) Cross-section in the vertical and lateral dimensions



b) View looking down

Figure 9-7. Hazardous gas release in a canyon between buildings.

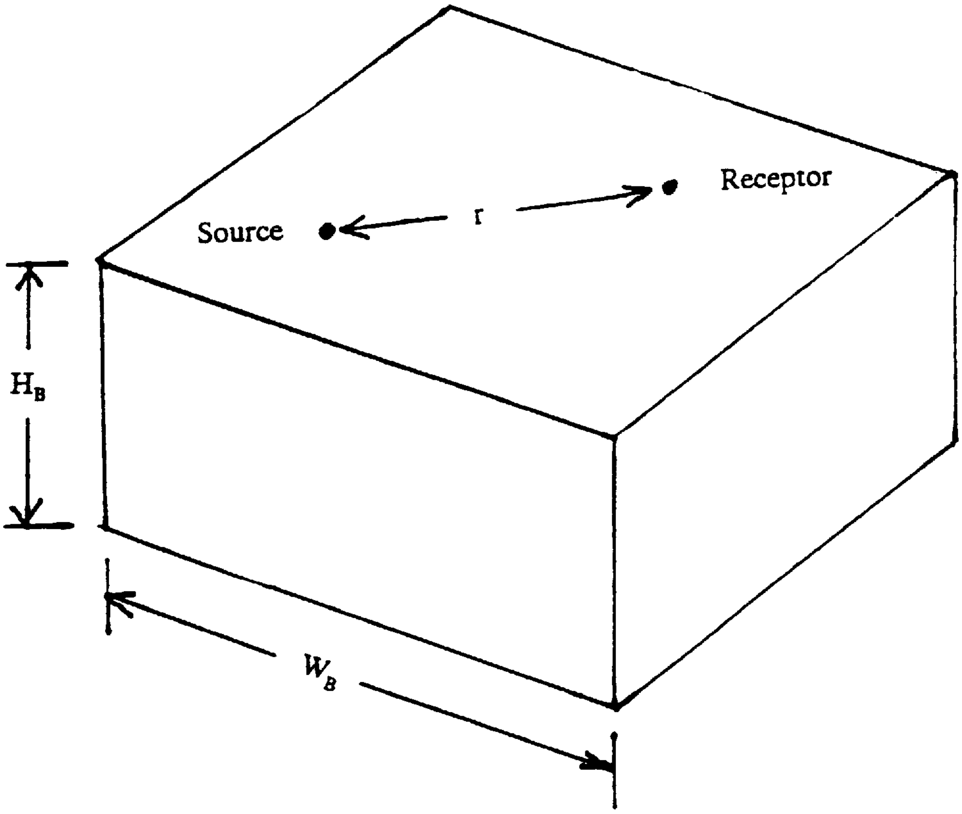


Figure 9-8. Definitions of parameters for calculating concentrations on building faces due to emissions from vents.

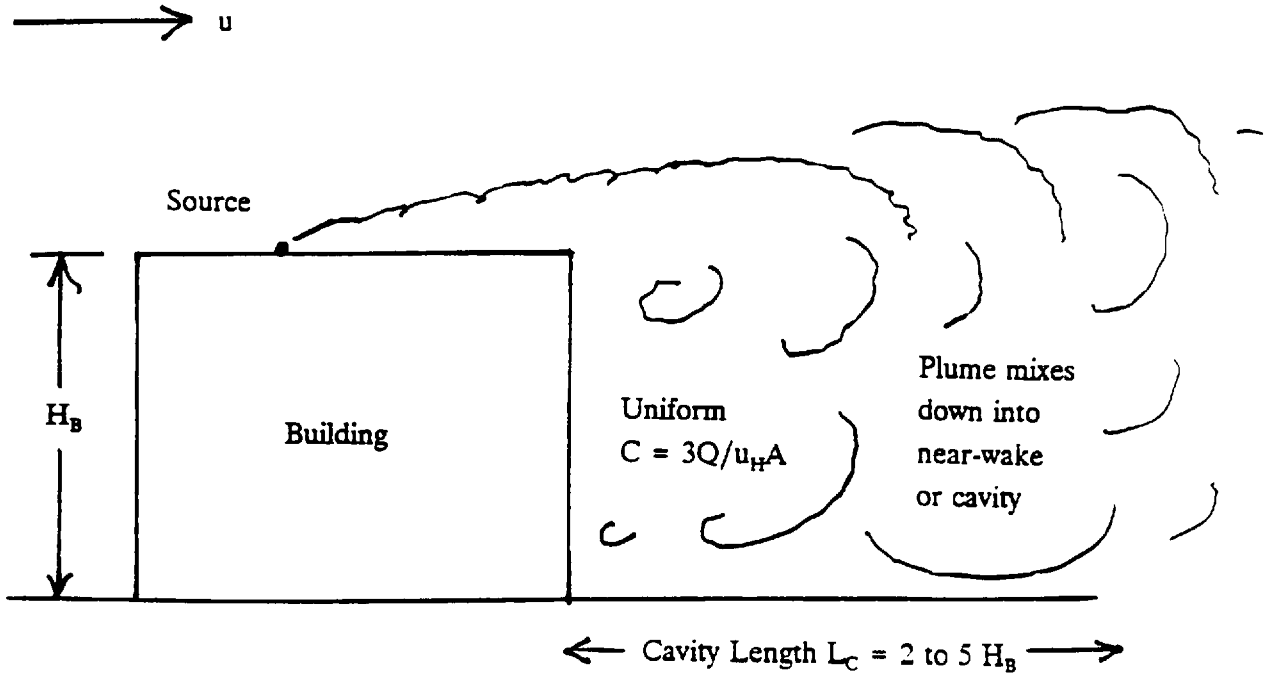


Figure 9-9. Schematic diagram of passive plume mixing into near-wake.

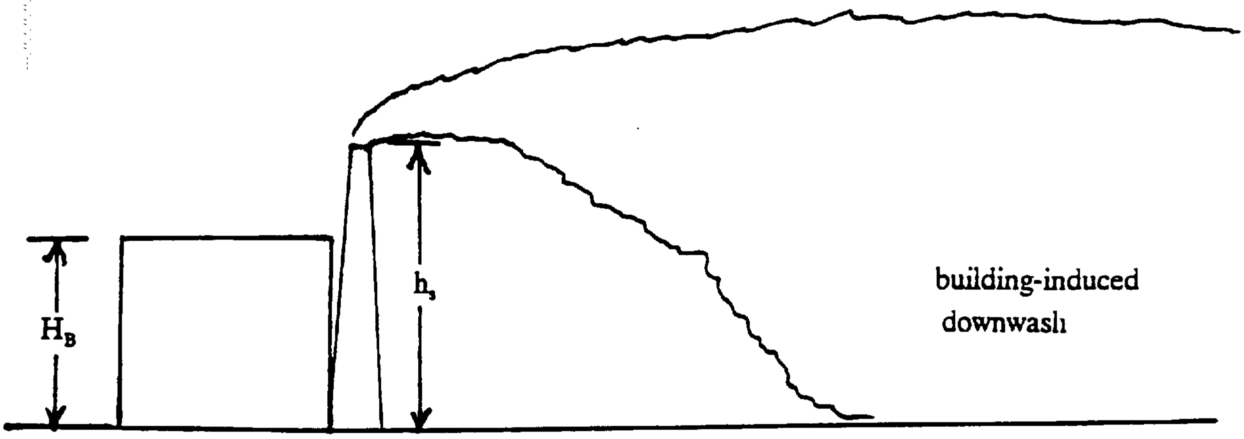


Figure 9-10. Scenario of dispersion in the far-wake, for which the ISC model downwash algorithms applicable.

10. HGSYSTEM VALIDATION

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10. HGSYSTEM VALIDATION

10.1. Objectives of model evaluation exercise

The primary objective of the work described in this section has been to evaluate the new HGSYSTEM version 3.0 package with data from full-scale field experiments. The performance has been compared with the performance of other hazardous gas models for limiting cases such as non-buoyant inert gases and non-reactive dense gases. As a result the typical accuracy's and relative uncertainties of the models can be estimated.

10.2. Evaluations with field data from eight sites

10.2.1. Models to be included

The new HGSYSTEM version 3.0 package has been included in all evaluations. Because nine independent dense gas models (DEGADIS, SLAB, AIRTOX, CHARM, FOCUS, GASTAR, PHAST, TRACE, Britter and McQuaid) had already been evaluated with the field data sets that were used, the performance statistics for HGSYSTEM 3.0 could be directly compared to performance statistics that existed in the files for these nine models (Hanna et al., 1993).

10.2.2. Description of field data sets

The set of field data used for this portion of the evaluations includes the eight experiments used by Hanna et al. (1993) in their evaluation of 14 hazardous gas models. The characteristics of these data sets are summarised in Table 10-1. It is seen that the data include non-buoyant releases (Prairie Grass and Hanford), continuous dense gas releases (Burro, Coyote, Desert Tortoise, Goldfish, Maplin Sands, and part of the Thorney Island tests), and instantaneous dense gas releases (Thorney Island). The three Goldfish trials involved releases of HF (about 4000 kg per trial). There are 41 separate field trials involving dense gases. These data are all stored on Earth Tech's computer files in a so-called Modelers Data Archive (MDA) that has been widely distributed to interested scientists and engineers throughout the world. We do not describe the details of these datasets here, but refer the reader to Section 3 of the Hanna et al. (1993) article, or to Volume II of the Hanna et al. (1991) project report prepared for the U.S. Air Force and the American Petroleum Institute.

The Hanna et al. (1993) model evaluation exercise included the 1990 version (indicated by NOV90 or version 1.0) of HGSYSTEM, which was applied to the eight field data sets listed in Table 10-1.

Table 10-1. Summary of characteristics of the datasets used by Hanna et al. (1993) in their model evaluations

	Burro	Coyote	Desert Tortoise	Goldfish	Hanford Kr^{85} (Continuous)	Maplin Sands	Prairie Grass	Thorney Island (Instantaneous)	Thorney Island (Continuous)
Number of Trials	8	3	4	3	5	4,8	44	9	2
Material	LNG	LNG	NH_3	HF	Kr^{85}	LNG, LPG	SO_2	Freon & N_2	Freon & N_2
Type of Release	Boiling Liquid (dense gas)	Boiling Liquid (dense gas)	2-Phase Jet (dense gas)	2-Phase Jet (dense gas)	Gas (non-buoyant)	Boiling Liquid (dense gas)	Gas Jet (non-buoyant)	Gas (dense gas)	Gas (dense gas)
Total Mass (kg)	10700-17300	6500-12700	10000-36800	3500-3800	11-24*	LNG 2000-6600 LPG 1000-3800	23-63	3150-8700	4800
Duration (s)	79-190	65-98	126-381	125-360	598-1191	60-360	600	Instantaneous	460
Surface	Water	Water	Soil	Soil	Soil	Water	Soil	Soil	Soil
Roughness (m)	.0002	.0002	.003	.003	.03	.0003	.006	.005-.018	.01
Stability Class	C-E	C-D	D-E	D	C-E	D	A-F	D-F	E-F
Max. Distance (m)	140-800	300-400	800**	3000	800	400-650	800	500-580	472
Min. Averaging Time (s)	1	1	1	66.6-88.3	38.4	3	Dosage	0.06	30
Max. Averaging Time (s)	40-140	50-90	80-300	66.6-88.3	270-845	3	600	0.06	30
Reference	Koopman et al. 1982	Goldwire et al. 1983	Koopman et al. 1985	Blewitt et al. 1987	Nickola et al. 1970	Puttock et al 1980	Barad, 1958	McQuaid and Roebuck, 1985	McQuaid and Roebuck, 1985

* Curies, rather than kg, are used as a measure of the amount of this radioactive tracer released

** Concentrations are measured beyond 800 m, but there are not well-instrumented measurement arcs.

Because one new module (HEGABOX for instantaneous sources) has been added to HGSYSTEM 3.0, one module (PLUME) has been superseded by another module (AEROPLUME), and most parts of the model have changed slightly, HGSYSTEM 3.0 has been re-evaluated with the eight sets of field data. The following component modules of HGSYSTEM have been applied to these data in our new model evaluation exercise.

Field Experiment and Source Type	**Applied HGSYSTEM Module**
Burro (evaporation area source of LNG)	HEGADAS-S
Coyote (evaporating area source of LNG)	HEGADAS-S
Desert Tortoise (NH_3 aerosol horizontal jet)	AEROPLUME/HEGADAS-S
Goldfish (HF aerosol horizontal jet)	HFPLUME/HEGADAS-S
Hanford Kr^{85} (trace gas from point)	HEGADAS-S (orifice diameter unknown)
Maplin Sands (evaporating area source of LNG & LPG)	HEGADAS-S
Prairie Grass (trace gas (SO_2) from point)	AEROPLUME/PGPLUME
Thorney Island (instantaneous volume source of Freon & N_2)	HEGABOX/HEGADAS-T
Thorney Island (continuous area source of Freon & N_2)	HEGADAS-S

The existing Modelers' Data Archive (MDA) contained sufficient input data (e.g., mass emission rate, wind speed) to carry out the HGSYSTEM runs described above. The MDA also contained the concentration observations that were necessary for the statistical evaluations.

10.2.3. Model output parameters that were evaluated

Of primary interest in the evaluation is the maximum near-ground-level concentration at each downwind distance; a measure (say the standard deviation) of the plume width and height at each downwind distance; and the geometric characteristics of particular contours of concentration or dosage. For a module (i.e., AEROPLUME) where uniform crosswind and vertical profiles are assumed, the average plume concentration is the same as the maximum centreline concentration.

10.2.4. Statistical model evaluation procedures to be used

The statistical model evaluation software, BOOT, applied in the study described by Hanna et al. (1993), was used. The software has been well-tested in a wide range of studies and is currently in use by a number of groups in the U.S., Europe, and Australia. It involves the use of the relative mean bias, the normalised mean-square-error, the correlation coefficient, and the fraction of predictions within a factor of two of observations. Confidence intervals on these performance measures are generated by bootstrap resampling. Section 4 of the reference describes these procedures in detail.

10.2.5. Standards for accepting or rejecting model performance

Air quality modelers have not yet agreed upon the magnitude of standards for accepting or rejecting model performance. In most cases a model is considered 'acceptable' if most of its predictions are within a factor of two of the observations. However, in the case of dense gas models, the study by Hanna et al. (1993) demonstrated that the performance measures for several models were within a range of acceptability shown in Figure 10-1, which is a reproduction of Figure 1a in Hanna et al. (1993). It is seen that most models fall in a cluster of fair performance, with 0.7 < geometric mean bias < 1.5 and 1.3 < geometric variance < 2.5. Consequently it is expected that, to be acceptable, the performance measures for the new model would at least fall within this same range.

10.2.6. Results of model evaluation at eight field sites

The BOOT model evaluation software produces many tables and figures. Here we have selected a set of figures in which the geometric variance, VG, is plotted versus the geometric mean bias, MG, for each model. These performance measures are calculated from the following formulas:

$$VG = \exp\overline{\left(\ln\left({C_0}/{C_p} \right) \right)^2} \quad (1)$$

$$MG = \exp\overline{\left(\ln\left({C_0}/{C_p} \right) \right)} \quad (2)$$

Therefore a 'perfect' model would have VG = MG = 1.0.

Five figures are presented. Figure 10-2a,b,c consists of a set of results for concentration predictions for three groups of data--a) continuous dense gas field data, b) continuous passive gas field data, and c) instantaneous dense gas field data. Figure 10-3a,b is concerned with predictions of plume width for groups a) and b).

Figure sets a) and b) show that there is very little difference between the results for the 'old' (version 1.0) and 'new' (version 3.0) HGSYSTEM models. Both versions overpredict the mean by about 20 to 40% with a geometric variance of about 2, and both versions are within the cloud of the five or six best-performing models. The biggest difference occurs for Figure 10-2c (instantaneous dense gas field data), where the 'old' model did not apply at all, while the 'new' model (with the addition of HEGABOX) now applies and is one of the three best-performing models (along with AIRTOX and the Britter and McQuaid nomograms).

Like the other dense gas models, HGSYSTEM overpredicts the dense gas plume widths by about 50% (see Figure 10-3a) and underpredicts the passive gas plume widths by about 30% (see Figure 10-3b).

It is concluded that the new version 3.0 of HGSYSTEM is among the better performing models, with a typical mean bias of about 20 to 40% and a typical scatter less than a factor of two.

10.3. References

S.R. Hanna, J.C. Chang and D.G. Strimaitis, Hazardous gas model evaluation with field observations. *Atmos. Environ.*, **27A**, 2265-2285, 1993.

S.R. Hanna, D.G. Strimaitis and J.C. Chang, *Hazard Response Modeling Uncertainty (A Quantitative Method) Vol. II, Evaluation of Commonly-Used Hazardous Gas Dispersion Models*, Sigma Research Corp., Concord, MA, 1991.

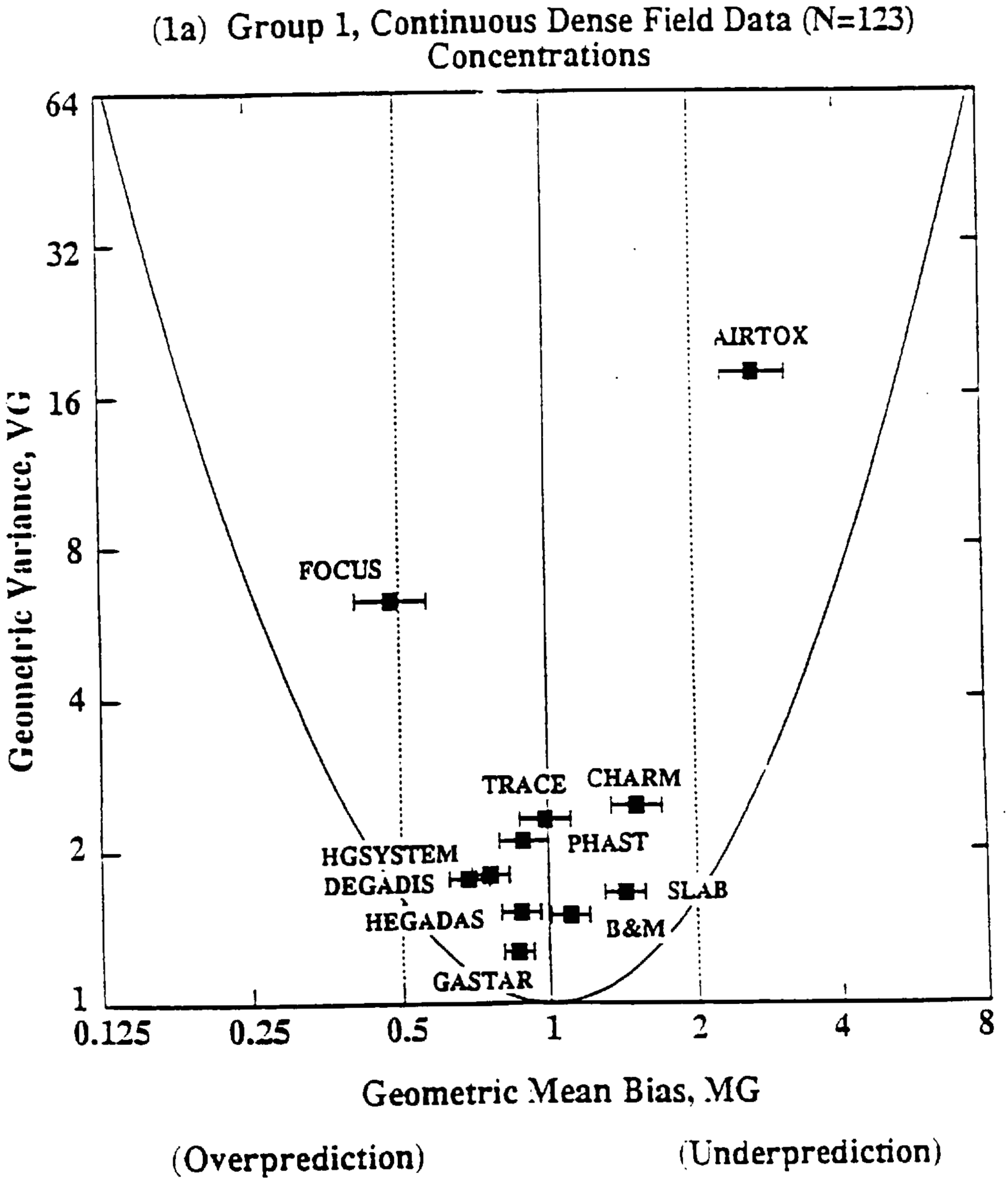

Figure 10-1. Example of presentation of model evaluation results from Hanna et al. (1993).

Group 1. Continuous Dense Field Data (N = 123) Concentrations

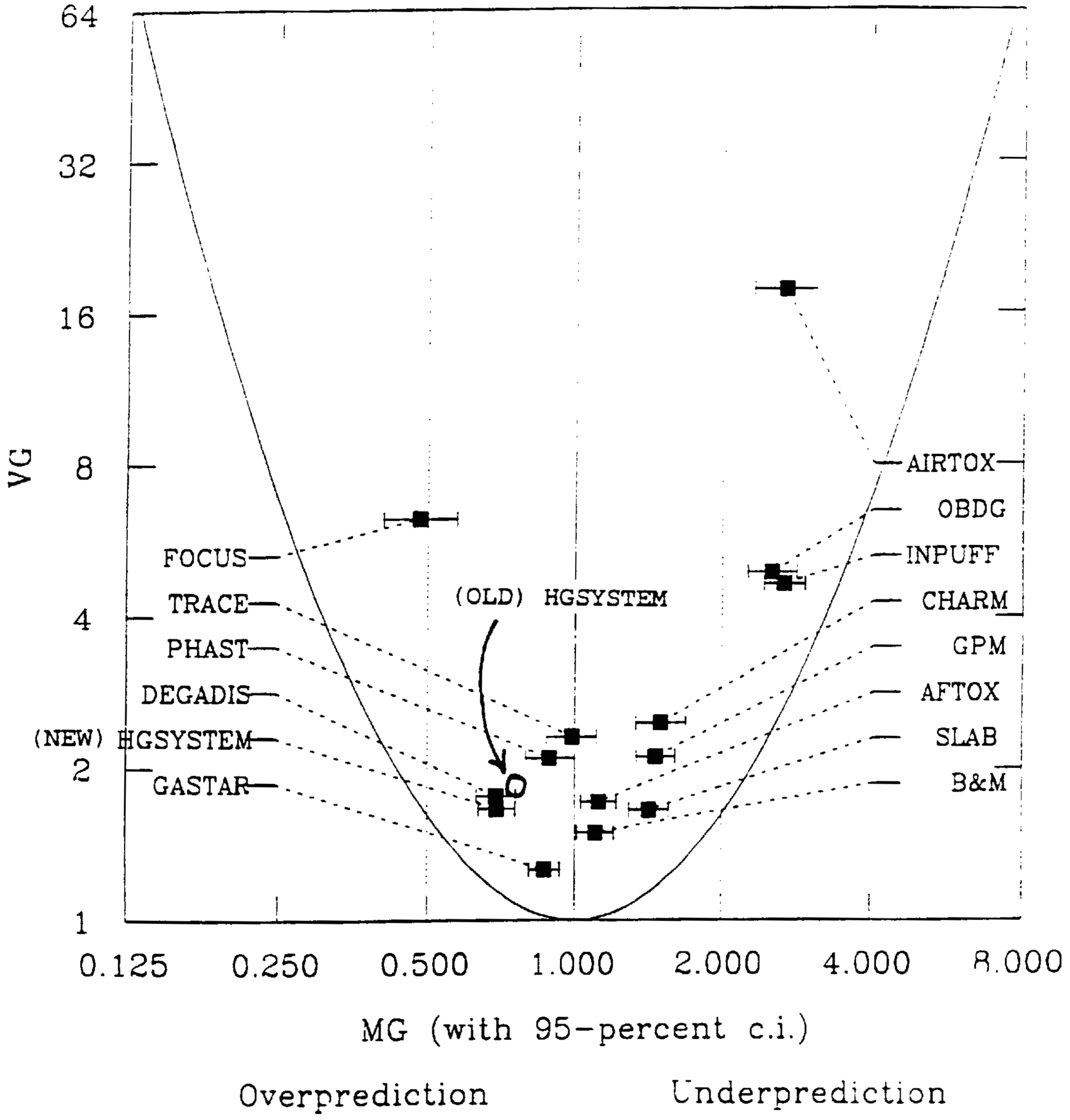

Figure 10-2a. Model performance measures, geometric mean bias MG and geometric variance VG, for maximum plume centreline concentration predictions and observations. 95% confidence intervals on MG are indicated by the horizontal lines. The solid parabola is the 'minimum VG' curve. The vertical dotted lines represent 'factor of two' agreement between mean predictions and observations. Group 1 - Continuous dense gas data sets (Burro, Coyote, Desert Tortoise, Goldfish, Maplin Sands, and Thorney Island), involving a total of 32 trials and 123 points for the shortest available instrument averaging times.

Group 2. Continuous Passive Field Data (N = 222) Concentrations

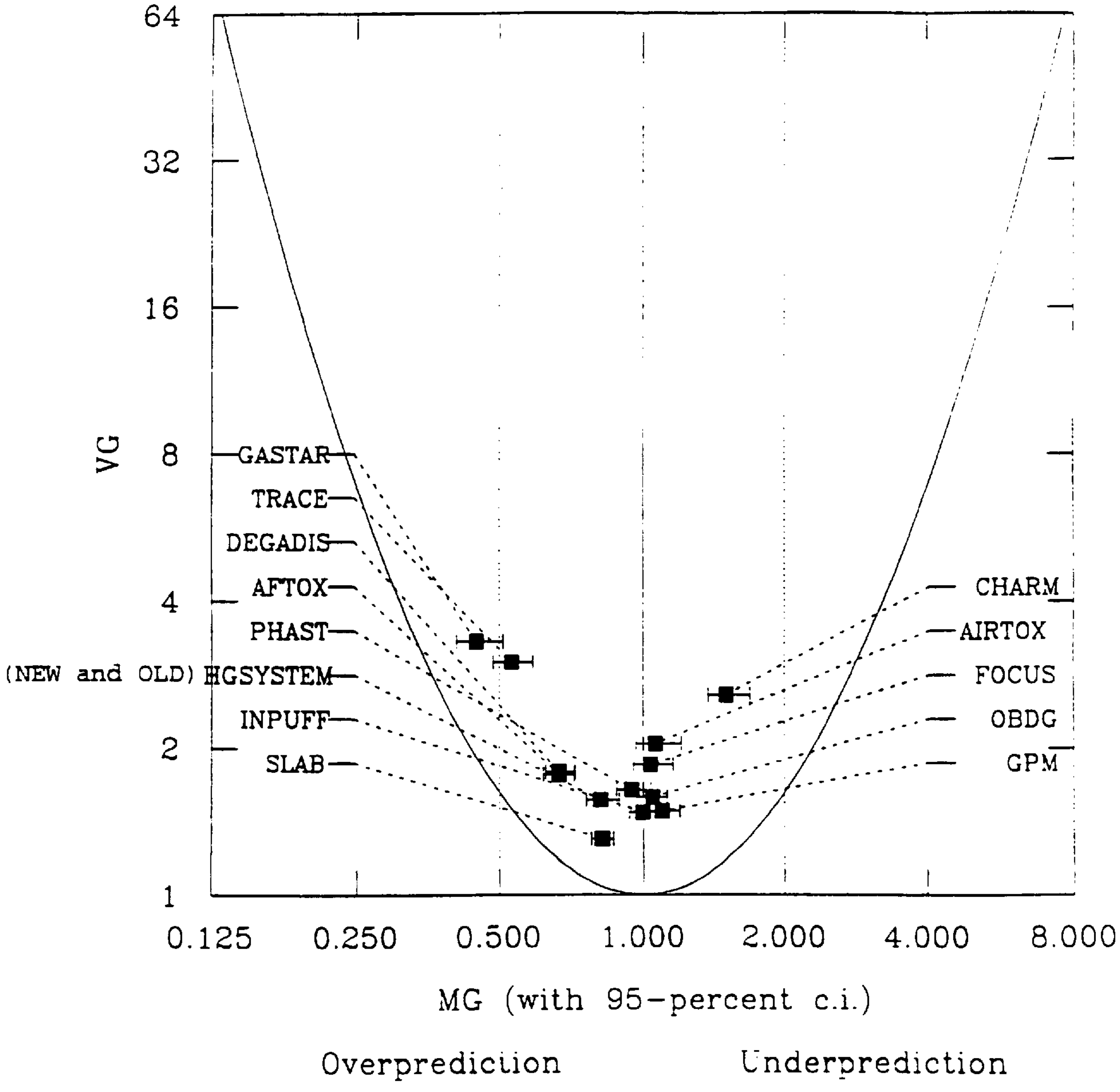

Figure 10-2b. Model performance measures, geometric mean bias MG and geometric variance VG, for maximum plume centreline concentration predictions and observations. 95% confidence intervals on MG are indicated by the horizontal lines. The solid parabola is the 'minimum VG' curve. The vertical dotted lines represent 'factor of two' agreement between mean predictions and observations. Group 2 - Continuous passive gas data sets (Prairie Grass and Hanford), involving a total of 49 trials and 222 points for the shortest available instrument averaging times.

Group 3. Instantaneous Dense Field Data (N = 61) Concentrations

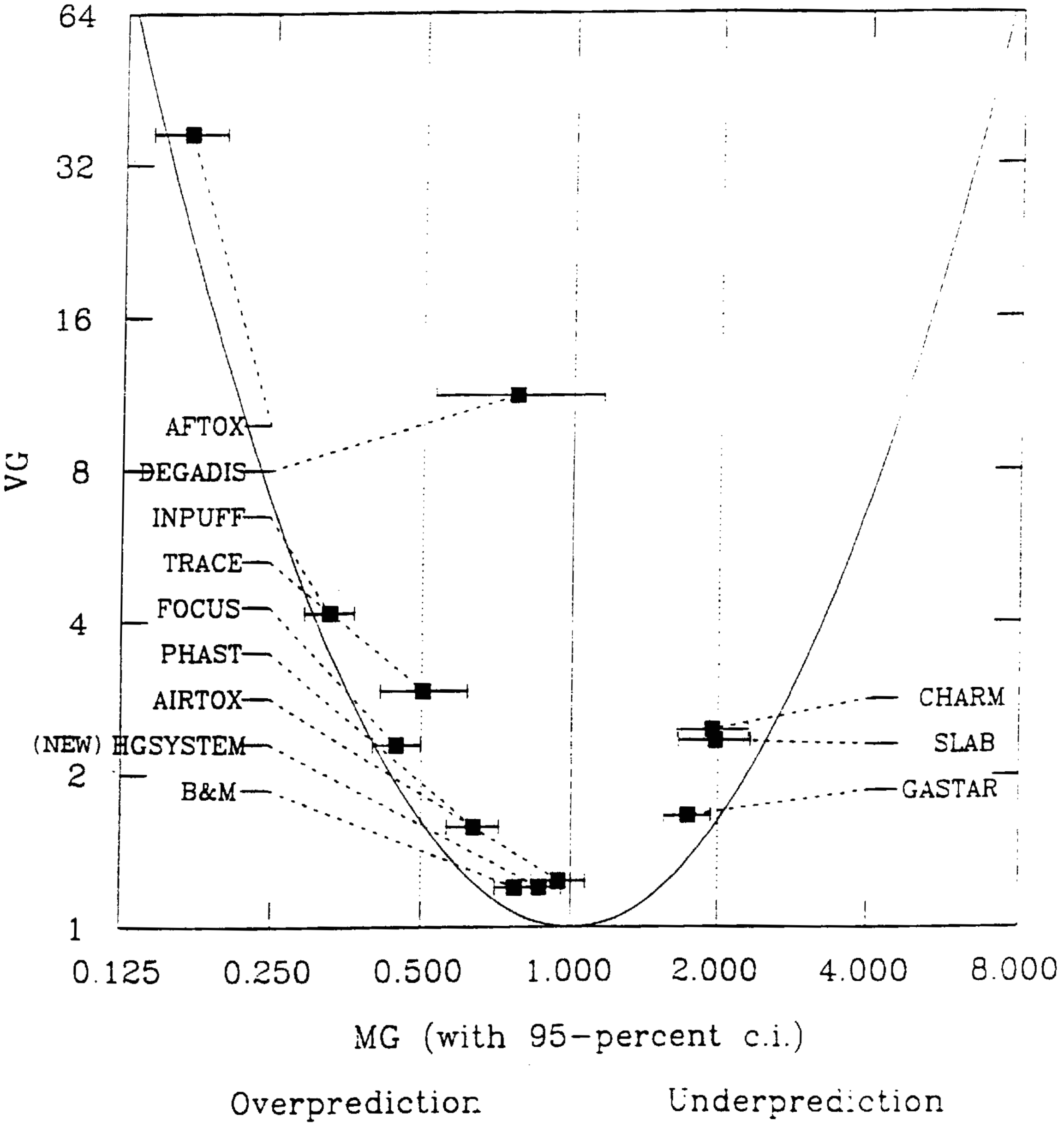

Figure 10-2c. Model performance measures, geometric mean bias MG and geometric variance VG, for maximum plume centreline concentration predictions and observations. 95% confidence intervals on MG are indicated by the horizontal lines. The solid parabola is the 'minimum VG' curve. The vertical dotted lines represent 'factor of two' agreement between mean predictions and observations. Group 3 - Instantaneous dense gas data set (Thorney Island), involving a total of 9 trials and 61 points for the shortest available instrument averaging times.

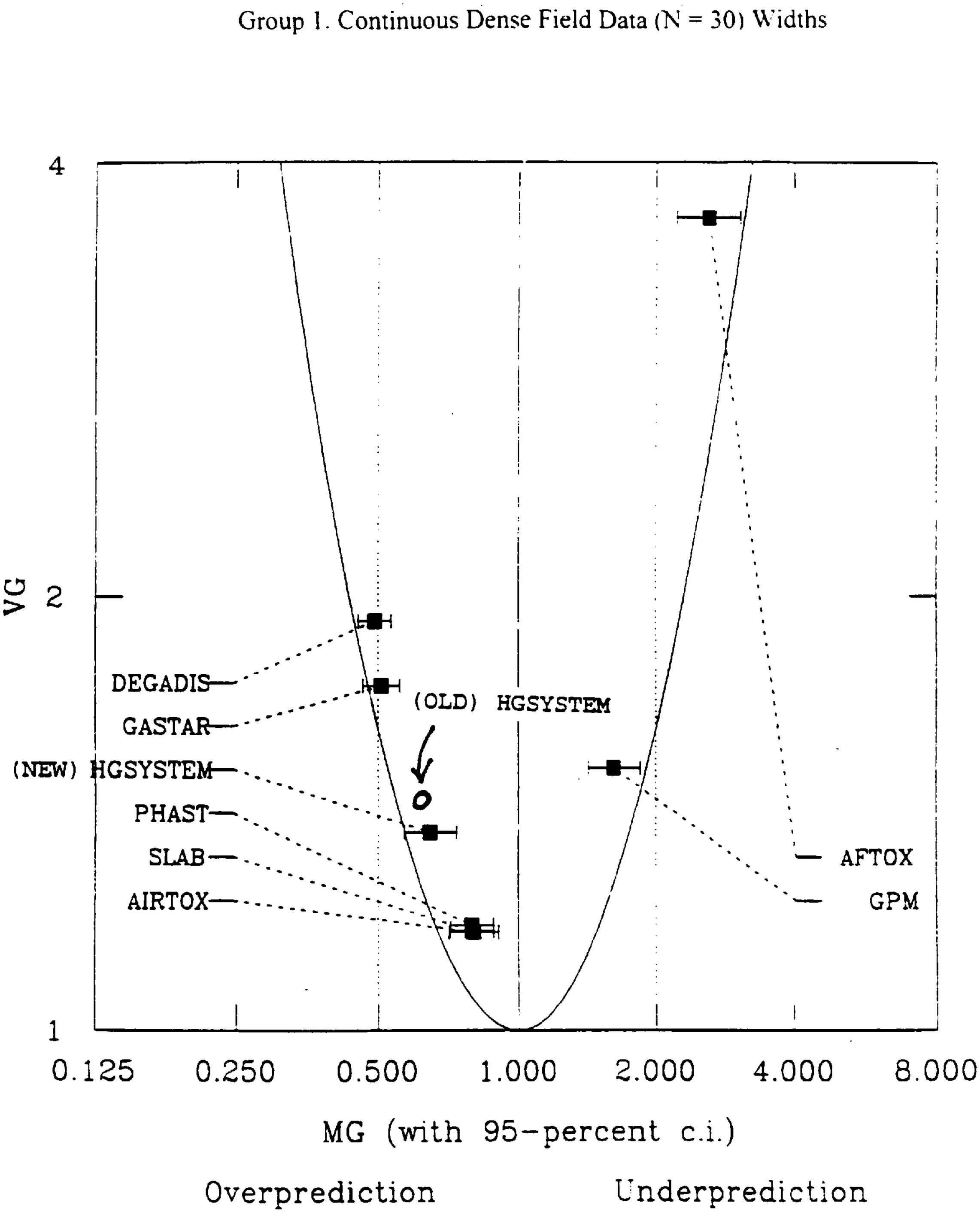

Figure 10-3a. Model performance measures, geometric mean bias MG and geometric variance VG, for plume width predictions and observations. 95% confidence intervals on MG are indicated by the horizontal lines. The solid parabola is the 'minimum VG' curve. The vertical dotted lines represent 'factor of two' agreement between mean predictions and observations. Group 1 - Continuous dense gas data sets (Burro, Coyote, Desert Tortoise, and Goldfish) involving 18 trials and 30 points.

Group 2. Continuous Passive Field Data (N = 85) Widths

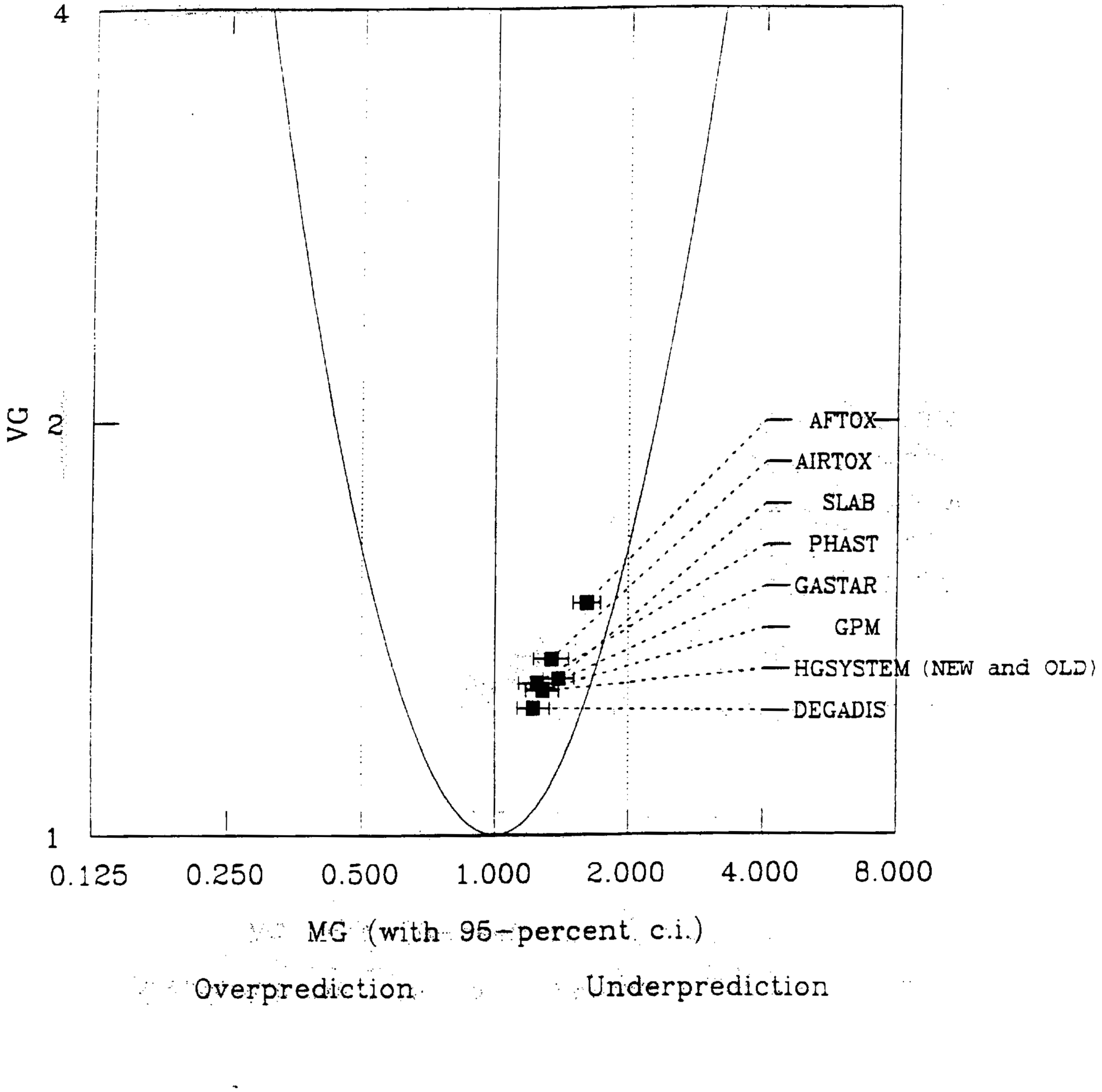

Figure 10-3b. Model performance measures, geometric mean bias MG and geometric variance VG, for plume width predictions and observations. 95% confidence intervals on MG are indicated by the horizontal lines. The solid parabola is the 'minimum VG' curve. The vertical dotted lines represent 'factor of two' agreement between mean predictions and observations. Group 2 - Continuous passive gas data sets (Prairie Grass and Hanford) involving a total of 49 trials and 85 points.

HGSYSTEM 3.0

User's Manual

by

L. Post

TNER.94.058

Shell Research Limited, Thornton Research Centre,
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HGSYSTEM 3.0

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John A. King, Shell Development Company
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The LPOOL model was made available by Exxon Research and Engineering Company.

EXECUTIVE SUMMARY

1. Historical background

As a result of many years in-house research, the gas dispersion group at Shell Research Ltd. Thornton (United Kingdom) has developed a package of mathematical models, called HGSYSTEM, to study the atmospheric dispersion of accidental pollutant releases with emphasis on denser-than-air materials. HGSYSTEM can be simulate different dispersion scenarios (jet dispersion, heavy gas dispersion, passive dispersion). The first version of HGSYSTEM was made freely available for use in November 1990. This version, called NOV90 or version 1.0, was prepared by Shell Research Ltd. for *The Industry Cooperative HF Mitigation/Assessment Program, Ambient Impact Assessment Subcommittee* as one component of a wider programme aimed at a better understanding of atmospheric dispersion, including hydrogen fluoride (HF) releases. HGSYSTEM can model the full HF chemistry and thermodynamics. Most of the modules in the HGSYSTEM package can also be used for more general, non-reactive (ideal gas) releases as well. Validation of the HF-related simulations has been done with the well-known Goldfish Test Series. Full documentation to the 1.0 version was given in the HGSYSTEM Technical Reference Manual and User's Manual.

After release of the 1.0 (NOV90) version, a version 1.1 was made available which contained minor changes to solve some program bugs. Several internal versions were also developed.

2. HGSYSTEM 3.0

HGSYSTEM is in wide use for simulation of atmospheric dispersion scenarios for HF and other pollutant releases. It has been assessed against other models and found to rank amongst the best available atmospheric dispersion models in the world. HGSYSTEM sets the standard for HF dispersion calculations. However, a number of topics were open for improvement and generalisation. With financial support of the *American Petroleum Institute, Air Modelling Task Force*, Shell Research has upgraded and updated the existing HGSYSTEM package, resulting in a new release called HGSYSTEM version 3.0. The following major changes have been made to HGSYSTEM 1.0 to obtain HGSYSTEM 3.0:

- The thermodynamical models available in HGSYSTEM have been extended. The full HF chemistry and thermodynamical model is now suitable for mixtures of HF, water and an inert ideal gas. The non-reactive ideal gas description has been extended to multi-compound liquid-vapour mixtures (aerosols).

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- A database containing physical properties for some 30 compounds has been added to HGSYSTEM. This database is needed when using the new two-phase multi-compound thermodynamical model.

- The PLUME model for pressurised releases has been extended to model jet dispersion of multi-compound, two-phase mixtures and is now called AEROPLUME.

- A new model describing the initial phase of instantaneous releases, HEGABOX, has been added to HGSYSTEM.

- A new model to calculate release rates from pressurised vessels, SPILL, is now available in HGSYSTEM version 3.0.

- The existing evaporating pool model EVAP has been replaced by a better model, LPOOL, for boiling and non-boiling pools and land and water. LPOOL is based on a model developed by Exxon Research and Engineering Company.

- The formulation of the lateral spreading in the heavy gas dispersion model HEGADAS has been reviewed and improved.

- Several options have been added to the time-dependent version of the heavy gas model HEGADAS making it easier to use and to evaluate the results.

- HGSYSTEM now contains three post-processors to generate data for graphical output after a pressurised jet release, steady state heavy gas release and a time-dependent heavy gas release respectively. These post-processors will improve the ease of use of the HGSYSTEM modules.

- Five additional options resulting from work done on HGSYSTEM as sponsored by Martin Marietta Energy Systems Inc (USA) are available to all HGSYSTEM users.

- A new HGSYSTEM 3.0 User's Manual and Technical Reference Manual have been written. These are now up-to-date and their format allows for easy future updating.

3. Modules available in HGSYSTEM 3.0

The following models are available in HGSYSTEM version 3.0:

Database program

DATAPROP	generates physical properties used in other HGSYSTEM models

Source term models

SPILL	transient liquid release from a pressurised vessel
HFSPILL	SPILL version specifically for hydrogen fluoride (HF)
LPOOL	evaporating multi-compound liquid pool model (unpressurised release)

Near-field dispersion models

AEROPLUME	high-momentum jet and elevated plume model
HFPLUME	AEROPLUME version specifically for hydrogen fluoride (HF)
HEGABOX	dispersion of instantaneous heavy gas releases

Far-field dispersion models

HEGADAS	heavy gas dispersion (steady-state and transient version)
PGPLUME	passive Gaussian plume dispersion

Utility programs

HFFLASH	flashing of hydrogen fluoride (HF) from pressurised vessel
POSTHS/POSTHT	post-processing of HEGADAS results (steady state and time-dependent version)
PROFILE	post-processor for concentration contours of air borne plumes
GET2COL	utility for data retrieval

4. Documentation

HGSYSTEM version 3.0 is documented in the following two manuals:

HGSYSTEM 3.0 User's Manual
L. Post
Shell Research Limited, Thornton Research Centre, TNER.94.058
1994

HGSYSTEM 3.0 Technical Reference Manual
L. Post (editor)
Shell Research Limited, Thornton Research Centre, TNER.94.059
1994

The User's Manual is thought to be the main reference document for normal us of the HGSYSTEM modules. It contains all information necessary to run the models and interpret the generated results. The Technical Reference Manual is intended as a source of background information for users who want to know more about the technical/scientific contents of the HGSYSTEM modules.

HGSYSTEM 3.0 Course Notes (TNER.94.060) are also available for use during possible HGSYSTEM training sessions.

HGSYSTEM USER's MANUAL

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1. GENERAL INTRODUCTION

1.1. About HGSYSTEM

The HGSYSTEM package is a PC based set of atmospheric dispersion models developed by Shell Research Ltd. It contains a wide range of models (or modules) to simulate source terms, near-field and far-field dispersion. HGSYSTEM can be used to study one particular aspect of a dispersion situation, using one of the available HGSYSTEM models. But by using several modules in sequence, HGSYSTEM can also be used to simulate a complete *scenario* starting from a release source, then modelling the near-field dispersion and finally calculate the far-field dispersion.

The thermodynamical descriptions available in HGSYSTEM are either a reactive hydrogen fluoride (HF) chemistry and thermodynamics model or a non-reactive two-phase multi-compound thermodynamics model.

The first public domain release of HGSYSTEM version 1.0 was in November 1990 and this version is also denoted as the NOV90 version. Some later versions of HGSYSTEM have been developed but were not made publicly available.

Version 3.0 is the second public domain version of HGSYSTEM. It is made available, both in executable form and in Fortran source code, to all interested parties, under copyright of Shell Internationale Research Maatschappij B.V., The Hague.

Please note that HGSYSTEM has a complete package has a version number, but the individual HGSYSTEM modlues all have their own version number as well. The module version numbers are usually different from the package version number.

1.2. About this User's Manual

This User's Manual is intended as a *concise* guide to all the HGSYSTEM modules, giving per chapter a short description of each model and more detailed information for all input parameters.

It can be used for **HGSYSTEM version 3.0** and later.

New users of HGSYSTEM are advised to read the first 4 chapters of this Manual before running HGSYSTEM models. Then they can read the more detailed information for a specific HGSYSTEM module in the corresponding chapter of the Manual.

Experienced HGSYSTEM users can read the chapter for the HGSYSTEM model they want to use.

Every user is strongly advised to study the information for the HGSYSTEM module to be used, as the description of the input parameters will also make clear what the program capabilities and limitations are.

1.3. HGSYSTEM modules

The HGSYSTEM package consists of several modules which can all be used as independent simulation models for a specific atmospheric dispersion situation. Some of the modules calculate release (or source) terms, others simulate different dispersion scenarios like evaporating liquid pools, jet dispersion and heavy gas dispersion.

Although all models can be run individually, it is often quite useful when simulating a complete dispersion *scenario* (source term calculation, near-field dispersion simulation and far-field dispersion simulation) to run models *consecutively*. HGSYSTEM offers several combinations of consecutive model runs. Each model is run separately, but information generated by one model can be communicated to a following model using so-called *link files*. See Chapter 4 on running HGSYSTEM scenarios.

The following models (or modules) are available in HGSYSTEM.

Database program

DATAPROP	generates physical properties used in other HGSYSTEM models

Source term models

SPILL	transient liquid release from a pressurised vessel
HFSPILL	SPILL version specifically for hydrogen fluoride (HF)
LPOOL	evaporating multi-compound liquid pool model ('unpressurised release')

Near-field dispersion models

AEROPLUME	high-momentum jet model
HFPLUME	AEROPLUME version specifically for hydrogen fluoride (HF)
HEGABOX	dispersion of instantaneous heavy gas releases

Far-field dispersion models

HEGADAS	heavy gas dispersion (steady-state and transient version)
PGPLUME	passive Gaussian dispersion

Utility programs

HFFLASH	flashing of hydrogen fluoride (HF) from pressurised vessel
POSTHS/POSTHT	post-processing of HEGADAS results (steady state and time-dependent version)
PROFILE	post-processor for concentration contours of air borne plumes
GET2COL	utility for data retrieval

Most of these models can be used as individual models (see Chapter 3 of the User's Manual). However, running them consecutively, as described in Chapter 4 of the User's Manual, adds considerably to the value of the models.

In figure 1 the main HGSYSTEM models are shown and also the possible links that can be made between the different models. For example, the database program DATAPROP generates physical properties for the used compounds in a mixture and communicates these via a link file to AEROPLUME, SPILL, LPOOL, HEGABOX and HEGADAS. In another example. first SPILL is used to calculate discharge rate from a pressurised vessel. Using this information an AEROPLUME run is made and this model makes a transition to HEGADAS. A complete scenario is thus simulated, starting from a source term description (SPILL), calculating near-field jet dispersion (AEROPLUME) and simulating far-field heavy gas dispersion (HEGADAS). For more details, see Chapter 4 on running HGSYSTEM scenarios.

1.4. Parameters describing atmospheric conditions

Most HGSYSTEM modules require specification of parameters describing the state of the ambient atmosphere. As not all users may be familiar with these a short description is given of the most important of these parameters.

Wind speed and ambient temperature

The speed of the ambient wind and the atmospheric temperature are measured at a given reference height (usually 10 m). These important atmospheric parameters can be obtained from meteorological data.

Both the reference wind speed and temperature are used in HGSYSTEM models to calculate the full boundary profiles for wind speed and temperature.

Atmospheric stability class.

In order to define meteorological conditions in a relative simple way, a system of stability classes has been introduced. These are called Pasquill-Gifford classes. They are given by the single characters A, B, C, D, E and F ranging from very unstable to stable conditions.

Table 1 gives an overview of the Pasquill stability classes and table 2 shows how the stability class depends on the meteorological conditions.

Surface roughness length

The surface roughness parameter is a measure for the ground surface roughness which determines the turbulence characteristics of the ambient boundary layer. It is taken to be about 1/10 to 1/30 of the height of a typical roughness element as present on the ground surface.

It is about 1 m for cities, forests and industrial sites, 10 cm for agricultural crops, 1 cm for grass and 1 mm for water or paved surfaces.

Monin-Obukhov length

This is a turbulent length scale depending on meteorological conditions. This parameter never has to be specified by the user when running HGSYSTEM models. If needed, it is calculated within the model itself.

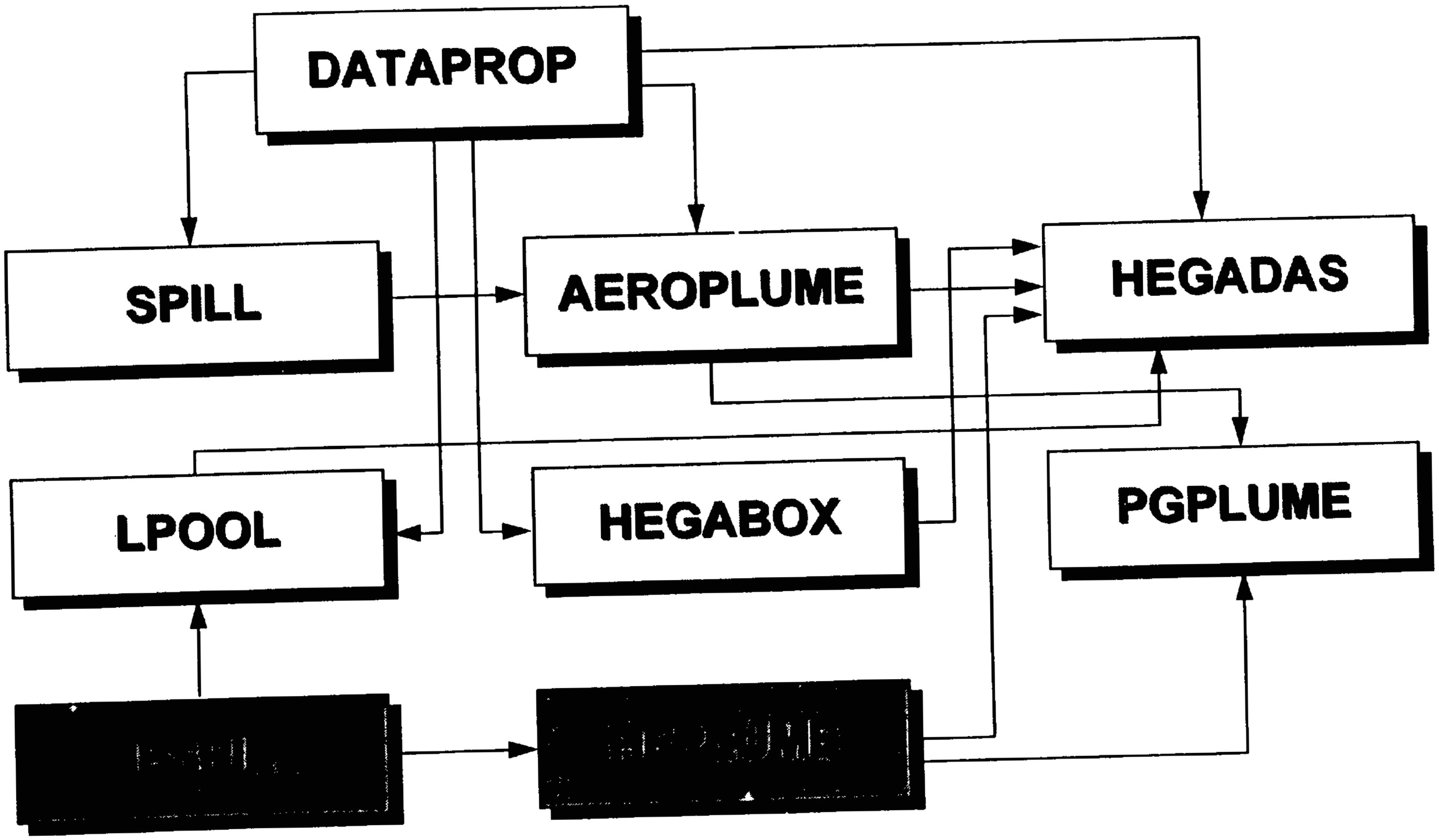

Figure 1. Main HGSYSTEM modules and links between them. HF specific modules indicated by darker shading.

A: Extremely unstable conditions	D: Neutral conditions
B: Moderately unstable conditions	E: Slightly stable conditions
C: Slightly unstable conditions	F: Moderately stable conditions

Table 1. Pasquill-Gifford stability classes

	Daytime insolation			Night-time conditions	
Surface wind speed (m/s)	Strong	Moderate	Slight	Thin overcast or > 4/8 low cloud	≤ 4/8 cloudiness
< 2	A	A - B	B		
2 - 3	A - B	B	C	E	F
3 - 4	B	B - C	C	D	E
4 - 6	C	C - D	D	D	D
> 6	C	D	D	D	D

Table 2. Meteorological conditions defining Pasquill stability classes.

2. INSTALLATION OF HGSYSTEM

2.1. Introduction

HGSYSTEM is a PC (personal computer) based package of models which can only be installed as a complete system. In the following installation description it is assumed that the user has a basic knowledge of DOS. As HGSYSTEM works with input files which have to be edited, the user must have a file editor available on his PC and the user must know how to make (simple) changes with this editor. HGSYSTEM does not run under Windows but is called directly from the DOS command line.

2.2. System requirements

HGSYSTEM 3.0 executable code is generated using the Microsoft Fortran Powerstation compiler. This means that the code will only run on a IBM compatible machine with an 80386 or 80486 processor running MS-DOS version 3.3 or later. *At least 4 Megabytes of memory is needed.* The code will use its own (extended) memory manager (DOSXMSF.EXE, available in the HGSYSTEM directory) while running. The PC should have at least 2.5 Megabyte of free disk space before installation of HGSYSTEM.

Although HGSYSTEM can be run on any machine that meets the above requirements, it is strongly recommended to install HGSYSTEM on a PC with a mathematical co-processor, as calculation times can become quite large if complicated simulations are being done on a machine without a co-processor.

HGSYSTEM 3.0 is delivered on a set of 1.44 MB (high density) 3.5-inch disks, thus an appropriate disk drive is needed for installation.

2.3. Installation

The user can install the executable code and, optionally for expert users, the program Fortran source code.

On the labels of every HGSYSTEM diskette, the correct installation command is given. It is assumed that the diskettes are installed from drive A to drive C, but if other drive names apply, they can be used instead of the default names without any problem. The installation should take place in the correct diskette order (starting with diskette HGSYSTEM-1).

After running the installation program, the PATH command in the AUTOEXEC.BAT file must be extended by adding the following path:

```
C:\HGSYSTEM
```

assuming HGSYSTEM is installed on the C drive (change if other drive has been used).

Please check that the FILES parameter in the CONFIG.SYS file is large enough (at least 50).

To use the colours in the interactive HGSYSTEM program, the ANSI.SYS driver should be installed in CONFIG.SYS (consult your DOS manual).

To update your PATH statement, your PC has to be rebooted.

After installation of the executable code, there are three new directories on the hard disk:

C:\HGSYSTEM	contains all the executable code (programs)
C:\HGSYSTEM\DATADICT	contains data dictionaries
C:\HGSYSTEM\STINPUT	contains example (partial) input files

Here it is assumed that HGSYSTEM has been installed on the C drive. Data dictionaries and input files will be discussed in Chapter 3.

It is strongly advised to create a separate working sub-directory (e.g. C:\HGWORK) to run the models. *Do not run the models in the three above mentioned directories.*

After installing the Fortran source code (optional, only for expert users) a directory named C:\HGSOURCE will have been created. This directory has several sub-directories, one for each model. The source code is installed in a compressed format. The utility program PKUNZIP, which is available in directory C:\HGSYSTEM, can be used to un-compress these files. Giving the command PKUNZIP without any parameters will bring up a information screen on how to use PKUNZIP.

3. RUNNING AN INDIVIDUAL HGSYSTEM MODEL

3.1. General introduction

HGSYSTEM is a software package with several modules. These modules are separate computer programs that can be run individually. Before any individual model can be run, an appropriate input file must have been prepared. For every model available in HGSYSTEM, example input file can be found in directory C:\HGSYSTEM\STINPUT. For file name conventions see below.

3.2. Running an individual HGSYSTEM model

As an example let us consider an individual run of the AEROPLUME model. From the tables 2 and 3 given below it can be seen that AEROPLUME input files always have the file extension API. The example AEROPLUME input file is called SKELETON.API.
Start by copying the example AEROPLUME input file to a file called EXAMPLE.API in a working directory (say C:\HGWORK):

```
COPY C:\HGSYSTEM\STINPUT\SKELETON.API C:\HGWORK\EXAMPLE.API
```

Now, using a file editor, the input file (EXAMPLE.API in this case) can be changed so that the input information corresponds to the case to be simulated. The general structure of input files will be discussed below. When the input file has been updated, running AEROPLUME with this input data is performed by giving the following command:

```
AEROPLUME EXAMPLE
```

In general, running HGSYSTEM model with name 'MODELNAME' in combination with an input file which has a file name 'CASENAME.EXT' is done by the command

```
MODELNAME CASENAME
```

The (up to eight-characters) 'CASENAME' part of the input file name can be freely specified by the user (following DOS file name conventions). The (three-character) 'EXT' part of any HGSYSTEM file follows a strict convention which will be discussed below. All model output names will have 'CASENAME' as the first part of their file name. As explained later, the type of file is indicated by the last character of the three-character extension. *Please note that using the same 'CASENAME' twice means that all model output files created during the first run will be overwritten during the second run of the model.* Preferably use different names for different model runs.

The 'MODELNAME' for any HGSYSTEM model is simply the name as it is used in this Manual. For HEGADAS-S and HEGADAS-T the names are HEGADASS and HEGADAST respectively.

In our current example, AEROPLUME is actually the name of a batch file AEROPLUM.BAT which can be found in the C:\HGSYSTEM directory. This batch file calls the programs that read in the input file, check the input data and perform the actual AEROPLUME calculations. The batch file also does all the file manipulations needed for a model run.

The program that reads in the input data from the input file and checks whether the input data is valid is called FFMAIN. FFMAIN can only check whether all necessary data is given and whether the data falls within the range specified in the so-called 'data dictionary' of the specific model. For example, the input file for AEROPLUME *must* contain the orifice diameter and this diameter must have a value between 0.001 and 5 meter. A missing value for the diameter or a value outside this range would cause FFMAIN to signal an input file error.

If an input file contains invalid data of this kind, the program execution will stop. The input file will now contain error messages at the appropriate positions in file. The user must correct the errors before restarting the model run. The user does *not* have to remove the error messages from the input file: these will be automatically deleted once the input data is found to be correct.

Every model will perform its own checks on input data *consistency*. If errors are found these will be reported in the model report file or in a specific error file. For example, if specified, the reservoir pressure in an AEROPLUME input file must exceed the ambient pressure.

Each HGSYSTEM model will produce several different *output* files. The model batch file will display a screen message, after the model run, naming all output files created during this run. Usually the most important one is the *report* file. This file contains calculated results and model run information. The user will be mainly interested in this information. Possible *link* files are also important as they contain information needed in subsequent runs of other HGSYSTEM models for a particular scenario (see Chapter 4). A *monitor* file, if created by the model, echoes all screen messages for later reference. *Error* and *warning* files will only be created if found necessary by the program.

Some files, containing information useful for expert users only, are deleted in the final part of the model batch file. Expert users may want to disable these DOS 'delete' commands by editing the corresponding batch files in the C:\HGSYSTEM directory.

File name conventions are discussed in a later paragraph of this chapter.

3.3. The interactive program HGINTER

The HGSYSTEM package comes with an interactive utility program that allows the user to run one or more HGSYSTEM models. This program is particularly useful if a complete scenario is followed (that is, several models are run consecutively to perform a complete source/near-field/far-field simulation), but it can also be used to run one model. The interactive program can be started by giving the following command:

```
HGSYSTEM CASENAME
```

In a question and answer session, the interactive program determines which models to run in what order. The user only has to modify standard input files to specify the parameters to be used for the model runs. More details on using HGINTER to run a series of models are given in Chapter 4.

3.4. Input files

All HGSYSTEM input files have the same structure. All input data is organised in input block, each with a unique keyword. Within every input block, several input values are entered. Every input value has a unique keyword, followed by the data value. The order of keyword within an input block is irrelevant. The order of input block within the input file is also irrelevant. Information beyond the '*' symbol is treated as a comment. Spaces and comma's can be used as delimiters. Input file are 'free format' or 'flat' files: input data does not have to be in a specific location or column. Input files are ASCII files: they can be edited by any file editor (*not* by a word processor).

In table 1 an example HGSYSTEM input file is given. This example is for the AEROPLUME model. The use of input blocks, block parameters and comments is clear. The input keywords in this example are: RESERVOIR, RELEASE, GASDATA, PIPE, AMBIENT, DISP, TERMINAT and MATCH. The RESERVOIR block, for example, has two parameters, TRES and PRES. These two parameters are given a value. The TITLE input block is slightly exceptional in that here it is the input block keyword itself which is given a value. The TITLE input block has no further parameters.

For all HGSYSTEM models a complete discussion of all input blocks and parameters in given in subsequent chapters of this User's Manual. The permitted range of every parameter is indicated as well as physical units if applicable. It is also clearly indicated whether a parameters is mandatory or optional and, if optional, what the default values are. Mandatory parameters are parameters that *must* be specified in every input file. Optional parameters need not occur in the input file. If all parameters of an input block are optional, then the whole input block is optional. Sometimes *precisely one* of two alternative input blocks *must* be specified. This will be clearly indicated in the description.

3.5. HGSYSTEM input and output file names

All DOS files names used in the HGSYSTEM environment for input and output of a model, follow a strict nomenclature system.
All input and output file names have the structure:

<casename>.MMK

where <casename> is an identifier of up to 8 characters specified by the user when calling an HGSYSTEM module. It can be freely chosen within the DOS file name conventions.

The 'MM' in the file extension is a two letter code, which is unique for every HGSYSTEM module. Table 2 shows the letter combinations that are used within HGSYSTEM.

The last letter K of the file extension indicates the *type* of the file. Table 3 shows the types of file that can occur during a run of an HGSYSTEM module.

Not all types of file will occur for all modules. Several files will normally be deleted in the batch files controlling a module run. Removing the appropriate 'delete' statements from the batch file will make the file available for inspection for more experienced users. Every module will have an *input* and *report* file for every model run. Almost always *link* files will also be generated.

Please note that link files will have the 'MM' code of the model which will *use* the link information, *not* of the model which generated the link file.

3.6. Data dictionaries

Pre-processed data dictionaries are all in the directory C:\HGSYSTEM. Their name is of the form DICT.'MM'D where the 'MM' is again as given in table 2. Data dictionary definition files are given in the directory C:\HGSYSTEM\DATADICT. These files can be modified using a file editor. Their name is of the form 'NNN'DDF.DCT. Every data dictionary definition file must be processed by a corresponding batch file to create a new pre-processed data dictionary. The batch files are named 'NNN'DD.BAT and are in the same directory as the definition files. The batch files use the program DDMAIN.

Normally the user will *not* have to be concerned about the data dictionaries. They are only used internally by the HGSYSTEM program. Expert users may want to change them, preferably after consultation with the HGSYSTEM developers.

```
TITLE          Example input file AEROPLUME

RESERVOIR                            * RESERVOIR FLUID THERMODYNAMIC STATE
     TRES        = 20.0              * Storage/reservoir temperature (°C).
     PRES        = 4.0               * Reservoir (absolute) pressure (atm).

*RELEASE                             * STACK RELEASE CONDITIONS
     *TSTACK     = 150.0 * Stack release temperature (°C).

GASDATA                              * ————————→ POLLUTANT DATA
     WATERPOL    = 1.0E-03           * Water in pollutant (mole fraction).
     CPGAS = 48.66 * J/MOLE/C  specific heat of dry pollutant.
     MMGAS       = 29.72 * KG/KMOLE  molecular mass of dry pollutant.
     HEATGR      = 26.53 * .....   heat group (used for HEGADAS link only).
     SPECIES     = METHANE    , 0.5990   , 8
                   35.41   , 63.28   , 6593.   , 190.6   , 45.35
                   -6.029  , 1.251   ,-0.9105  , -1.233  , 16.04   , 354.6
     SPECIES     = ISO-OCTANE , 0.1000   , 8
                   186.7   , 255.3   , 3.3361E+04, 543.8  , 25.29
                   -7.489  , 1.434   , -3.267  , -2.452  , 114.2   , 658.5

PIPE                                 * PIPE EXIT-PLANE CONDITIONS
     DMDT  = -1.0                    * Mass (discharge) flow-rate (kg/s).
     DEXIT  = 0.03200                * (Effective) release orifice diameter (m).
     ZEXIT  = 1.0                    * Height of release above level ground (m).
     ANGLE = 0.0              * Angle of release to horizontal (degrees).
     DURATION    = 100.0 * Release duration (negative steady) (s).

AMBIENT                              * ATMOSPHERIC AMBIENT CONDITIONS
     Z0          = 2.0               * Reference height for measurements (m).
     U0          = 3.0               * Wind-speed at reference height (m/s).
     AIRTEMP     = 20.0              * Air temperature at reference height (C).
     AIRPRESS    = 1.00              * Atmosphere pressure at release height (atm).
     RHPERC      = 70.0              * Relative humidity at release height (%).

DISP                                 * DISPERSION DATA
     PQSTAB      = D                 * Pasquill/Gifford stability class (-).
     ZR          = 0.003 * Ground surface roughness (m).

TERMINAT                      * JET/PLUME DEVELOPMENT TERMINATION CRITERIA
     XLST        = 100               * Last required downwind (horizontal) distance (m).
     SLST        = -1.0              * Last required distance along plume axis (m).
     ULST        = -1.0              * Last required plume velocity (m/s).

MATCH                         * MATCHING CRITERIA FOR HEGADAS/PGPLUME
     RULST = 0.1              * Matching criterion based on velocities (-).
     RELST = 0.3              * Matching criterion based on entrainment (-).
     RGLST = 0.3              * Matching constraint based on buoyancy (-).
     RNLST = 0.1              * Matching criterion for heavy-gas/neutral limit (-).
     RALST = 0.2              * Constraint based upon aspect ratio (-).
```

Table 1. Example of HGSYSTEM input file (AEROPLUME model).

Module name	Code MM
DATAPROP	DP
SPILL	SP
HFSPILL	HL
HFFLASH	HF
LPOOL	LP
AEROPLUME	AP
HFPLUME	HP
HEGABOX	HB
HEGADAS-S	HS
HEGADAS-T	HT
PGPLUME	PG
POSTHS	PS
POSTHT	PT
PROFILE	PR
GET2COL	G2

Table 2. Two-character combinations used in HGSYSTEM model files.

Type of file	Code K
Input file	I
Partial input file	P
Report file	R
Monitor or Model Output file	M
Link file	L
Warning messages	W
Error messages	E
Match data (jet models)	1
Match data (jet models)	2
Mixture composition (AEROPLUME)	3
Matching criteria (jet models)	Z
Spreadsheet data or expansion info	X
NAESOL messages	N
Emission rates (LPOOL)	T
Heat transfer details (LPOOL)	H
Cloud composition (LPOOL)	C
SPRINT messages or pool composition	S
Debug information	D

Table 3. Types of files that can occur during an HGSYSTEM model run.

4. HGSYSTEM SCENARIOS; RUNNING MODELS IN SEQUENCE

4.1. HGSYSTEM scenarios

There are two important situations in which information generated by one HGSYSTEM module will be used by a second (subsequent) module:

1. Physical properties for a multi-compound mixture, generated by DATAPROP, must be passed on to an HGSYSTEM module using this information in its thermodynamical calculations.

2. Models are run in sequence to simulate a complete scenario. A *scenario* in this context is a complete simulation of a release/near-field/far-field dispersion event. This situation can of course include the above mentioned use of DATAPROP to generate physical properties.

In HGSYSTEM the following scenarios are currently available:

(DATAPROP ➨) SPILL ➨ AEROPLUME ➨ HEGADAS or PGPLUME

For liquid releases from a pressurised vessel with a near-field jet dispersion analysis followed by a far-field dispersion analysis. Multi-compound aerosol thermodynamics. No liquid pool formation on the ground.

(DATAPROP ➨) AEROPLUME ➨ HEGADAS or PGPLUME

Same as above but instead of using SPILL's source calculation, now using AEROPLUME's own discharge model or stack calculation. Multi-compound aerosol thermodynamics.

(DATAPROP ➨) LPOOL ➨ HEGADAS-T

Evaporation of a liquid pool ('unpressurised release') followed by a heavy gas dispersion analysis. Multi-compound two-phase thermodynamics.

(DATAPROP ➨) HEGABOX ➨ HEGADAS-T

Near-field analysis for instantaneous release of initially stagnant cloud followed by far-field heavy gas dispersion analysis. Multi-compound aerosol thermodynamics *or* HF chemistry and thermodynamics.

HFSPILL ➨ HFPLUME ➨ HEGADAS or PGPLUME

For HF releases from a pressurised vessel with a near-field jet dispersion analysis followed by a far-field dispersion analysis. HF chemistry and thermodynamics.

HFSPILL ➨ LPOOL ➨ HEGADAS-T

HF releases from a vessel leading to an evaporating pool, followed by a heavy gas dispersion analysis. HF chemistry and thermodynamics.

It is always possible to consider only part of the mentioned scenarios.

Please note that there is no scenario going from SPILL to LPOOL. The SPILL to AEROPLUME scenario assumes that all momentum of the pressurised release is conserved. If the momentum is destroyed, that is if a liquid pool rather than a jet forms, then the discharge model within LPOOL can be used to calculate discharge rates. The discharge correlations used in LPOOL are very similar to the ones used in SPILL.

In all of the above mentioned situations it is necessary to transfer information generated by one HGSYSTEM module to the next one to be run. In HGSYSTEM this is done by using so-called *link files*. After running the first model, a link file is created by this model. A link file contains all information available to the first model and needed by subsequent models. Thus a link file for a model contains *part of* the information needed in a complete input file. The additional data needed to build a complete input file is given in a so-called *partial input file*. Therefore to run a subsequent model in a series, both a link file and a partial input file must be available to make the necessary input data complete.
Example partial input files are available in directory C:\HGSYSTEM\STINPUT for all possible situations as discussed above.

4.2. Running subsequent (linked) models using the interactive program

The easiest way to run a series of subsequent HGSYSTEM models is by using the interactive utility program HGINTER. This program starts a question-and-answer session and based on the information given by the user it will determine which HGSYSTEM modules to run and in what order. The interactive program deals with link files and partial input files and their concatenation completely automatically. The user is given the opportunity to change (partial) input files based on the example files given in C:\HGSYSTEM\STINPUT. The user will also be given the choice to look at intermediate report files on the screen after a model has been run.
To start an interactive session, the user simply gives the following command from a working directory:

```
HGSYSTEM CASENAME
```

where all files generated during this interactive session will have a file name starting with CASENAME. All files will be created in the directory where the command is given. *Please do not give this command while in an HGSYSTEM (sub)directory.* It is strongly advised to create a separate working directory (for example C:\HGWORK) to run HGSYSTEM models from.

Using the interactive utility is strongly recommended for novice users of HGSYSTEM.

More experienced users can use manual linking of subsequent HGSYSTEM modules as will be explained in the next paragraph.

4.3. Manual linking of subsequent HGSYSTEM modules

Once a link file and a partial input file have been created, the subsequent model can be run by the following command:

```
MODELNAME  OLDNAME.MML  OLDNAME.MMP  (NEWNAME)
```

where MODELNAME is the name of the subsequent HGSYSTEM module (see Chapter 3), OLDNAME.MML is the name of the link file and OLDNAME.MMP the name of the partial input file. NEWNAME will be the new case name for this run. NEWNAME is optional. MM is a two-character code which corresponds to the model MODELNAME that is being used.

For file name conventions see Chapter 3. In Chapter 3 the correct characters for MM, depending on the MODELNAME used, are also given.
The last character of the three-character file name extension for a link file is always an 'L'. For a partial input file it is always a 'P'.

Following this command, the MODELNAME batch file will *'concatenate'* (combine, merge) the link file and the partial input file into a single input file and then execute the HGSYSTEM model MODELNAME in the usual way.
The user can merge the link file and partial input file manually by using a file editor but this is not necessary.

As an example consider running AEROPLUME using data generated by DATAPROP. Suppose a DATAPROP input file EXAMPLE.DPI has been created. First DATAPROP is run using the command:

```
DATAPROP EXAMPLE
```

DATAPROP will generate a report file EXAMPLE.DPR and several link files. One of the link files is intended for AEROPLUME and is called EXAMPLE.APL. A partial input file. supplementing the input data in EXAMPLE.APL, can be found in the HGSYSTEM sub-directory C:\HGSYSTEM\STINPUT. A partial input file for AEROPLUME has the file extension APP (see Chapter 3 on file name conventions). The sub-directory contains two file with this extension: STDP.APP and STSPILL.APP. The first partial input file supplements data generated by DATAPROP and the second one supplements data generated by SPILL. See the scenarios mentioned above to check that both DATAPROP and SPILL can provide a link to AEROPLUME.

In this example we need the STDP.APP partial input file. This file can be copied to a working directory and be edited to update parameter values as required. Assuming the name of this partial input file has been changed to NEWCASE.APP, the AEROPLUME model can be run with the link file data and the partial input data by the command:

```
AEROPLUME EXAMPLE.APL NEWCASE.APP NEWNAME
```

All files created by AEROPLUME will now have a filename beginning with NEWNAME.
AEROPLUME will create a new input file NEWNAME.API which is the combination of EXAMPLE.APL and NEWCASE.APP. The rest of the program execution is as usual (see Chapter 3).

4.4. General batch command for HGSYSTEM modules

The command given above to run an HGSYSTEM model using two data files (a link file and a partial input file) is a special case of the following general command:

```
MODELNAME FILE1.EXT FILE2.EX2 ... FILEn.EXn NEWNAME
```

where n is an integer number ≥ 1.

The n files FILE1.EX1 etc. all contain some input blocks for the model MODELNAME. The files will all be combined (concatenated) to one new input file NEWNAME.MMI before the model will be run.

It is possible to have several specifications for a certain input parameter occurring in several of the used files. If this parameter can only occur once in an input file, then the *last* specified value will be used in the new input file. If the parameter can occur more than once, then all specified values will be used. If in this case the total number of parameter specifications is too high, an error message will be generated by FFMAIN in the usual way.

5. DATAPROP

General introduction

DATAPROP is the HGSYSTEM database program which generates physical properties for the chemical species that are available. DATAPROP generates a report file containing information on the user-specified chemical compounds. However, its main purpose is to generate *link files* for all other HGSYSTEM modules, except the HF-specific ones. These link files contain the pollutant physical data, usually specified in the GASDATA input block, needed for the two-phase multi-compound thermodynamics.

Range of applications and limitations

A maximum of ten (10) compounds can be specified per DATAPROP run.

A list of all the compounds available in DATAPROP is given at the end of this chapter.

For compounds not available in DATAPROP the user is advised to specify the physical properties directly using the SPECIES keyword of the relevant HGSYSTEM module. New compounds may be added but this should be done by expert users only after consulting the HGSYSTEM developers. See end of section 2.A.1 of the HGSYSTEM 3.0 Technical Reference Manual for a reference on adding new compounds to DATAPROP.

Guidance for use

Whenever the two-phase, multi-compound thermodynamical description is used in a HGSYSTEM module, it is strongly recommended to use DATAPROP to generate the necessary input parameters.
Please note that when the user specifies the chemical compound DRY_AIR, the link files will contain *two* compounds: NITROGEN and OXYGEN.

DATAPROP INPUT FILE PARAMETERS

A description of all the input parameters that can occur in a DATAPROP input file will be given.

The DATAPROP input file has the DOS filename 'casename.DPI' where 'casename' is the user-supplied name of the problem.

In the following, actual keywords are given in *capitals* and in *bold*.

All parameters, except **TITLE**, occur in blocks preceded by a specific block keyword. For DATAPROP these block keywords are: **POLLUTANT** and **OUTPUT**.

The **TITLE** keyword does *not* occur in a parameter block.

TITLE	The title of the current problem to be run with DATAPROP. At most 50 alphanumeric characters. Optional, no default.

The **POLLUTANT** block contains the name and molar percentage of every compound present in the total pollutant mixture.

SPECIES This keyword should be specified for *every* compound in the pollutant mixture (including water). There must be at least one (1) SPECIES keyword and there can be at most ten (10).
Following the **SPECIES** keyword for a certain compound, a set of 2 parameters (#1 and #2, separated by a comma) *must* be specified:

#1 DATAPROP compound name (at most 12 alphanumeric characters).

#2 mole percentage of this compound in the reservoir mixture (%).
$0 \leq \#2 \leq 100$.
Note: the sum of all the mole percentages per DATAPROP run *must* be equal to 100%. DATAPROP will check if this condition is met.

The **OUTPUT** block specifies the temperature range for which the temperature dependent properties of each user-specified compound are printed in the DATAPROP report file. Data is given for a temperature interval [MINTEMP,MAXTEMP] with stepsize DIFTEMP.

MINTEMP	Minimum output temperature (°C). -273 ≤ **MINTEMP** ≤ 800. Optional, default is -273.
MAXTEMP	Maximum output temperature (°C). -273 ≤ **MAXTEMP** ≤ 1000. Optional, default is 300.
DIFTEMP	Output step for temperature (°C). 0.001 ≤ **DIFTEMP** ≤ 300. Optional, default is 20.

COMPOUNDS AVAILABLE IN DATAPROP

5 July 1993

Nr.	DATAPROP name	Chemical name
0	DRY_AIR	Dry air (79 vol% nitrogen, 21 vol% oxygen)
1	WATER	Water (H_2O)
2	CHLORINE	Chlorine (Cl_2)
3	CO2	Carbon dioxide (CO_2)
4	AMMONIA	Ammonia (NH_3)
5	NITROGEN	Nitrogen (N_2)
6	OXYGEN	Oxygen (O_2)
7	SO2	Sulphur dioxide (SO_2)
8	METHANE	Methane (CH_4)
9	ETHANE	Ethane (C_2H_6)
10	PROPANE	Propane (C_3H_8)
11	N-BUTANE	N-butane (C_4H_{10})
12	ISO-BUTANE	Iso-butane, 2-methylpropane (C_4H_{10})
13	N-PENTANE	N-pentane (C_5H_{12})
14	ISO-PENTANE	Iso-pentane, 2-methylbutane (C_5H_{12})
15	N-HEXANE	N-hexane (C_6H_{14})
16	N-HEPTANE	N-heptane (C_7H_{16})
17	N-OCTANE	N-octane (C_8H_{18})
18	ISO-OCTANE	Iso-octane, 2,2,4-trimethylpentane (C_8H_{18})
19	N-NONANE	N-nonane (C_9H_{20})
20	N-DECANE	N-decane ($C_{10}H_{22}$)
21	ETHENE	Ethene (C_2H_4)
22	PROPENE	Propene (C_3H_6)
23	BENZENE	Benzene (C_6H_6)
24	HF	Hydrogen fluoride (HF), full thermodynamics
25	HFIDEALGAS	Hydrogen fluoride (HF) as inert, ideal gas
26	CO	Carbon monoxide (CO)
27	HYDROGEN	Hydrogen (H_2)
28	H2S	Hydrogen sulfide (H_2S)
29	FREON-11	Freon-11, Trichlorofluoromethane (CCl_3F)
30	FREON-12	Freon-12, Dichlorodifluoromethane (CCl_2F_2)

6. SPILL

General introduction

SPILL is a utility program to calculate time-dependent liquid (and vapour) discharge rates from a pressurised vessel assuming a high-momentum jet arises from this release. During discharge the pressure in the reservoir will drop and temperature, mixture composition and discharge rate will all be functions of time.
It is assumed that a liquid jet rather than a liquid pool will form. See below.

SPILL uses the standard HGSYSTEM multi-compound, two-phase aerosol model.

SPILL will create a link file for AEROPLUME. The choice of a representative discharge rate to be used by AEROPLUME is not trivial as AEROPLUME is a steady-state model. See chapter on SPILL in Technical Reference Manual.

Range of applications and limitations

SPILL should be used as a utility to estimate the time-dependence of the discharge mass flow rate directly from an orifice in a pressurised vessel. It is not suitable for cases where there is pipework between the reservoir and the discharge orifice.

For vessel discharges having low momentum (that is, not resulting in a dispersing jet but rather in a pool on the ground), the HGSYSTEM evaporating liquid pool model LPOOL should be used insteda of SPILL. LPOOL is also fully time-dependent, but will link to HEGADAS-T rather than to AEROPLUME.

In the SPILL model it is assumed that all liquid remains within the jet: dropout of large liquid particles is not accounted for. Within the AEROPLUME model a deposition model is now available, see the MMESOPT input block in the AEROPLUME Chapter and Chapter 9 of the HGSYSTEM 3.0 Technical Reference Manual.

The heat transfer modelling assumes an infinitely thin vessel wall. The mixture temperature is assumed to be equal to the vessel wall temperature. These assumptions are not valid anymore for vessels filled with vapour-only mixtures.

Guidance for use

The SPILL model proves to be reasonably robust. For mixtures with many compounds (more than say 3), run times can be quite long.

SPILL INPUT FILE PARAMETERS

A description of all the input parameters that can occur in a SPILL input file will be given.

The SPILL input file has the DOS filename 'casename.SPI' where 'casename' is the user-supplied name of the problem.

In the following, actual keywords are given in *capitals* and in *bold*. The descriptions of less important parameters or parameters that need not normally be set by the user, are given in a *smaller font*.

All parameters, except **TITLE**, occur in blocks preceded by a specific block keyword. For SPILL these block keywords are: **RESERVOIR**, **GASDATA**, **PIPE**, **AMBIENT** and **TERMINAT**.

The **TITLE** keyword does *not* occur in a parameter block.

TITLE	The title of the current problem to be run with SPILL. At most 50 alphanumeric characters. Optional, no default.

The **RESERVOIR** block contains the parameters which describe the reservoir fluid thermodynamic state.

TRES	Initial temperature of the reservoir fluid (°C). $-50 \leq$ **TRES** ≤ 1500. Mandatory.
PRES	Initial absolute pressure within the reservoir (atm). $-200 \leq$ **PRES** ≤ 500. Mandatory. A negative value of **PRES** serves as a flag to SPILL: the program will calculate the saturation pressure of the specified mixture assuming all compounds are in the liquid-only state and use this as the value for the reservoir pressure. This option is only available when the two-phase (aerosol) thermodynamics model is being used, in other words when the **SPECIES** keyword is being used in the **GASDATA** block as discussed below. It is the user's responsibility to judge whether these assumptions in calculating the reservoir pressure are reasonable or not. When **PRES** is positive, it must always be greater than **AIRPRESS** of the **AMBIENT** block.
VRES	Reservoir volume (m^3) $0.001 \leq$ **VRES** ≤ 10000 Mandatory
MRES	Reservoir mass contents (tonnes, 1 tonne = 1000 kg). $0.1 \leq$ **MRES** ≤ 10000. Optional. If **MRES** is not specified then SPILL will calculate the maximum mass contents of the reservoir based on current values of **PRES**, **TRES** and **VRES** and on mixture composition as given in **GASDATA** block. SPILL also checks whether **MRES** is consistent with other reservoir data. If necessary the mixture composition will be changed by adding dry air to the mixture. A user-specified value of **MRES** is only used if the **SPECIES** keyword is used in the **GASDATA** input block *and* if the initial reservoir mixture is denser than dry air. In all other cases, **MRES** is calculated by the program based on mixture composition and **VRES**, **TRES** and **PRES**.

The **GASDATA** block contains the initial composition of the reservoir mixture and the relevant thermodynamic data.

WATERPOL	Initial mole fraction water (liquid plus vapour) in reservoir mixture (mole water per mole mixture). 0 ≤ **WATERPOL** ≤ 1.0. Optional, default is 0.0.
CPGAS	Initial specific heat at constant pressure of the *dry* reservoir mixture (J/(mole K)). 5 ≤ **CPGAS** ≤ 300. Mandatory if **SPECIES** keyword is not used (vapour-only mixture), *no default*. If **SPECIES** keyword is used then **CPGAS** is needed when a link file to HEGADAS is being made by AEROPLUME. Thus in practice **CPGAS** must almost always be specified. Using HGSYSTEM module DATAPROP to find **CPGAS** and other keywords is strongly recommended.
MMGAS	Initial molar mass of *dry* reservoir mixture (kg/kmole). 2 ≤ **MMGAS** ≤ 200. Same comments as for **CPGAS** apply. Again, use of DATAPROP to calculate **MMGAS** is recommended.
HEATGR	Natural convection heat transfer group $(\mathrm{J} \cdot \mathrm{m}^{\frac{2}{3}} / (\mathrm{s}^{\frac{1}{3}} \cdot \mathrm{K}^{\frac{5}{3}} \cdot \mathrm{kmole}))$ 5 ≤ **HEATGR** ≤ 100. Optional, *no default*. Not used by SPILL or AEROPLUME model but written to HEGADAS link file if this is being made after AEROPLUME run. Use of DATAPROP to calculate **HEATGR** is strongly recommended.
SPECIES	Reservoir mixture compound properties. Using this keyword at least once implies the use of the full two-phase (aerosol) model or a mixture consisting of at least one compound (excluding water). If the **SPECIES** keyword is *not* specified, ideal gas thermodynamics is used with gas properties given by **CPGAS** and **MMGAS**. Condensation or freezing of *water* is still taken into account. The **SPECIES** keyword plus parameters must be specified *for every compound* in the mixture, except water. The sum of the molar fractions (see parameter #2 below) *must* equal 1.0-**WATERPOL**. The use of DATAPROP to generate the input parameters when the **SPECIES** keyword is being used, is strongly recommended. Currently a maximum of 8 species can be specified (excluding water). Please note that DATAPROP allows for more species to be specified. DATAPROP also splits *dry air* (if specified) up into nitrogen and oxygen, thus generating *two* compounds instead of one. Thus the

SPILL link file generated by DATAPROP could contain the **SPECIES** keyword more than 8 times. The user should combine or remove compounds if this occurs.

Within the above-mentioned restrictions, there are no restrictions within SPILL concerning the number of aerosols forming or the number of compounds per aerosol.

Following the **SPECIES** keyword for a certain compound, a block of 14 parameters (#1 to #14) *must* be specified:

#1 compound name (maximum of 12 characters).
#2 initial mole fraction of this compound in the reservoir mixture (-).
$0 \leq \#2 \leq 1$.
#3 aerosol class (-).
$-1 \leq \#3 \leq 50$.
#4 specific heat of vapour (J/(mole K)).
$5 \leq \#4 \leq 300$.
#5 specific heat of liquid (J/(mole K)).
$0 \leq \#5 \leq 10^3$.
#6 heat of vaporisation (J/mole)
$0 \leq \#6 \leq 10^5$
#7 critical temperature (K).
$0 \leq \#7 \leq 10^4$.
#8 critical pressure (atm).
$0 \leq \#8 \leq 10^3$.
#9 vapour pressure function coefficient B1.
$-10^8 \leq \#9 \leq 10^8$.
#10 vapour pressure function coefficient B2.
$-10^8 \leq \#10 \leq 10^8$.
#11 vapour pressure function coefficient B3.
$-10^8 \leq \#11 \leq 10^8$.
#12 vapour pressure function coefficient B4.
$-10^8 \leq \#12 \leq 10^8$.
#13 molar mass (kg/kmole).
$2 \leq \#13 \leq 200$.
#14 liquid density (kg/m^3).
$1 \leq \#14 \leq 10^5$.

Note: the saturated vapour pressure of the compound is described by the Wagner function:

$$P_v(T) = P_c \cdot \exp\left\{\left[B_1 \cdot Q + B_2 \cdot Q^{1.5} + B_3 \cdot Q^3 + B_4 \cdot Q^6\right] / T_r\right\}$$

where T is the vapour temperature, P_c the critical pressure, T_c the critical temperature, $T_r = T/T_c$ and $Q = 1 - T_r$.

The **PIPE** block contains the release pipe/orifice exit-plane conditions.

DEXIT	Effective orifice diameter of the discharge pipe (m). $0.001 \leq$ **DEXIT** ≤ 5. Mandatory.
CDG	Discharge coefficient for vapour only releases (-). $0.0 \leq$ **CDG** ≤ 1.0. Optional, default is 1.0. SPILL uses discharge coefficients to calculate values for the mass discharge rate, the user might want to change the default values of these coefficients.
CDL	Discharge coefficient for liquid or two-phase releases (-). $0.0 \leq$ **CDL** ≤ 1.0. Optional, default is 0.61. See remark above.

The **AMBIENT** block contains parameters describing the conditions of the ambient atmosphere.

AIRPRESS	Ambient air pressure at release height (atm). $0.7 \leq$ **AIRPRESS** ≤ 1.1. Optional, default is 1.0 atm. **AIRPRESS** must be less than **PRES** of the **RESERVOIR** block.
TATM	Temperature ambient air for heat transfer only (°C). $-50 \leq$ **TATM** ≤ 50. Optional, default is 20 °C. Used to calculate radiative and convective heat transfer between reservoir and surrounding air.
QSOLAR	Direct solar heat flux to reservoir (W/m^2). $0 \leq$ **QSOLAR** ≤ 3000 Optional, default is 0 W/m^2. Used in reservoir heat balance.
EMISS	Radiative emissivity of reservoir surface (-). $0 \leq$ **EMISS** ≤ 1.0. Optional, default is 0.8. Used to calculate radiative heat flux.
AREA	Surface area over which heat transfer takes place (m^2). $0 \leq$ **AREA** ≤ 10000. Optional, default is 0.0: no heat transfer between reservoir and surrounding air.

The **TERMINAT** block sets reservoir release termination criteria. Normally these are all *inactive* (by setting them to a negative value) and the SPILL run will only end when the reservoir is exhausted or when the reservoir pressure falls below the ambient pressure. Sometimes, however, it can be useful to stop the run before this occurs. The **TERMINAT** parameters can be used for this purpose.

TLST	Last required elapsed time after release start (s). $-1000 \leq$ **TLST** ≤ 2000. Optional, default is -1.0 (criterion inactive) If set to a negative value, the termination criterion will not be used.
MLST	Last required reservoir mass content (tonnes, 1 tonne = 1000 kg). $-1000 \leq$ **MLST** ≤ 1000 Optional, default is -1.0 (criterion inactive) If set to a negative value, the termination criterion will not be used
LLST	Last required reservoir total liquid mole fraction (%). $-1000 \leq$ **LLST** ≤ 100. Optional, default is -1.0 (criterion inactive) If set to a negative value, the termination criterion will not be used.
PLST	Last required reservoir pressure (Pa). $-1000 \leq$ **PLST** ≤ 1000. Optional, default is -1.0 (criterion inactive) If set to a negative value, the termination criterion will not be used.
RLST	Last required reservoir mixture density (kg/m^3). $-1000 \leq$ **RLST** ≤ 1000. Optional, default is -1.0 (criterion inactive) If set to a negative value, the termination criterion will not be used.

7. HFSPILL

General introduction

HFSPILL is the HF-specific counterpart of SPILL. It calculates the time-dependent release rate from a pressure vessel filled with HF and water.
The vessel mixture is assumed to be in one of the following two states:

(1) a subcooled (not saturated or superheated) liquid consisting of HF and water
(2) an equilibrium vapour mixture of HF vapour, water vapour and nitrogen.

HFSPILL can prepare link files for HFPLUME or LPOOL, depending on the release scenario.

Range of applications and limitations

HFSPILL should be used as a utility to estimate the time-dependence of the discharge mass flow rate directly from an orifice in a pressurised vessel resulting in a dispersing jet rather than a pool on the ground. It is not suitable for cases where there is pipework between the reservoir and the discharge orifice.

Contrary to SPILL, in HFSPILL heat exchange of the vessel with the ambient atmosphere is *not taken into account.*

HFSPILL INPUT FILE PARAMETERS

A description of all the input parameters that can occur in a HFSPILL input file will be given.

The HFSPILL input file has the DOS filename 'casename.HLI' where 'casename' is the user-supplied name of the problem.

In the following, actual keywords are given in *capitals* and in *bold.* The descriptions of less important parameters or parameters that need not normally be set by the user, are given in a *smaller font.*

All parameters, except **TITLE**, occur in blocks preceded by a specific block keyword. For SPILL these block keywords are: **RESERVOIR**, **LIQUID**, **VAPOUR**, **PIPE** and **AMBIENT**.

The **TITLE** keyword does *not* occur in a parameter block.

TITLE	The title of the current problem to be run with HFSPILL. At most 50 alphanumeric characters. Optional, no default.

The **RESERVOIR** block contains the parameters which describe the reservoir fluid thermodynamic state.

TRES	Initial temperature of the reservoir fluid (°C). $-50 \leq$ **TRES** ≤ 150. Mandatory.
PRES	Initial absolute pressure within the reservoir (atm). $0.7 \leq$ **PRES** ≤ 20. Mandatory. **PRES** must exceed **AIRPRESS** in the **AMBIENT** block.
VRES	Reservoir volume (m^3) $0.1 \leq$ **VRES** ≤ 500. Mandatory. HFSPILL checks whether the input data is consistent: **VRES** should be compatible with the user-specified vessel contents at the given **TRES** and **PRES**.

The **LIQUID** block contains data from which HFSPILL determines the vessel equilibrium state when liquid is present. The user has to specify the mass percentage of water in the vessel, the rest of the mixture is assumed to be (anhydrous) hydrogen fluoride acid HF.
The user should either specify a **LIQUID** or a **VAPOUR** input block. If there is liquid present in the vessel, the **LIQUID** input block should be used, otherwise the **VAPOUR** block. The user should *not* specify *both* blocks in one run.

MFH2O	Mass percentage water in the reservoir mixture (%). 0 ≤ **MFH2O** ≤ 100. Mandatory.
MLRES	Total reservoir mass (tonnes, 1 tonne = 1000 kg). 0.1 ≤ **MLRES** ≤ 200. Mandatory.

The **VAPOUR** block contains data from which HFSPILL determines the vessel equilibrium state when only vapour is present. The user has to specify the mass percentage of water and HF in the vessel, the rest of the mixture is assumed to be nitrogen.
The user should either specify a **LIQUID** or a **VAPOUR** input block. If there is liquid present in the vessel, the **LIQUID** input block should be used, otherwise the **VAPOUR** block. The user should *not* specify *both* blocks in one run.

MFHF	Mass percentage HF vapour in the (gaseous) reservoir mixture (%). 0 ≤ **MFHF** ≤ 100. Mandatory.
MFH2O	Mass percentage water vapour in the (gaseous) reservoir mixture (%). 0 ≤ **MFH2O** ≤ 100. Mandatory.

Note: Total reservoir mass is calculated by HFSPILL. Phase stability is checked by the program.

The **PIPE** block contains the release pipe/orifice exit-plane conditions.

DEXIT	Effective orifice diameter of the discharge pipe (m). $0.001 \leq$ **DEXIT** ≤ 0.5. Mandatory.
DTLINK	Time duration step used in HFSPILL/LPOOL link file (s). $0.0 \leq$ **DTLINK** $\leq 10^8$. Optional. default is 200 s. As LPOOL can deal with up to 5 spill data records SPILDATA. it is important to choose a corect value for **DTLINK**. DTLINK should be chosen in such a way that the SPILDATA records in the LPOOL input file give a good representation of the release history. For **DTLINK** too large, not enough SPILDATA records will be used, for **DTLINK** too small the whole release history might not be covered. The user needs to run HFSPILL at least once to be able to find a good value for **DTLINK**.
CDG	Discharge coefficient for vapour only releases (-). $0.0 \leq$ **CDG** ≤ 1.0. Optional, default is 1.0. SPILL uses discharge coefficients to calculate values for the mass discharge rate. the user might want to change the default values of these coefficients.
CDL	Discharge coefficient for liquid or two-phase releases (-). $0.0 \leq$ **CDL** ≤ 1.0. Optional, default is 0.61. See remark above.

The **AMBIENT** block contain one parameter describing the conditions of the ambient atmosphere.

AIRPRESS	Ambient air pressure at release height (atm). 0.7 ≤ **AIRPRESS** ≤ 1.1. Optional, default is 1.0 atm. **AIRPRESS** must be less than **PRES** in the **RESERVOIR** block.

8. HFFLASH

General introduction

The HFFLASH model is an HF-specific utility program that can be used to calculate post-flash temperature and liquid fraction upon release of anhydrous hydrogen fluoride (HF).
HFFLASH main use is to create a link file to the HEGADAS (-S, -T) dispersion program. This file contains the post-flash temperature and liquid fraction. Together with evaporating pool data from LPOOL this information is needed to give a source term description needed in HEGADAS.

Range of applications and limitations

The HFFLASH/HEGADAS combination should be used for *unpressurised* (low-momentum) releases where a liquid pool forms on the ground. Pool data can be generated using the LPOOL model.
For *pressurised* releases the HFPLUME model should be used followed by a HEGADAS or PGPLUME run if required.
The flash calculations assume that ambient pressure is 1 atm.

HFFLASH INPUT PARAMETERS

A description of all the input parameters that can occur in an HFFLASH input file will be given.

The HFFLASH input file has the DOS filename 'casename.HFI' where 'casename' is the user-supplied name of the problem.

In the following, actual keywords are given in *capitals* and in *bold*.
All parameters, except **TITLE**, occur in blocks preceded by a specific block keyword. For HFFLASH these block keywords are: **RESERVOIR** and **PIPE**.

The **TITLE** keyword does *not* occur in a parameter block.

TITLE	The title of the current problem to be run with HFFLASH. At most 50 alphanumeric characters. Optional, no default.

The **RESERVOIR** block contains the parameters which describe the reservoir thermodynamic state of the anhydrous HF.

TRES	Temperature of the HF in the reservoir (°C). -50 ≤ **TRES** ≤ 150. Mandatory.
PRES	Absolute pressure within the reservoir (atm). 0.7 ≤ **PRES** ≤ 20. Note: ambient pressure is assumed to be 1.0 atm.

The **PIPE** block contains the release pipe/orifice exit-plane conditions.

DMDTHF	Mass discharge rate of HF (kg/s). $0.01 \leq$ **DMDTHF** $\leq 10^3$. Mandatory. The HFSPILL model might be used to estimate **DMDTHF**.
DEXIT	Effective orifice diameter of the discharge pipe (m). $0.001 \leq$ **DEXIT** ≤ 5. Mandatory.

9. LPOOL

General introduction

The LPOOL model simulates the time-dependent evaporation of a multi-component liquid pool on land or water. The pool can be boiling or non-boiling. Dikes can be modelled as well. The pool is assumed to be well-mixed (no concentration gradients within the pool).

LPOOL replaces the EVAP model as available in previous version of HGSYSTEM. The program is functionally the same as the LSM90 model, developed by Exxon Research & Engineering Company.

Apart from the evaporating pool calculations, LPOOL can calculate liquid spill rates from a reservoir, using either a choked flow equation or a Bernoulli liquid flow equation. The user can specify prescribed spill rates, if required.

Range of applications and limitations

For more details on the validation of the LSM90 model, see the original LSM90 references in the Technical Reference Manual chapter on LPOOL.

Like the EVAP model, LPOOL can not model the full HF chemistry and thermodynamics. However, similar to the EVAP model, it can do a post-HFSPILL run using the relevant physical properties of HF.

LPOOL is a fully time-dependent code, it *can not be run in steady-state mode*. Therefore only a link file to the time-dependent dispersion model HEGADAS-T is created by LPOOL. If the user judges that the pool evaporation can be represented by a steady-state release, a HEGADAS-S input file can be prepared based on the example input files available in the HGSYSTEM\STINPUT subdirectory.

LPOOL is intended to be used for evaporating liquid pools. If the mixture at reservoir conditions (also) contains compounds which are always vapour-only (e.g. nitrogen, oxygen, methane), numerical problems may occur or results may be incorrect. *Only* include in the mixture specification those compounds (GASDATA input block) which will form *part of the liquid pool* upon release.

Guidance for use

If numerical problems occur during LPOOL runs, changing the input parameters slightly might help. Also check that the input data is consistent. See remarks for specific keywords below. HEGADAS-T will print a warning if the spill data from LPOOL imply that the pool has not dried up completely at the end of the simulation time. The user can try to find values for MAXTIM and DTLINK (see below) so that a complete pool description is obtained.

The report file 'casename.LPR' contains a reprint of the input data and a summary of the average pool evaporation results. The file 'casename.LPT' contains time-dependent results like evaporation rate and mass in pool. The file 'casename.LPC' shows the composition of the cloud above the pool as a function of time (molar and mass fractions, all compounds) and 'casename.LPS' gives the same information for the pool mixture.

LPOOL INPUT PARAMETERS

A description of all the input parameters that can occur in a LPOOL input file will be given.

The LPOOL input file has the DOS filename 'casename.LPI' where 'casename' is the user-supplied name of the problem.

In the following, actual keywords are given in *capitals* and in *bold*. The descriptions of less important parameters or parameters that need not normally be set by the user, are given in a *smaller font*.
All parameters, except **TITLE**, occur in blocks preceded by a specific block keyword. For LPOOL these block keywords are: **CONTROL**, **SPILL**, **RESERVOIR**, **GROUND**, **GASDATA**, **FLASH** and **AMBIENT**.

The **TITLE** keyword does *not* occur in a parameter block.

TITLE	The title of the current problem to be run with LPOOL. At most 50 alphanumeric characters. Optional, no default.

The **CONTROL** input block contains several general control parameters.

MAXTIM	Maximum simulation time for this LPOOL run (s). $0.1 \le$ **MAXTIM** $\le 10^{10}$. Mandatory.
MINFILM	Minimum (film) thickness of pool (mm = 10^{-3} m). $0.1 \le$ **MINFILM** $\le 10^{4}$. Optional, default is 1 mm. Although simulation results do depend on the value of **MINFILM**, its precise value for any given compound is unfortunately rather insecure. Theoretically it should never be lower than the capillary depth $h_c = \sqrt{\sigma_L / (g \cdot \rho_L)}$ where σ_L is the surface tension (N/m), g the gravitational acceleration (9.8 m/s^2) and ρ_L the liquid density (kg/m^3). Usually **MINFILM** is taken to be order h_c.
DTLINK	Time step for pool data in HEGADAS-T link file (s). $0 \le$ **DTLINK** $\le 10^{4}$ Optional, default is 20 s. LPOOL creates a link file for HEGADAS-T which contains pool data printed at time intervals of **DTLINK** s. The maximum number of pool data records that HEGADAS-T can use is 100. It is probably necessary to run LPOOL at least once to be able to find a value of **DTLINK** that generates sufficient pool data records for HEGADAS-T so that a good representation of the pool history is communicated to HEGADAS-T.

The **GROUND** block contains the parameters which describe the ground composition and the dike composition and size (if present).

GRCOMP	Ground composition (-). **GRCOMP** = 1, 2, 3, 4, 5, 6 or 7. Optional, default is 3 (concrete). The possible ground surface materials are: 1: wet sand 2: dry sand 3: concrete 4: insulated concrete 5: steel 6: insulated plastic 7: water
GRTEMP	Ground surface temperature (°C). -50 ≤ **GRTEMP** ≤ 50. Mandatory.
DIKEPRES	Dike (bund) presence indicator (-). **DIKEPRES** = 0 (*no* dike) or 1 (dike). Optional, default is 0 (no dike).
DIKECOMP	Dike composition (-). **DIKECOMP** = 0, 1, 2, 3, 4, 5, or 6. Optional, default is 0 (indicating *no dike*). The possible dike materials are: 1: wet sand 2: dry sand 3: concrete 4: insulated concrete 5: steel 6: insulated plastic Only relevant if **DIKEPRES** = 1. Will be set to 0 if **DIKEPRES** = 0.
DIKEHEIGHT	Height of dike (m). 0 ≤ **DIKEHEIGHT** ≤ 10^3. Mandatory if **DIKEPRES** = 1.
DIKERADIUS	Radius of dike (m). 0 ≤ **DIKERADIUS** ≤ 10^3. Mandatory if **DIKEPRES** = 1.

The **SPILL** block contains the parameters which describe the discharge details for a release of liquid from a reservoir.

SPTYPE	Spill rate type (-). **SPTYPE** = 0, 1 or 2 Mandatory. **SPTYPE** = 0 indicates a fully user-specified spill rate using the **SPILDATA** parameters below. **SPTYPE** = 1 indicates that LPOOL will use a choked flow model to calculate the discharge rate. In this case **PRES** *must* exceed **PATM!** **SPTYPE** = 2 indicates that LPOOL will use a standard liquid Bernoulli relation to determine the spill rate.
CD	Spill discharge coefficient (-). $0.0 \leq$ **CD** ≤ 1.0 Optional, default is 0.6.
DURATION	Spill duration (s). $10^{-6} \leq$ **DURATION** $\leq 10^{5}$ Optional, default is **MAXTIM** + 100. Specify only if spill stops before exhaustion (e.g. to simulate plugging of leak). Otherwise set larger than **MAXTIM**. Normally LPOOL calculates spill duration. Not relevant if **SPTYPE** = 0.
SPILDATA	User-specified spill rates and durations. Mandatory if **SPTYPE** = 0. The **SPILDATA** keyword *must* be followed by two parameters (#1 and #2): #1 spill rate (m^3/s) $0 \leq \#1 \leq 10^6$. #2 spill duration (s). $0 \leq \#2 \leq 10^6$. The **SPILDATA** keyword with its pair of parameters can be specified up to five (5) times. Only relevant if **SPTYPE** = 0.

The **RESERVOIR** block contains the parameters which describe the reservoir (tank) containing the liquid to be released. The reservoir is assumed to be a vertical cylinder.

TRES	Temperature of the reservoir fluid (°C). $-50 \le$ **TRES** ≤ 200. Mandatory.
PRES	Absolute pressure within the reservoir (atm). $0 \le$ **PRES** ≤ 200. Mandatory. **PRES** must be equal or larger than the ambient pressure **PATM**. For a vented tank they will be equal and in this case the only driving force for the spill is the liquid height. If **SPTYPE** = 1, then **PRES** *must* exceed **PATM**.
RRADIUS	Radius of the cylindrical tank (m). $10^{-6} \le$ **RRADIUS** $\le 10^{3}$. Mandatory. **RRADIUS** must not exceed **DIKERADIUS** of the **GROUND** block.
RFLHEIGHT	Initial fluid level in the cylindrical tank (m). $10^{-6} \le$ **RFLHEIGHT** $\le 10^{3}$. Mandatory. Must be larger than **ZEXIT**.
DEXIT	Equivalent diameter of reservoir (tank) orifice (m). $10^{-6} \le$ **DEXIT** $\le 10^{3}$. Mandatory.
ZEXIT	Elevation (height) of orifice (m). $0 \le$ **ZEXIT** $\le 10^{3}$. Mandatory. **ZEXIT** must be less than **RFLHEIGHT**. **ZEXIT** must be greater than **DEXIT**/2.

N.B. **RFLHEIGHT** and **ZEXIT** measured with respect to ground level

The **AMBIENT** block contains parameters describing the conditions of the ambient atmosphere.

TATM	Ambient air temperature at height 10 m (°C). $-50 \le$ **TATM** ≤ 100. Mandatory.
UATM	Ambient wind velocity at height of 10 m (m/s). $1.0 <$ **UATM** ≤ 20. Mandatory.
PATM	Ambient air pressure (atm). $0.7 \le$ **PATM** ≤ 1.1. Optional, default is 1.0 atm. **PATM** must be less than or equal to **PRES** of the **RESERVOIR** block.
RHPERC	Relative air humidity (%). $0.0 \le$ **RHPERC** ≤ 100. Optional, default is 70 %. Used in aerosol calculation and to write HEGADAS-T link file.
CLCOVER	Fraction of sky covered by clouds (-) $0.0 \le$ **CLCOVER** ≤ 1.0. Optional, default is 1.0.
SPSTART	Spill starting time (24 hour clock) $0.0 \le$ **SPSTART** ≤ 24.0 Optional, default is 12.0.
SUNRISE	Sun rise (24 hour clock) $0.0 \le$ **SUNRISE** ≤ 24.0. Optional, default is 6.0.
SUNSET	Sun set (24 hour clock) $0.0 \le$ **SUNSET** ≤ 24.0 Optional, default is 18.0.

Note: **SPSTART, SUNRISE** and **SUNSET** are decimals indicating time using a 24 hour clock. Example: 7:30 am is given by 7.50 and 7:15 pm is 19.25.

The **FLASH** block contains parameters concerning the flashing and aerosol formation of the spilled liquid.

FLASHFRAC	User-specified flash fraction (-). 0.0 < **FLASHFRAC** ≤ 1.0. Optional. default is 0. Only used if **AUTOFLASH** = 0.
AEROSFRAC	User-specified aerosol fraction (-). 0.0 < **AEROSFRAC** ≤ 1.0. Optional, default is 0. Only used if **AUTOAEROS** = 0.

The **GASDATA** block contains the fluid composition and thermodynamic data. LPOOL will always assume the tank contains (some) liquid and the calculations will always use two-phase thermodynamics. Tanks containing only vapour can *not* be modelled.
A mixture containing some volatile compounds which are vapour-only at reservoir conditions (e.g. methane, nitrogen) may cause numerical problems or give incorrect results. *Only* include in the mixture specification those compounds which will form *part of the liquid pool* upon release.
Using the HGSYSTEM module DATAPROP to find the values for **GASDATA** parameters is strongly recommended.

WATERPOL	Mole fraction water in fluid (-). $0 \leq$ **WATERPOL** ≤ 1.0. Optional, default is 0.0.
CPGAS	Specific heat at constant pressure of fluid *without water* (J/(mole K)). $5 \leq$ **CPGAS** ≤ 300. Mandatory for writing the link file to HEGADAS-T. Thus in practice **CPGAS** must always be specified. Using the HGSYSTEM module DATAPROP to find **CPGAS** is strongly recommended.
MMGAS	Molar mass of FLUID *without water* (kg/kmole). $2 \leq$ **MMGAS** ≤ 200. Same comments as for **CPGAS** apply. Again, use of DATAPROP to calculate **MMGAS** is recommended.
HEATGR	Natural convection heat transfer group $(\mathrm{J} \cdot \mathrm{m}^{\frac{2}{3}} / (\mathrm{s}^{\frac{1}{3}} \cdot \mathrm{K}^{\frac{4}{3}} \cdot \mathrm{kmole}))$ $5 \leq$ **HEATGR** ≤ 100. Same comments as for **CPGAS** apply. Again, use of DATAPROP to calculate **HEATGR** is recommended.
SPECIES	Fluid component properties. Contrary to other HGSYSTEM modules (SPILL, HEGABOX, AEROPLUME and HEGADAS) LPOOL always uses two-phase thermodynamics. Vapour-only calculations are not possible. It is assumed that the tank always contains (some) liquid. The **SPECIES** keyword plus parameters must be specified *for every compound* in the fluid mixture, *except water.* The sum of the molar fractions used in the **SPECIES** (see parameter #2 below) *must* equal 1.0 - **WATERPOL.** Again, the use of DATAPROP to generate the input parameters when the **SPECIES** keyword is being used, is strongly recommended. Currently a maximum of 8 components can be specified (excluding water). Please note that DATAPROP allows for more compounds to be specified. DATAPROP also splits *dry air* (if specified) up into nitrogen and oxygen, thus generating *two* compounds instead of one.

Thus the LPOOL link file generated by DATAPROP could contain the **SPECIES** keyword more than 8 times. The user should combine or remove compounds if this occurs.

Within the above-mentioned restrictions, there are no restrictions within LPOOL concerning the number of aerosols forming or the number of compounds per aerosol. Please note that HEGADAS *does* have restrictions: either a single two-compound aerosol or a number of separate one-compound aerosols are allowed (not regarding water and dry air), other combinations are not supported.

Following the **SPECIES** keyword of a certain compound a block of 16 parameters (#1 to #16) *must* be specified:

#1 compound name (maximum of 12 characters).
#2 mole fraction in fluid mixture (-).
$0 \leq \#2 \leq 1$.
#3 aerosol class (-).
$-1 \leq \#3 \leq 50$.
#4 specific heat of vapour (J/(mole K)).
$5 \leq \#4 \leq 300$.
#5 specific heat of liquid (J/(mole K)).
$0 \leq \#5 \leq 10^3$.
#6 heat of vaporisation (J/mole)
$0 \leq \#6 \leq 10^5$
#7 critical temperature (K).
$0 \leq \#7 \leq 10^4$.
#8 critical pressure (atm).
$0 \leq \#8 \leq 10^3$.
#9 vapour pressure function coefficient B1.
$-10^8 \leq \#9 \leq 10^8$.
#10 vapour pressure function coefficient B2.
$-10^8 \leq \#10 \leq 10^8$.
#11 vapour pressure function coefficient B3.
$-10^8 \leq \#11 \leq 10^8$.
#12 vapour pressure function coefficient B4.
$-10^8 \leq \#12 \leq 10^8$.
#13 molar mass (kg/kmole).
$2 \leq \#13 \leq 200$.
#14 liquid density (kg/m^3).
$1 \leq \#14 \leq 10^5$.
#15 normal atmospheric boiling point (K).
$0 \leq \#14 \leq 10^4$.
#16 vapour viscosity (Pa·s = kg/m/s).
$0 \leq \#14 \leq 10^5$.

Note: the saturated vapour pressure of the compound is described by the Wagner function:

$$P_v(T) = P_c \cdot \exp\left\{\left[B_1 \cdot Q + B_2 \cdot Q^{1.5} + B_3 \cdot Q^3 + B_4 \cdot Q^6\right] / T_r\right\}$$

where T is the vapour temperature, P_c the critical pressure, T_c the critical temperature, $T_r = T/T_c$ and $Q = 1 - T_r$.

10. AEROPLUME

General introduction

The AEROPLUME model can be used to simulate the near-field atmospheric dispersion of high-momentum jets. AEROPLUME is a steady-state model.
Both vapour-only and two-phase jets can be modelled. AEROPLUME uses the standard HGSYSTEM multi-compound, two-phase thermodynamical model.
Dense, neutral and buoyant jets can be simulated for different release angles.

AEROPLUME has its own reservoir discharge model to calculate (steady-state) release rates from a pressurised reservoir. The used relations are identical to the ones used in the SPILL model. The user can specify discharge rates if required.
AEROPLUME will also calculate post-flash conditions using its two-phase thermodynamical model.
Instead of the reservoir calculations, it is also possible to do stack calculations with the AEROPLUME model, where post-flash conditions are user-specified.

AEROPLUME simulates near-field dispersion. In the far field, the code will automatically generate a link file either for PGPLUME or for HEGADAS-S. See documentation on these models. The AEROPLUME model will determine automatically when to make a far-field transition.

AEROPLUME replaces the old PLUME model in HGSYSTEM version 1.0 (also called NOV90 version). PLUME could only describe the dispersion of ideal gas releases.

The HF-specific version of AEROPLUME is a separate model called HFPLUME.

Range of applications and limitations

The AEROPLUME model should not be used for very low-speed jets (slower than ambient wind speed), as wake-effects will be important.

AEROPLUME should not be used for *unpressurised* releases, or for any releases where exit velocities are small compared to ambient wind speed or where initial momentum is quickly destroyed by impact with the ground. In those cases the evaporating liquid pool model LPOOL should be used.

Jets touching the ground at high speed or very steep angles should also not be simulated with AEROPLUME.

It is *very important* when interpreting AEROPLUME results to realise that all physical quantities (concentration, density, temperature etc.) are always *average* quantities over the plume cross-section. As a general rule of thumb, peak (that is, centre-line) concentrations will be about a factor 1.3-1.4 higher than the cross-sectional mean concentrations as given in the AEROPLUME report file.

In the AEROPLUME model it is assumed that all liquid remains within the jet: dropout of large liquid particles is not accounted for. However, it is possible to use the optional deposition model developed by Earth Technology and available in HGSYSTEM. See the MMESOPT input block and Chapter 9 in the HGSYSTEM 3.0 Technical Reference Manual.

Guidance for use

It is *very* important to realise that when the SPECIES keyword in the GASDATA input block is *not* specified, AEROPLUME will perform *vapour-only* calculations (except for any water present in the jet). There is usually a *large difference* in dispersion results between a vapour-only and a two-phase jet. If any (non-water) two-phase behaviour is relevant then a SPECIES keyword for the corresponding compound *must be specified.* Serious underpredictions will result if two-phase behaviour is appropriately neglected.

Although the AEROPLUME model is reasonably robust, under certain circumstances the non-linear solver SPRINT used in AEROPLUME, might not be able to find a (physical) solution. This especially occurs for very dense, touch down jets or for plumes which entrain themselves due to strong bending over. Upwind directed releases of dense jets may also cause severe numerical problems.

Numerical difficulties can sometimes be overcome by slightly changing the input parameters. It should be realised that the influence of atmospheric parameters (wind speed, stability class) and also of surface roughness, on the near-field dispersion is not very strong for high-momentum jets. Therefore changing these parameters will not have large effects on calculated near-field AEROPLUME results, but might solve numerical problems.

For two-phase releases, the calculation time to simulate the first few meters of the jet dispersion can be high compared to calculations further downwind.

AEROPLUME INPUT PARAMETERS

A description of all the input parameters that can occur in an AEROPLUME input file will be given.

The AEROPLUME input file has the DOS filename 'casename.API' where 'casename' is the user-supplied name of the problem.

In the following, actual keywords are given in *capitals* and in *bold*. The descriptions of less important parameters or parameters that need not normally be set by the user, are given in a *smaller font*.

All parameters, except **TITLE**, occur in blocks preceded by a specific block keyword. For AEROPLUME these block keywords are: **RESERVOIR**, **RELEASE**, **GASDATA**, **PIPE**, **AMBIENT**, **DISP**, **MMESOPT**, **TERMINAT** and **MATCH**.

The **TITLE** keyword does *not* occur in a parameter block.

TITLE	The title of the current problem to be run with AEROPLUME. At most 50 alphanumeric characters. Optional, no default.

The **RESERVOIR** block contains the parameters which describe the reservoir fluid thermodynamic state.

TRES	Temperature of the reservoir fluid (°C). -50 ≤ **TRES** ≤ 1500. Mandatory.
PRES	Absolute pressure within the reservoir (atm). -1 ≤ **PRES** ≤ 200. Mandatory. A negative value of **PRES** serves as a flag to AEROPLUME: the program will calculate the saturation pressure of the specified mixture assuming all compounds are in the liquid-only state and use this as the value for the reservoir pressure. This option is only available when the two-phase (aerosol) thermodynamics model is being used, in other words when the **SPECIES** keyword is being used in the **GASDATA** block as discussed below. It is the user's responsibility to judge whether these assumptions in calculating the reservoir pressure are reasonable or not. PRES must always be greater than **AIRPRESS** of the **AMBIENT** block.

The **RESERVOIR** block can be omitted if the **RELEASE** block, discussed on the next page, is being specified.

Adding the **RELEASE** input block to the parameter file causes AEROPLUME to skip the reservoir and discharge calculations. The data of the **RESERVOIR** block (if specified) is *ignored*. The pollutant mass flow rate **DMDT** in the **PIPE** block must be positive when using the **RELEASE** block.
This input block is useful for vent stack simulations.

TSTACK	Temperature of the stack release fluid (°C). -50 ≤ **TSTACK** ≤ 1500. Mandatory.

The **GASDATA** block contains the pollutant composition and thermodynamic data. The reservoir or initial stack mixture consists of 100 % wet pollutant by definition. Wet pollutant is defined to consist of the dry pollutant *plus* any water present in pollutant (as specified by **WATERPOL**).

WATERPOL	Mole fraction water (liquid plus vapour) in *wet* pollutant (-). $0 \leq$ **WATERPOL** ≤ 1.0. Optional, default is 0.0.
CPGAS	Specific heat at constant pressure of the *dry* pollutant (J/(mole K)). $5 \leq$ **CPGAS** ≤ 300. Mandatory if **SPECIES** keyword is not used (gas-only mixture), *no default*. If **SPECIES** keyword is used then **CPGAS** is needed when a link file to HEGADAS is being made. Thus in practice **CPGAS** must almost always be specified. Using HGSYSTEM module DATAPROP to find **CPGAS** and other keywords is strongly recommended.
MMGAS	Molar mass of *dry* pollutant (kg/kmole). $2 \leq$ **MMGAS** ≤ 200. Same comments as for **CPGAS** apply. Again, use of DATAPROP to calculate **MMGAS** is recommended.
HEATGR	Natural convection heat transfer group $(\mathrm{J} \cdot \mathrm{m}^{\frac{2}{3}} / (\mathrm{s}^{\frac{1}{3}} \cdot \mathrm{K}^{\frac{5}{3}} \cdot \mathrm{kmole}))$ $5 \leq$ **HEATGR** ≤ 100. Optional, *no default*. Not used by AEROPLUME model but written to HEGADAS link file if this is being made. Use of DATAPROP to calculate **HEATGR** is strongly recommended.
SPECIES	Pollutant compound properties. Using this keyword at least once implies the use of the full two-phase (aerosol) model or a mixture consisting of at least one compound (excluding water). If the **SPECIES** keyword is *not* specified, ideal gas thermodynamics is used with gas properties given by **CPGAS** and **MMGAS**. Condensation or freezing of *water* is still taken into account. The **SPECIES** keyword plus parameters must be specified *for every compound* in the mixture, except water. The sum of the molar fractions used in the **SPECIES** keywords (see parameter #2 below) *must* equal 1.0 - **WATERPOL.** The use of DATAPROP to generate the input parameters when the **SPECIES** keyword is being used, is strongly recommended. Currently a maximum of 8 species can be specified (excluding water). Please note that DATAPROP allows for more species to be specified. DATAPROP also splits *dry air* (if specified) up into nitrogen and oxygen, thus generating *two* compounds instead of one. Thus the AEROPLUME link file generated by DATAPROP could contain the

SPECIES keyword more than 8 times. The user should combine or remove compounds if this occurs.

Within the above-mentioned restrictions, there are no restrictions within AEROPLUME concerning the number of aerosols forming or the number of compounds per aerosol. Please note that HEGADAS *does* have restrictions: either a single two-compound aerosol or a number of separate one-compound aerosols are allowed (not regarding water and dry air), other combinations are not supported. See the description of the SPECIES keyword for the HEGADAS model.

Following the **SPECIES** keyword of a certain compound a block of 14 parameters (#1 to #14) *must* be specified:

#1 compound name (maximum of 12 characters).
#2 mole fraction in pollutant mixture (-).
$0 \le \#2 \le 1$.
#3 aerosol class (-).
$-1 \le \#3 \le 50$.
#4 specific heat of vapour (J/(mole K)).
$5 \le \#4 \le 300$.
#5 specific heat of liquid (J/(mole K)).
$0 \le \#5 \le 10^3$.
#6 heat of vaporisation (J/mole)
$0 \le \#6 \le 10^5$
#7 critical temperature (K).
$0 \le \#7 \le 10^4$.
#8 critical pressure (atm).
$0 \le \#8 \le 10^3$.
#9 vapour pressure function coefficient B1.
$-10^8 \le \#9 \le 10^8$.
#10 vapour pressure function coefficient B2.
$-10^8 \le \#10 \le 10^8$.
#11 vapour pressure function coefficient B3.
$-10^8 \le \#11 \le 10^8$.
#12 vapour pressure function coefficient B4.
$-10^8 \le \#12 \le 10^8$.
#13 molar mass (kg/kmole).
$2 \le \#13 \le 200$.
#14 liquid density (kg/m^3).
$1 \le \#14 \le 10^5$.

Note: the saturated vapour pressure of the compound is described by the Wagner function:

$$P_v(T) = P_c \cdot \exp\left\{\left[B_1 \cdot Q + B_2 \cdot Q^{1.5} + B_3 \cdot Q^3 + B_4 \cdot Q^6\right] / T_r\right\}$$

where T is the vapour temperature, P_c the critical pressure, T_c the critical temperature, $T_r = T/T_c$ and $Q = 1 - T_r$.

The **PIPE** block contains the release pipe/orifice exit-plane conditions.

DMDT	Steady wet pollutant mass discharge rate (kg/s). $-10^3 \le$ **DMDT** $\le 10^5$. Mandatory. A non-positive value for **DMDT** serves as a flag to AEROPLUME: the program will in this case use a literature correlation to calculate **DMDT**. However, the maximum value of **DMDT**, calculated using AEROPLUME's own discharge model, will never be exceeded. If the user has specified the **RELEASE** block, then **DMDT** *must* be *positive*.
DEXIT	Effective orifice diameter of the discharge pipe (m). $0.001 \le$ **DEXIT** ≤ 10. Mandatory.
ZEXIT	Height above ground level of discharge opening (m). $0.0 \le$ **ZEXIT** ≤ 600. Mandatory. **ZEXIT** should be greater than **ZR** in the **DISP** block because otherwise model assumptions used in some atmospheric correlations will be violated.
ANGLE	Inclination of release opening with respect to horizontal (°). $-180 \le$ **ANGLE** ≤ 180. Optional, default is 0° (downwind horizontal release). E.g. for a vertically upward release **ANGLE** is 90°.
DURATION	Duration of pollutant release (s). $-10^6 \le$ **DURATION** $\le 10^6$. Optional, default is -1 (steady release). If **DURATION** ≤ 0, then a steady release is assumed (infinite duration). Please note that this is not always a realistic scenario as the total amount of released pollutant can become very large. AEROPLUME does not use **DURATION** itself as it only simulates steady releases, but for a proper transition to HEGADAS-S or HEGADAS-T the value of **DURATION** is needed.
CDG	Discharge coefficient for vapour only releases (-). $0.0 \le$ **CDG** ≤ 1.0. Optional, default is 1.0. AEROPLUME uses discharge coefficients to estimate value for **DMDT**, the user might want to change the default values of these coefficients.
CDL	Discharge coefficient for liquid or two-phase releases (-). $0.0 \le$ **CDL** ≤ 1.0. Optional, default is 0.61. AEROPLUME uses discharge coefficients to estimate value for **DMDT**, the user might want to change the default values of these coefficients.

The **AMBIENT** block contains parameters describing the conditions of the ambient atmosphere.

Z0	Reference height for atmospheric data in this block (m). $0.1 \leq \textbf{Z0} \leq 200$. Mandatory.
U0	Ambient wind velocity at height **Z0** (m/s). $0.0 < \textbf{U0} \leq 20$. Mandatory. Please note that **U0** can be small but never *equal* to 0.
AIRTEMP	Ambient air temperature at height **Z0** (°C). $-50 \leq \textbf{AIRTEMP} \leq 50$. Mandatory.
AIRPRESS	Ambient air pressure at release height **ZEXIT** (atm). $0.7 \leq \textbf{AIRPRESS} \leq 1.1$. Optional, default is 1.0 atm. **AIRPRESS** must be less than **PRES** of the **RESERVOIR** block.
RHPERC	Relative air humidity at release height **ZEXIT** (%). $0.0 \leq \textbf{RHPERC} \leq 100$. Mandatory.

The **DISP** block contains parameters describing the dispersion characteristics.

ZR	Land surface roughness (m). $10^{-5} \leq$ **ZR** ≤ 1. Mandatory. **ZR** must be less than **ZEXIT** of the **PIPE** block.
PQSTAB	Pasquill/Gifford stability class. **PQSTAB** = A, B, C, D, E or F (character). Mandatory.

The **MMESOPT** block contains the 'switches' which indicate the use of the extra options developed by Earth Technology and sponsored by Martin Marietta Energy Systems. An indicator value of 1 means that the corresponding option is used, a value of 0 means that the option is inactive.

IMETP	Indicator for use of meteorological pre-processor (-). **IMETP** = 0 or 1. Optional, default is 0. For **IMETP** = 1, an additional file 'casename.MET' *must* be supplied. See Chapter 18 for a description of the data which must be given in this file.
IDEP	Indicator for use of wet and dry deposition model (-). **IDEP** = 0 or 1. Optional, default is 0. For **IDEP** = 1, an additional file 'casename.DEP' *must* be supplied. See Chapter 18 for a description of the data which must be given in this file.
ICANY	Indicator for calculation of canyon effects (-). **ICANY** = 0 or 1. Optional, default is 0. For **ICANY** = 1, an additional file 'casename.CNY' *must* be supplied. See Chapter 18 for a description of the data which must be given in this file.
IFLUC	Indicator for calculation of centre-line concentration fluctuations (-). **IFLUC** = 0 or 1. Optional, default is 0. For **IFLUC** = 1, an additional file 'casename.PTL' *must* be supplied. See Chapter 18 for a description of the data which must be given in this file.
ILIFT	Indicator for use of plume lift-off description (-). **ILIFT** = 0 or 1. Optional, default is 0. No additional data needed. When **ILIFT** = 0, AEROPLUME will stop program execution when plume lift-off is detected for a plume after touch-down. When **ILIFT** = 1, a plume is allowed to become air-borne again after touch-down. See Chapter 9 in the HGSYSTEM 3.0 Technical Reference Manual for details.

The **TERMINAT** block sets plume development termination criteria. Normally these are all *inactive* (by setting them to a negative value) and the AEROPLUME run will only end when a transition can be made to HEGADAS or to PGPLUME. Sometimes, however, it can be useful to stop the run before this transition occurs. The **TERMINAT** parameters can be used for this purpose.

DLST	Last required plume diameter (m). $-1000 \leq \mathbf{DLST} \leq 1000$. Optional, default is -1.0 (criterion inactive). If set to a negative value, the termination criterion will not be used.
SLST	Last required displacement measured along plume axis (m). $-1000 \leq \mathbf{SLST} \leq 2000$. Optional, default is -1.0 (criterion inactive). If set to a negative value, the termination criterion will not be used
ZLST	Last required plume centroid height (m). $-1000 \leq \mathbf{ZLST} \leq 1000$. Optional, default is -1.0 (criterion inactive). If set to a negative value, the termination criterion will not be used.
XLST	Last required horizontal displacement (m). $-1000 \leq \mathbf{XLST} \leq 2000$. Optional, default is -1.0 (criterion inactive). If set to a negative value, the termination criterion will not be used.
ULST	Last required plume velocity (m/s). $-1000 \leq \mathbf{ULST} \leq 500$. Optional, default is -1.0 (criterion inactive). If set to a negative value, the termination criterion will not be used.
CPOLST	Last required pollutant concentration (kg/m^3). $-1000 \leq \mathbf{CPOLST} \leq 1000$. Optional, default is -1.0 (criterion inactive). If set to a negative value, the termination criterion will not be used.
VPOLST	Last required volumetric pollutant concentration (vol%). $-1000 \leq \mathbf{VPOLST} \leq 100$. Optional, default is -1.0 (criterion inactive). If set to a negative value, the termination criterion will not be used.

The **MATCH** block parameters contain the criteria that determine when the transition from AEROPLUME to one of the far-field models (HEGADAS and PGPLUME) will occur.
Normally the user should not change these parameters.
However, if the user wants to influence the transition location, then the **MATCH** parameters should be modified. This is only recommended for expert users or after seeking expert advice.

RULST	Excess velocity ratio (-). $10^{-3} \leq$ **RULST** ≤ 1.0. Optional, default is 0.1.
RELST	Entrainment ratio (-). $10^{-3} \leq$ **RELST** ≤ 1.0. Optional, default is 0.3.
RGLST	Buoyancy effect for advection (-). $10^{-3} \leq$ **RGLST** ≤ 1.0. Optional, default is 0.3.
RNLST	Buoyancy effect for passive diffusion (-). $10^{-3} \leq$ **RNLST** ≤ 1.0. Optional, default is 0.1.
RALST	Aspect ratio for passive diffusion (-). $10^{-3} \leq$ **RALST** ≤ 1.0. Optional, default is 0.2.

The **CONCS** block contains the minimum and maximum volumetric concentrations that are used to generate extra plume information concerning the contents of pollutant and total mixture within the cloud.

VCMAX	Maximum volumetric concentration (%). $0 \leq$ **VCMAX** ≤ 100. Optional, default is 100. E.g. higher flammability limit.
VCMIN	Minimum volumetric concentration (%). $0 \leq$ **VCMIN** ≤ 100. Optional, default is 0. E.g. lower flammability limit.

11. HFPLUME

General introduction

The HFPLUME model is the HF-specific version of AEROPLUME which can be used to simulate pressurised jet releases from a reservoir containing a mixture of HF, water, an inert ideal gas and dry air. HFPLUME uses the full chemistry and thermodynamics of a reacting system of HF/water/inert gas mixture. The HGSYSTEM 3.0 Technical Reference Manual contains a chapter which gives details about the HF chemistry model.

HFPLUME is a steady-state program.

HFPLUME calculations start from user-specified reservoir conditions. A reservoir discharge calculation plus a flash calculation will precede the actual atmospheric dispersion calculation.

The HFPLUME program will generate a link file to one of the far-field HGSYSTEM models (PGPLUME or HEGADAS) if possible. This is done completely automatically.

Range of applications and limitations

The HFPLUME model should not be used for very low-speed jets (slower than ambient wind speed), as wake-effects will be important.

HFPLUME should not be used for *unpressurised* releases, or for any releases where exit velocities are small compared to ambient wind speed or where initial momentum is quickly destroyed by impact with the ground. In those cases the evaporating liquid pool model LPOOL should be used.

Jets touching the ground at high speed and very steep angles should also not be simulated with HFPLUME.

It is *very important* when interpreting HFPLUME results to realise that all physical quantities (concentration, density, temperature etc) are always *average* quantities over the plume cross-section. As a general rule of thumb, peak concentrations will be about a factor 1.3-1.4 higher than the cross-sectional mean concentrations as given in the HFPLUME report file.

Guidance for use

See the AEROPLUME chapter for general information.
The HFPLUME model is not as robust as the AEROPLUME model, mainly due to the complicated HF chemistry and thermodynamics involved.
Numerical difficulties can sometimes be overcome by slightly changing the input parameters. It should be realised that the influence of atmospheric parameters (wind speed, stability class) and also of surface roughness, on the near-field dispersion is not very strong for high-momentum jets. Therefore changing these parameters will not have large effects on calculated near-field HFPLUME results, but might solve numerical problems.

HFPLUME INPUT PARAMETERS

A description of all the input parameters that can occur in an HFPLUME input file will be given.

The HFPLUME input file has the DOS filename 'casename.HPI' where 'casename' is the user-supplied name of the problem.

In the following, actual keywords are given in *capitals* and in *bold*. The descriptions of less important parameters or parameters that need not normally be set by the user, are given in a *smaller font*.
All parameters, except **TITLE**, occur in blocks preceded by a specific block keyword. For HFPLUME these block keywords are: **RESERVOIR**, **GASDATA**, **PIPE**, **AMBIENT**, **DISP**, **MMESOPT**, **TERMINAT** and **MATCH**.
Some of these blocks are identical or very similar to the corresponding AEROPLUME input blocks.

The **TITLE** keyword does *not* occur in a parameter block.

TITLE	The title of the current problem to be run with HFPLUME. At most 50 alphanumeric characters. Optional, no default.

The **RESERVOIR** block contains the parameters which describe the reservoir fluid thermodynamic state.

TRES	Temperature of the reservoir mixture (°C). $-50 \le$ **TRES** ≤ 150. Mandatory.
PRES	Absolute pressure within the reservoir (atm). $0.7 \le$ **PRES** ≤ 20. Mandatory. **PRES** must be greater than **AIRPRESS** in the **AMBIENT** block.
HFRES	Mass percentage HF in reservoir (%) $0 \le$ **HFRES** ≤ 100. Mandatory
HCRES	Mass percentage inert ideal gas in reservoir (%) $0 \le$ **HCRES** ≤ 100. Mandatory
H2ORES	Mass percentage water in reservoir (%) $0 \le$ **H2ORES** ≤ 100. Mandatory

Note: The sum of **HFRES**, **HCRES** and **H2ORES** need not be exactly equal to 100 %. If the sum is smaller, the HFPLUME program will add *dry air* to the reservoir mixture to get a 100 % mixture. Too large values will be changed by the program and messages will be generated accordingly. For numerical reasons, the mass percentage dry air in the mixture should preferably be larger than about 1 %.

The **GASDATA** block only contains data concerning the inert ideal gas that can be specified in the **RESERVOIR** block. All other chemical species data is included in the HF chemistry description of HFPLUME.

CPGAS	Specific heat at constant pressure of the inert ideal gas (J/(mole·K)). 5 ≤ **CPGAS** ≤ 200. Mandatory.
MMGAS	Molar mass of the inert ideal gas (kg/kmole). 5 ≤ **MMGAS** ≤ 200. Mandatory.

The **PIPE** block contains the release pipe/orifice exit-plane conditions.

DMDT	Steady mass discharge rate (kg/s). $0.01 \le$ **DMDT** ≤ 1000. Mandatory.
DEXIT	Effective orifice diameter of the discharge pipe (m). $0.001 \le$ **DEXIT** ≤ 5. Mandatory.
ZEXIT	Height above ground level of discharge opening (m). $0.0 \le$ **ZEXIT** ≤ 50. Mandatory. **ZEXIT** should be greater than **ZR** in the **DISP** block because otherwise model assumptions used in some atmospheric correlations will be violated.
ANGLE	Inclination of release opening with respect to horizontal (°). $-180 \le$ **ANGLE** ≤ 180. Optional, default is 0° (downwind horizontal release). E.g. for a vertically upward release **ANGLE** is 90°.
DURATION	Duration of pollutant release (s). $-10^6 \le$ **DURATION** $\le 10^6$. Optional, default is -1 (steady release). If **DURATION** ≤ 0, then a steady release is assumed (infinite duration). Please note that this is not always a realistic scenario as the total amount of released pollutant can become very large. HFPLUME does not use **DURATION** itself as it only simulates steady releases, but for a proper transition to HEGADAS-S or HEGADAS-T the value of **DURATION** is needed.

The **AMBIENT** block contains parameters describing the conditions of the ambient atmosphere.

Z0	Reference height for atmospheric data in this block (m). 0.1 ≤ **Z0** ≤ 50. Mandatory.
U0	Ambient wind velocity at height **Z0** (m/s). 0.5 < **U0** ≤ 20. Mandatory. Please note that **U0** can be small but never *equal* to 0.
AIRTEMP	Ambient air temperature at height **Z0** (°C). -50 ≤ **AIRTEMP** ≤ 50. Mandatory.
AIRPRESS	Ambient air pressure at release height **ZEXIT** (atm). 0.7 ≤ **AIRPRESS** ≤ 1.1. Optional, default is 1.0 atm. **AIRPRESS** must be less than **PRES** in the **RESERVOIR** block.
RHPERC	Relative air humidity at release height **ZEXIT** (%). 0.0 ≤ **RHPERC** ≤ 100. Mandatory.

The **DISP** block contains parameters describing the dispersion characteristics.

ZR	Land surface roughness (m). $10^{-5} \leq$ **ZR** ≤ 1. Mandatory. **ZR** must be less than **ZEXIT** of the **PIPE** block.
PQSTAB	Pasquill/Gifford stability class. **PQSTAB** = A, B, C, D, E or F (character). Mandatory.

The **MMESOPT** block contains the 'switches' which indicate the use of the extra options developed by Earth Technology and sponsored by Martin Marietta Energy Systems. An indicator value of 1 means that the corresponding option is used, a value of 0 means that the option is inactive.

ILIFT	Indicator for use of plume lift-off description (-). **ILIFT** = 0 or 1. Optional, default is 0. No additional data needed. When **ILIFT** = 0, HFPLUME will stop program execution when plume lift-off is detected for a plume after touch-down. When **ILIFT** = 1, a plume is allowed to become air-borne again after touch-down. See Chapter 9 in the HGSYSTEM 3.0 Technical Reference Manual for details.

The **TERMINAT** block sets plume development termination criteria. Normally these are all *inactive* (by setting them to a negative value) and the HFPLUME run will only end when a transition can be made to HEGADAS or to PGPLUME. Sometimes, however, it can be useful to stop the run before this transition occurs. The **TERMINAT** parameters can be used for this purpose.

DLST	Last required plume diameter (m). -1000 ≤ **DLST** ≤ 1000. Optional, default is -1.0 (criterion inactive) If set to a negative value, the termination criterion will not be used.
SLST	Last required displacement measured along plume axis (m). -1000 ≤ **SLST** ≤ 1000. Optional, default is -1.0 (criterion inactive) If set to a negative value, the termination criterion will not be used
ZLST	Last required plume centroid height (m). -1000 ≤ **ZLST** ≤ 1000. Optional, default is -1.0 (criterion inactive) If set to a negative value, the termination criterion will not be used.
XLST	Last required horizontal displacement (m). -1000 ≤ **XLST** ≤ 1000. Optional, default is -1.0 (criterion inactive) If set to a negative value, the termination criterion will not be used.
ULST	Last required plume velocity (m/s). -1000 ≤ **ULST** ≤ 500. Optional, default is -1.0 (criterion inactive) If set to a negative value, the termination criterion will not be used.
HFLST	Last required HF concentration (mole %). -1000 ≤ **HFLST** ≤ 100. Optional, default is -1.0 (criterion inactive) If set to a negative value, the termination criterion will not be used.
HCLST	Last required inert gas concentration (mole %). -1000 ≤ **HCLST** ≤ 100. Optional, default is -1.0 (criterion inactive) If set to a negative value, the termination criterion will not be used.

The **MATCH** block parameters contain the criteria that determine when the transition from HFPLUME to one of the far-field models (HEGADAS and PGPLUME) will occur.
Normally the user should not change these parameters.
However, if the user wants to influence the transition location, then the **MATCH** parameters should be modified.
This is only recommended for expert users or after seeking expert advice.

RULST	Excess velocity ratio (-). $10^{-3} \leq$ **RULST** ≤ 1.0. Optional, default is 0.1.
RELST	Entrainment ratio (-). $10^{-3} \leq$ **RELST** ≤ 1.0. Optional, default is 0.3.
RGLST	Buoyancy effect for advection (-). $10^{-3} \leq$ **RGLST** ≤ 1.0. Optional, default is 0.3.
RNLST	Buoyancy effect for passive diffusion (-). $10^{-3} \leq$ **RNLST** ≤ 1.0. Optional, default is 0.1.
RALST	Aspect ratio for passive diffusion (-). $10^{-3} \leq$ **RALST** ≤ 1.0. Optional, default is 0.2.

12. HEGABOX

General introduction

HEGABOX is the HGSYSTEM model that describes the initial phase in the spreading of an initially stagnant, dense cloud. For an *instantaneous* release like this, gravity driven spreading dominates during the first phase of the dispersion process.

HEGABOX is a fully time-dependent model.

HEGABOX either uses the full hydrogen fluoride (HF) chemistry and thermodynamics or the standard HGSYSTEM multi-compound, two-phase aerosol thermodynamics model. See the Technical Reference Manual for details on the two thermodynamical descriptions.

HEGABOX can only simulate the initial cloud behaviour where the influence of ambient turbulence is still small. For longer times, a transition to a far-field model must be made. As HEGABOX models transient, dense gas dispersion, a link to HEGADAS-T, the time-dependent heavy gas dispersion model, will be made. The transition to HEGADAS-T will be made when the Richardson number reaches a critical value (normally 10). Note that when linking to HEGADAS-T, both a link file (.HTL) and an observer data file (.HBO) are needed. HEGABOX will create these files automatically.

Range of applications and limitations

HEGABOX can only be used for the very specific release conditions it was developed for. The initial cloud must be (almost) stagnant and dense. Possible scenarios are: dense gas releases with low momentum at low wind speeds and sudden releases of large quantities of dense gas.

HEGABOX has been validated with the Thorney Island data. See the HEGABOX chapter in the Technical Reference Manual.

Problems with significant liquid pools on the ground cannot be dealt with as liquid dropout from the cloud to the ground is not being modelled. If the initial cloud composition as found by HEGABOX results in a cloud with a very high liquid fraction then increasing the user-specified initial entrainment (see input parameter discussion below) might be helpful. For evaporation of liquid pools the LPOOL model of HGSYSTEM should be used.

HEGABOX INPUT PARAMETERS

A description of all the input parameters that can occur in a HEGABOX input file will be given.

The HEGABOX input file has the DOS filename 'casename.HBI' where 'casename' is the user-supplied name of the problem.

In the following, actual keywords are given in *capitals* and in *bold*. The descriptions of less important parameters or parameters that need not normally be set by the user, are given in a *smaller font*.

All parameters, except **TITLE**, occur in blocks preceded by a specific block keyword. For HEGABOX these block keywords are: **CONTROL, SPILL, GASDATA, AMBIENT, DISP** and **MMESOPT**.

The **TITLE** keyword does *not* occur in a parameter block.

TITLE	The title of the current problem to be run with HEGABOX. At most 50 alphanumeric characters. Optional, no default.

The optional **CONTROL** block contains several run control parameters.

TLAST	Maximum time for which HEGABOX calculates cloud dispersion (s). 0.01 ≤ **TLAST** ≤ 9000. Optional, default is 500 s. If during the calculation the time variable reaches the value **TLAST**, the run will be stopped. Usually **TLAST** is set sufficiently large so that the run ends because the Richardson number stop criterion has been met.
DTMAX	Maximum time step in output table and numerical integration (s). 0.01 ≤ **DTMAX** ≤ 100. Optional, default is 2 s. Only to be changed if the output table produced by HEGABOX in the report file ('casename.HBR'), is too long or too short, depending on the time scale of the problem.
PRTCODE	Output printing control code. **PRTCODE** = 0, 1, or 2. Optional, default is 1. Normally not to be changed. **PRTCODE** = 0 suppresses printout and with **PRTCODE** = 2 debug printout is generated.
RIMIN	Final (termination) Richardson number (-). 0.01 ≤ **RIMIN** ≤ 50. Optional, default is 10. When during the HEGABOX run the Richardson number falls below RIMIN, the run is ended, creating a link file for HEGADAS-T. This is the standard way to end the HEGABOX run. The default value of 10 should normally not be changed by the user.

The **SPILL** block contains data to describe the spill of pollutant. Wet pollutant = dry pollutant plus water contained in the pollutant (set by **WATERPOL**).

SPILLTOT	Spill size (excluding water pickup) (kg of wet pollutant). $1 \leq$ **SPILLTOT** $\leq 10^6$. Mandatory.
RSTART	Initial cloud radius (m). $10^{-2} \leq$ **RSTART** $\leq 10^3$. Mandatory. Note that in HEGABOX the cloud is always assumed to be a cylinder. The user might want to use the HGSYSTEM module LPOOL to find an estimated value for **RSTART**.

The **AMBIENT** block specifies the conditions of the ambient atmosphere.

Z0	Reference height for windspeed **U0** (m). 0.1 ≤ **Z0** ≤ 50. Mandatory.
U0	Ambient wind velocity at height **Z0** (m/s). 1.0 ≤ **U0** ≤ 20. Mandatory.
ZAIRTEMP	Reference height for temperature **AIRTEMP** (m). 0 ≤ **ZAIRTEMP** ≤ 50. Mandatory.
AIRTEMP	Ambient air temperature at height **ZAIRTEMP** (°C). -50 ≤ **AIRTEMP** ≤ 50. Mandatory.
RHPERC	Relative humidity of ambient air (%). 0.0 ≤ **RHPERC** ≤ 100. Optional, default is 0.
TGROUND	Temperature of the earth's surface (°C). -50 ≤ **TGROUND** ≤ 50. Mandatory.

The **DISP** block contains the atmospheric dispersion parameters. Note that the ambient pressure is always taken to be 1.0 atm (760 mm Hg).

ZR	Land surface roughness (m). $10^{-5} \le$ **ZR** ≤ 1. Mandatory.
PQSTAB	Pasquill/Gifford stability class (single character). **PQSTAB** = A, B, C, D, E or F. Mandatory.
MONIN	Monin-Obukhov length (m). $-500 \le$ **MONIN** $\le 10^{20}$. Optional, default calculated by HEGABOX based on **ZR** and **PQSTAB**. The user can override the correlation-based value that HEGABOX normally will use, e.g. if measurements are available.

In the **GASDATA** block we specify the physical properties of the pollutant. Most of the parameter values can be generated using DATAPROP and for a pollutant consisting of several compounds it is strongly recommended to use DATAPROP prior to HEGABOX to generate these values.

THERMOD	Thermodynamical model used (-). **THERMOD** = 1, 2. Optional, default is 1 (non-reactive aerosol model). **THERMOD** = 1 implies the use of the standard HGSYSTEM non-reactive, multi-compound two-phase thermodynamic model. In the absence of an aerosol, ideal gas relations will hold. For **THERMOD** = 2 the full HF thermodynamical model will be used.
TGAS	Initial wet pollutant temperature (°C). -273 ≤ **TGAS** ≤ 100. Mandatory. **TGAS** is the wet pollutant temperature before any dilution with ambient wet air (see **INICONC** below) and before water pickup (see **WPICKUP** below). Wet pollutant = dry pollutant plus water contained in the pollutant.
WATERPOL	Mole fraction water (liquid plus vapour) in wet pollutant (-). 0 ≤ **WATERPOL** ≤ 0.2. Optional, default is 0.0. **WATERPOL** refers to the released pollutant only, it should not take the water pickup into account (see **WPICKUP** below).
WPICKUP	Mole fraction water picked up from earth's surface during release (-). 0 ≤ **WPICKUP** ≤ 0.2. Optional, default is 0.0. **WPICKUP** is extra water added to the (wet pollutant) mixture during release, the original pollutant may already contain water (see **WATERPOL** above). The picked up water has temperature **TGROUND**.
INICONC	Dilution by initial entrainment (mole wet pollutant plus water pickup per mole total mixture). 10^{-5} ≤ **INICONC** ≤ 1.0. Optional, default is 1.0. The mixture after water pickup can be diluted by an initial entrainment with wet ambient air. The air composition and temperature are as specified in the **AMBIENT** block. Useful for very 'violent' releases where at the start of the HEGABOX simulation significant entrainment already has occurred.
MMGAS	Molecular mass of the dry pollutant (kg/kmole). 2 ≤ **MMGAS** ≤ 200. Mandatory. Will be generated by DATAPROP.
CPGAS	Specific heat at constant pressure of the dry pollutant (J/(mole K)).

	$5 \le$ **CPGAS** ≤ 200. Mandatory. Will be generated by DATAPROP.
DIFFDT2	Thermal diffusivity of the dry pollutant at a representative temperature T, divided by T^2 ($m^2/s/K^2$). $3 \cdot 10^{-11} \le$ **DIFFDT2** $\le 3 \cdot 10^{-9}$ Mandatory. Division by T^2 is used to try to scale out the temperature dependency of the thermal diffusivity. Used in calculation of natural convection heat flux. Will be generated by DATAPROP.
VISCDT2	Kinematic viscosity of the dry pollutant at a representative temperature T, divided by T^2 ($m^2/s/K^2$). $2 \cdot 10^{-11} \le$ **VISCDT2** $\le 3 \cdot 10^{-9}$. Mandatory. Division by T^2 is used to try to scale out the temperature dependency of the kinematic viscosity. Used in calculation of natural convection heat flux. Will be generated by DATAPROP The value of **HEATGR** (communicated to HEGADAS-T) is calculated as: **HEATGR** = (**DIFFDT2**·**VISCDT2**)$^{2/3}$·**CPGAS**·1000/**VISCDT2**. The factor 1000 arises because we want the specific heat per kmole. **HEATGR** is not a HEGABOX keyword, but it is a HEGADAS keyword.
SPECIES	Pollutant compound properties. Using this keyword at least once implies the use of the full two-phase (aerosol) model for a mixture consisting of at least one compound (excluding water). If the **SPECIES** keyword is not specified, ideal gas thermodynamics is used with gas properties given by **CPGAS** and **MMGAS**. Condensation or freezing of water is still taken into account. The SPECIES keyword plus parameters must be specified for every compound in the mixture, except water. The sum of the molar fractions (see parameter #2 below) must equal 1.0 - **WATERPOL**. The use of DATAPROP to generate the input parameters when the **SPECIES** keyword is being used, is strongly recommended. Currently a maximum of 8 species can be specified (excluding water). Please note that DATAPROP allows for more species to be specified. DATAPROP also splits dry air (if specified) up into nitrogen and oxygen, thus generating two compounds instead of one. Thus the HEGABOX link file generated by DATAPROP could contain the **SPECIES** keyword more than 8 times. The user should combine or remove compounds if this occurs.

Please note that. in contrast with SPILL and AEROPLUME. HEGABOX and HEGADAS do have some restrictions: either a single two-compound aerosol or a number of separate one-compound aerosols are allowed (not regarding water and dry air), other combinations are not supported.

Following the SPECIES keyword of a certain compound a block of 12 parameters (#1 to #12) must be specified:

#1 compound name (maximum of 12 characters).
#2 mole fraction in pollutant mixture (-).
$0 \leq \#2 \leq 1$.
#3 aerosol class (-).
$-1 \leq \#3 \leq 50$.
#4 specific heat of vapour (J/(mole.K)).
$5 \leq \#4 \leq 300$.
#5 specific heat of liquid (J/(mole.K)).
$0 \leq \#5 \leq 10^3$.
#6 heat of vaporisation (J/mole).
$0 \leq \#6 \leq 10^5$
#7 critical temperature (K)
$0 \leq \#7 \leq 10^4$
#8 critical pressure (atm)
$0 \leq \#8 \leq 10^3$
#9 vapour pressure function coefficient B1
$-10^8 \leq \#9 \leq 10^8$
#10 vapour pressure function coefficient B2
$-10^8 \leq \#10 \leq 10^8$
#11 vapour pressure function coefficient B3
$-10^8 \leq \#11 \leq 10^8$
#12 vapour pressure function coefficient B4
$-10^8 \leq \#12 \leq 10^8$

<u>Note</u>: the saturated vapour pressure of the compound is described by the Wagner function:

$$P_v(T) = P_c \cdot \exp\left\{\left[B_1 \cdot Q + B_2 \cdot Q^{1.5} + B_3 \cdot Q^3 + B_4 \cdot Q^6\right] / T_r\right\}$$

where T is the vapour temperature, P_c the critical pressure, T_c the critical temperature, $T_r = T/T_c$ and $Q = 1 - T_r$.

The **MMESOPT** block contains the 'switches' which indicate the use of the extra options developed by Earth Technology and sponsored by Martin Marietta Energy Systems. An indicator value of 1 means that the corresponding option is used a value of 0 means that the option is inactive.

IMETP	Indicator for use of meteorological pre-processor (-). **IMETP** = 0 or 1. Optional, default is 0. For **IMETP** = 1, an additional file 'casename.MET' *must* be supplied. See Chapter 18 for a description of the data which must be given in this file.
IDEP	Indicator for use of wet and dry deposition model (-). **IDEP** = 0 or 1. Optional, default is 0. For **IDEP** = 1, an additional file 'casename.DEP' *must* be supplied. See Chapter 18 for a description of the data which must be given in this file.
ICANY	Indicator for calculation of canyon effects (-). **ICANY** = 0 or 1. Optional, default is 0. For **ICANY** = 1, an additional file 'casename.CNY' *must* be supplied. See Chapter 18 for a description of the data which must be given in this file.
IFLUC	Indicator for calculation of centre-line concentration fluctuations (-). **IFLUC** = 0 or 1. Optional, default is 0. For **IFLUC** = 1, an additional file 'casename.PTL' *must* be supplied. See Chapter 18 for a description of the data which must be given in this file.

13. HEGADAS

General introduction

HEGADAS is the HGSYSTEM model for heavy gas dispersion from area sources. It is one of the oldest and most complex HGSYSTEM models and has many features and options.

HEGADAS has a steady-state version, called HEGADAS-S, and also a time-dependent (transient) version, called HEGADAS-T. Parameters of both versions are discussed in this chapter. HEGADAS-S can also be used for finite-duration releases.

HEGADAS can use *either* the standard HGSYSTEM multi-compound, two-phase aerosol thermodynamical model *or* the full hydrogen fluoride (HF) chemistry and thermodynamics. Both descriptions are discussed in separate chapters of the Technical Reference Manual.

HEGADAS can be used for three scenarios:
(1) evaporating pool scenario
(2) post-HEGABOX run
(3) post-AEROPLUME/HFPLUME run

In case (1), source term data generated from LPOOL (and HFFLASH if applicable) can be used. LPOOL (and HFFLASH) will generate link files with this information.
In case (2), HEGABOX will generate a link file plus an observer data file which will be used by HEGADAS-T.
Case (3) occurs when the near-field jet model (AEROPLUME or HFPLUME) makes a transition to HEGADAS at the end of the jet simulation. Relevant data is again communicated through a link file.

HEGADAS uses the concept of 'breakpoints'. Using a breakpoint, HEGADAS calculations can be interrupted or initiated at a specified downwind location. At a 'partial' breakpoint some variables may be changed (e.g. surface roughness). At a 'full' breakpoint a complete HEGADAS run is initiated, typically after running a jet model, this happens in scenario (3) above. More details on 'breakpoints' can be found in the HGSYSTEM 3.0 Technical Reference Manual section 7.A.3.4.1., 7.A.4. and 7.C.3.1.

POSTHS and POSTHT are the HGSYSTEM version 3.0 post-processors to plot HEGADAS results. They are discussed in Chapter 15.

Range of applications and limitations

HEGADAS is intended for heavy gas dispersion simulations. It should not be used for buoyant clouds or clouds that become buoyant. It should also not be used for clouds which have considerable momentum of their own.

Guidance for use

HEGADAS is a complicated model. To appreciate its full capabilities the user should read some of the technical background information in the Technical Reference Manual.

Use of defaults for many parameters is strongly advised (see discussion below).

The HEGADAS-T model is quite complex to use and interpret. For every new case the user wants to analyse, it is usually necessary to run the model several times to get a feeling for the results. Run times will be long (several minutes), especially for HF runs.
Concentration and cloud information will only be given for certain output times. The choice of the output times is important in interpreting results. Using the option to generate output times automatically is recommended.

For finite-duration releases where the travel time to a distance of concern is greater than the release duration, HEGADAS-T should be used instead of HEGADAS-S.

The HEGADAS code is quite robust: numerical problems seldom occur. If numerical problems do occur (especially for HF), slightly changing the input parameters might be helpful.

The report file use the following nomenclature:

DISTANCE	m	downwind distance fron source (x coordinate)
CONC	-	ground level centre-line concentration; % molar fraction of pollutant (all HF assumed to be monomer)
SZ	m	vertical dispersion coefficient S_z
SY	m	vertical dispersion coefficient S_y
MIDP	m	half-width b of the middle part of the cross-wind concentrtion profile (see Figure 7.A.1)
YCU, YCL	m	cross-wind distance from cloud centre-line (y coordinate) at which CONC is equal to CU or CL respectively. See CLOUD input block for CU and CL.
ZCU, ZCL	m	height at which CONC is equal to CU or CL respectively (m).
RIB	-	bulk Richardson number Ri,
TMP	°C	ground level centre-line temperature
CA	kg/m^3	ground level centreiline concentration

HEGADAS INPUT PARAMETERS

A description of all the input parameters that can occur in a HEGADAS input file will be given. Some parameters are specific for either the transient or steady-state model. Unless specified, parameters apply to both versions.

The HEGADAS-S input file has the DOS filename 'casename.HSI' where 'casename' is the user-supplied name of the problem. For HEGADAS-T the file name is 'casename.HTI'.

In the following, actual keywords are given in *capitals* and in *bold*. The descriptions of less important parameters or parameters that need not normally be set by the user, are given in a *smaller font*.

All parameters, except **TITLE**, occur in blocks preceded by a specific block keyword.
For HEGADAS-S these block keywords are: **CONTROL**, **AMBIENT**, **GASDATA**, **DISP**, **CLOUD**, **TRANSIT** and **POOL**.
For HEGADAS-T these block keywords are: **CONTROL**, **AMBIENT**, **DISP**, **CLOUD**, **GASDATA**, **CALC**, **TRANSIT**, **TIMEDATA**, **AUTOTIM**, and **MMESOPT**.

The **TITLE** keyword does *not* occur in a parameter block.

TITLE	The title of the current problem to be run with AEROPLUME. At most 50 alphanumeric characters. Optional, no default.

The **CONTROL** block contains the parameters which controlling the type of calculations performed in the HEGADAS run.

ISURF	Indicator for surface heat effects and water vapour effects (-). **ISURF** = 2, 3 or 4. Optional, default is 3. **ISURF** = 2: no heat transfer or water-vapour effects. *Only* for isothermal problems without HF. **ISURF** = 3: heat transfer from ground to cloud is taken into account, but not water vapour effect. **ISURF** = 4: in addition to heat effect, also water vapour transfer from ground to cloud is accounted for. Use this value for dispersion over water (no HF). For a run involving HF, **ISURF** must always be 3.
ICNT	Concentration data print indicator (-) **ICNT** = 0 (inactive) or 1 (active). Optional, default is 0. When **ICNT** = 1, concentration data is written to a file 'casename.HS1' or 'casename.HT1'. The following is written at every reporting downwind distance: - y-co-ordinates (y_{cu},y_{cl}) where ground-level concentration equals **CU** or **CL**, - heights (z_{cu},z_{cl}) where ground-level concentration equals **CU** or **CL**, - cumulative volumes (V_{cu},V_{cl}) (m^3) where concentrations exceed **CU** or **CL** for the part of the cloud up to present downwind position, - cumulative vapour contents (M_{cu},M_{cl}) (kg) where concentrations exceed **CU** or **CL** for the part of the cloud up to present downwind position.
IMTYPE	Type of HEGADAS run (-). **IMTYPE** = 1, 2 or 3. Optional, always set by HEGADAS program itself. **IMTYPE** = 1 for a HEGADAS-S run, 2 for a HEGADAS-T run and 3 for a post-HEGABOX run.
PRTOBSD	Print observer data indicator (-) **PRTOBSD** = 0 (inactive) or 1 (active) Optional, default is 0. HEGADAS-T only. When **PRTOBSD** = 1, observer dispersion data is written to a file 'casename.HT2'.
ICSCOR	Cloud shape correction indicator (-) **ICSCOR** = 0 (inactive) or 1 (active) Optional, default is 1, should normally not be changed. HEGADAS-T only
OBSEPS	Convergence tolerance for observer concentrations (-) $0.005 \le$ **OBSEPS** ≤ 0.2. Optional, default is 0.05. HEGADAS-T only. Only change if observer setting fails. Program will clearly indicate this.

The **AMBIENT** block contains parameters describing the conditions of the ambient atmosphere. In HEGADAS ambient pressure is always taken to be 1.0 atm.

Z0	Reference height for ambient wind speed **U0** (m). $0.1 \leq$ **Z0** ≤ 50. Mandatory.
U0	Ambient wind velocity at height **Z0** (m/s). $1.5 \leq$ **U0** ≤ 20. Mandatory.
AIRTEMP	Ambient air temperature at height **ZAIRTEMP** (°C). $-50 \leq$ **AIRTEMP** ≤ 50. Mandatory.
ZAIRTEMP	Height at which ambient air temperature is given (m). $0 \leq$ **ZAIRTEMP** ≤ 50. Optional, default is 0.
TGROUND	Ground (substrate) temperature (°C). $-50 \leq$ **TGROUND** ≤ 50. Optional, default is ambient air temperature at ground level ($z = 0$).
RHPERC	Relative air humidity (%). $0.0 \leq$ **RHPERC** ≤ 100. Optional, default is 0.

The **DISP** block contains parameters describing the dispersion characteristics.

ZR	Land surface roughness (m). $10^{-5} \leq$ **ZR** ≤ 1. Mandatory.
PQSTAB	Pasquill/Gifford stability class. **PQSTAB** = A, B, C, D, E or F (character). Optional, default is D.
AVTIMC	Concentration averaging time (s). $0 \leq$ **AVTIMC** ≤ 3600. Optional, default is 600. **AVTIMC** should not be specified by the user if the **CROSSW** parameter **DELTA** (δ) is specified below.

Specifying **AVTIMC** will only affect the calculation of the *cross wind diffusion* in HEGADAS.
For HEGADAS-T, if the user wants to apply time-averaging (or time-smoothing) of calculated concentrations c(t) to obtain (average) concentrations $c_{av}(t)$, where $c_{av}(t) = \frac{1}{\mathbf{AVTIMC}} \int_{t-\mathrm{AVTIMC}/2}^{t+\mathrm{AVTIMC}/2} c(\tau)d\tau$, then the post-processor POSTHT should be used.
For HEGADAS-S **AVTIMC** is *only* used if the user requests a finite duration correction in the postprocessor POSTHS (input block **ERRORFUN**).

MONIN		Monin-Obukhov length (m). $-500 \leq$ **MONIN** $\leq 10^9$. Optional, normally HEGADAS itself calculates the Monin-Obukhov length based on the value of **PQSTAB**.
CROSSW		Cross-wind dispersion coefficient. Following this keyword, three parameters can be specified: **MODSY**, **DELTA** and **BETA**. They specify the formula used for the cross-wind diffusion coefficient.
	MODSY	Power law (1) or Briggs law (2) indicator (-). **MODSY** = 1 or 2. Optional, default is 2.
	DELTA	First coefficient in formula (m^{1-BETA} or -). $0.02 \leq$ **DELTA** ≤ 0.6. Optional, default calculated by HEGADAS.
	BETA	Second coefficient in formula (- or 1/m). $10^{-6} \leq$ **BETA** ≤ 1.0. Optional, default calculated by HEGADAS. Normally the user only has to specify **MODSY**. Choose a value of 2 if the HEGADAS analysis involves distances larger than 1 km, otherwise set **MODSY** to 1. The values of **DELTA** and **BETA** should normally not be user-specified.
CE		Gravity spreading law constant (-). $1.0 \leq$ **CE** ≤ 1.3. Optional, default is 1.15 and should normally *not* be changed.

CD
Gravity spreading law constant (-).
$0 \leq \textbf{CD} \leq 10^6$.
Optional, default is 5 and should normally *not* be changed.

SIGX
Downwind dispersion coefficient formula.
Following this keyword, three parameters can be specified which specify the formula used to calculate downwind (x-direction) diffusion.
HEGADAS-T only.

MODSX
Formula indicator (-).
MODSX = 1, 2 or 3.
MODSX = 1 uses the original HEGADAS-4 formulation.
MODSX = 2 uses the Ermak/Wilson's formulation.
MODSX = 3 uses the adapted Chatwin/Wilson's formulation.
Optional, default is 2.

ASIGX
Bulk Richardson number (-).
$0 \leq \textbf{ASIGX} \leq 1000$.
Optional, default calculated by HEGADAS.

BSIGX
Second coefficient b in formula (-).
$10^{-4} \leq \textbf{BSIGX} \leq 1.2$.
Optional, default calculated by HEGADAS.
Normally the user should not set any of these parameters.

The **GASDATA** block contains the source emission data, pollutant composition and thermodynamic data. The reservoir or initial stack mixture consists of 100 % wet pollutant by definition. Wet pollutant is defined to consist of the dry pollutant *plus* any water present in pollutant (as specified by **WATERPOL**).

THERMOD	Thermodynamics model indicator (-). **THERMOD** = 1 (no HF) or 2 (HF). Optional, default is 1. **THERMOD** = 1 means that the normal ideal gas or aerosol thermodynamics will be used. **THERMOD** = 2 indicates that the full HF chemistry and thermodynamics will be used.
GASFLOW	Dry pollutant source emission rate (kg/s). $10^{-7} \leq$ **GASFLOW** $\leq 10^{5}$. Must be specified if **FLUX** is not given. Either **GASFLOW** or **FLUX** must be specified.
FLUX	Dry pollutant source emission rate (kg/s/m^2). $10^{-7} \leq$ **FLUX** ≤ 10. Can be specified instead of **GASFLOW** if **POOL** block is given. Either **GASFLOW** or **FLUX** must be specified.
WATERPOL	Mole fraction water (liquid plus vapour) in *wet* pollutant (-). $0 \leq$ **WATERPOL** ≤ 1.0. Optional, default is 0.0.
WPICKUP	Mole fraction of initial pick-up of liquid water by pollutant (-). $0 \leq$ **WPICKUP** ≤ 1.0. Optional, default is 0.0.
TEMPGAS	Pollutant temperature (°C). $-270 \leq$ **TEMPGAS** ≤ 150. Either **TEMPGAS** or **ENTPOL** must be user-specified.
ENTPOL	Pollutant enthalpy (J/mole). $-10^{9} \leq$ **ENTPOL** $\leq 10^{9}$. Either **TEMPGAS** or **ENTPOL** must be user-specified.
HFLIQFR	Liquid mass fraction in initial HF release (-). $0 \leq$ **HFLIQFR** ≤ 1. Optional, default is 0. Only relevant when using HF thermodynamics (**THERMOD** = 2). **TEMPGAS** must also be specified using this parameter. For a pool of liquid HF, **HFLIQFR** should be set to 1.0 and **TEMPGAS** to the pool temperature. For a pressurised releases with HF flashing off, **HFLIQFR** is the post-flash liquid in the original HF and **TEMPGAS** the post-flash

temperature. The modules HFPLUME or HFFLASH can be used to find these parameters.

CPGAS

Specific heat at constant pressure of the *dry* pollutant (J/(mole K)).
$5 \le$ **CPGAS** ≤ 300.
Mandatory. Using HGSYSTEM module DATAPROP to find **CPGAS** is strongly recommended.

MWGAS

Molar mass of *dry* pollutant (kg/kmole).
$2 \le$ **MWGAS** ≤ 200.
Mandatory. Again, use of DATAPROP to calculate **MWGAS** is recommended.

HEATGR

Natural convection heat transfer group $(\mathrm{J \cdot m^{\frac{4}{3}} / (s^{\frac{1}{3}} \cdot K^{\frac{5}{3}} \cdot kmole)})$
$5 \le$ **HEATGR** ≤ 100.
Optional, default is 24.
Use of DATAPROP to calculate **HEATGR** is strongly recommended.

SPECIES

Pollutant compound properties. Using this keyword at least once implies the use of the full two-phase (aerosol) model or a mixture consisting of at least one compound (excluding water). If the **SPECIES** keyword is *not* specified, ideal gas thermodynamics is used with gas properties given by **CPGAS** and **MWGAS**. Condensation or freezing of *water* is still taken into account.

Only relevant if **THERMOD** = 1.

The **SPECIES** keyword plus parameters must be specified *for every compound* in the mixture, except water. The sum of the molar fractions used in the **SPECIES** keywords (see parameter #2 below) *must* equal 1.0 - **WATERPOL**.

The use of DATAPROP to generate the input parameters when the **SPECIES** keyword is being used, is strongly recommended.

Currently a maximum of 8 species can be specified (excluding water). Please note that DATAPROP allows for more species to be specified. DATAPROP also splits *dry air* (if specified) up into nitrogen and oxygen, thus generating *two* compounds instead of one. Thus the HEGADAS link file generated by DATAPROP could contain the **SPECIES** keyword more than 8 times. The user should combine or remove compounds if this occurs.

Please note that HEGADAS has *restrictions* concerning the aerosol structure: either a single two-compound aerosol (two compounds with the same aerosol class) or a number of separate one-compound aerosols (a series of compounds with *all a* different aerosol class) are allowed (not regarding water and dry air), other combinations are not

supported. Sometimes this restriction can cause a fatal HEGADAS error message during a post-AEROPLUME run, because AEROPLUME has no such restrictions and allows any combination of at most eight compounds.
For example: propane and butane can be combined (two-compound aerosol, both compounds have same aerosol class). Propane, butane and oxygen can *not* be combined because propane and butane have the same aerosol class and for more than two compounds all aerosol classes must be different.

Following the **SPECIES** keyword of a certain compound a block of 12 parameters (#1 to #12) *must* be specified:

#1 compound name (maximum of 12 characters).
#2 mole fraction in pollutant mixture (-).
$0 \le \#2 \le 1$.
#3 aerosol class (-).
$-1 \le \#3 \le 50$.
#4 specific heat of vapour (J/(mole K)).
$5 \le \#4 \le 300$.
#5 specific heat of liquid (J/(mole K)).
$0 \le \#5 \le 10^3$.
#6 heat of vaporisation (J/mole)
$0 \le \#6 \le 10^5$
#7 critical temperature (K).
$0 \le \#7 \le 10^4$.
#8 critical pressure (atm).
$0 \le \#8 \le 10^3$.
#9 vapour pressure function coefficient B1.
$-10^8 \le \#9 \le 10^8$.
#10 vapour pressure function coefficient B2.
$-10^8 \le \#10 \le 10^8$.
#11 vapour pressure function coefficient B3.
$-10^8 \le \#11 \le 10^8$.
#12 vapour pressure function coefficient B4.
$-10^8 \le \#12 \le 10^8$.

Note: the saturated vapour pressure of the compound is described by the Wagner function:

$$P_v(T) = P_c \cdot \exp\left\{\left[B_1 \cdot Q + B_2 \cdot Q^{1.5} + B_3 \cdot Q^3 + B_4 \cdot Q^6\right] / T_r\right\}$$

where T is the vapour temperature, P_c the critical pressure, T_c the critical temperature, $T_r = T/T_c$ and $Q = 1 - T_r$.

The optional **CLOUD** block controls the output of gas cloud information.

NSOURCE	Number of report interval along vapour blanket (secondary source) (-). $1 \leq$ **NSOURCE** ≤ 20. Optional, default is 4. HEGADAS-S only.
NFIX	Number of fixed-sized report intervals with length **DXFIX** (-). $1 \leq$ **NFIX** $\leq 10^5$. Optional, default is calculated by HEGADAS. HEGADAS-S only.
DXFIX	Length of the **NFIX** fixed-sized report intervals (m). $10^{-4} \leq$ **DXFIX** $\leq 10^5$. Optional, default is L/5, where L is downwind length, calculated by HEGADAS. HEGADAS-S only.
XGEOM	Geometrical factor to increase reporting interval (-). $1.0 \leq$ **XGEOM** ≤ 2.0. Optional, default is 4. HEGADAS-S only. Applies to downwind distances after **NFIX·DXFIX** meter. Reporting interval is **NFIX·DXFIX** + $(\mathbf{XGEOM})^i \cdot$**DXFIX**, where i = 1, 2, ...
XEND	Last downwind distance for HEGADAS-S calculations (-). $0.01 \leq$ **XEND** $\leq 10^6$. Optional, default is 10^6. HEGADAS-S only.
XSTEP	Reporting interval in downwind direction (HEGADAS-T) (m). $0.01 \leq$ **XSTEP** $\leq 10^4$. Optional, default is 25. HEGADAS-T only.
XSFACT	Multiplication factor in variable **XSTEP** algorithm (-). $0.01 \leq$ **XSFACT** ≤ 100. Optional, default is 1.0 (algorithm not used). HEGADAS-T only. IF **XSFACT** is 1.0, then variable **XSTEP** algorithm is invoked, otherwise **XSTEP** is a constant for this HEGADAS-T run.
XSEPS	Tolerance in variable **XSTEP** algorithm (-). $10^{-5} \leq$ **XSEPS** ≤ 100. Optional, default is 0.05. HEGADAS-T only.

If **XSFACT** is 1.0. then variable **XSTEP** algorithm is invoked and **XSEPS** will be used, otherwise **XSTEP** is a constant for this HEGADAS-T run.

CAMIN	Termination ground level concentration (kg/m^3). $10^{-7} \leq$ **CAMIN** ≤ 5.0. Optional, default is that HEGADAS will use **COMIN**. Calculations do not go further downwind when concentration **CAMIN** is reached. Calculations will never go beyond **XEND** (HEGADAS-S).
CU	Upper concentration limit for output (kg/m^3). $10^{-7} \leq$ **CU** ≤ 5.0. Optional, default is that HEGADAS will use **CUV**. For iso-concentration output and cumulative cloud data. See **ICNT** keyword.
CL	Lower concentration limit for output (kg/m^3). $10^{-7} \leq$ **CU** ≤ 5.0. Optional, default is that HEGADAS will use **CLV**. For iso-concentration output and cumulative cloud data. See **ICNT** keyword.
COMIN	Volumetric equivalent of **CAMIN** (vol-%). $10^{-5} \leq$ **COMIN** ≤ 100.0. Optional, default is 0.1 %. Calculations do not go further downwind when concentration **COMIN** is reached. Calculations will never go beyond **XEND** (HEGADAS-S).
CUV	Volumetric equivalent of **CU** (vol-%). $10^{-5} \leq$ **CUV** ≤ 100.0. Optional, default is 2.0 %. For iso-concentration output and cumulative cloud data. See **ICNT** keyword.
CLV	Volumetric equivalent of **CL** (vol-%). $10^{-5} \leq$ **CLV** ≤ 100.0. Optional, default is 0.1 %. For iso-concentration output and cumulative cloud data. See **ICNT** keyword.

The **CALC** block specifies the output times. It is applicable for HEGADAS-T only. To specify output times in HEGADAS-T the user *must* use either the **CALC** block or the **AUTOTIM** block, but *not both*.

TSTAR	Output time for which cloud data is calculated and printed (s). $1.0 \leq$ **TSTAR** $\leq 10^6$. Mandatory if **AUTOTIM** block not used. This keyword must be repeated for each output time in increasing order. Up to 20 output times can be specified.

The **AUTOTIM** block applies to HEGADAS-T only. It instructs HEGADAS-T to calculate an 'optimal' set of output times between two user-specified limits. To specify output times in HEGADAS-T the user *must* use either the **CALC** block or the **AUTOTIM** block, but *not both*.

TFIRST	First output time in automatic output time algorithm (s). $1.0 \le$ **TFIRST** $\le 10^6$. Mandatory if **CALC** block not used.
TLAST	Last output time in automatic output time algorithm (s). $1.0 \le$ **TLAST** $\le 10^6$. Mandatory if **CALC** block not used.
DTMIN	Initial (minimum) step between output times (s). $10^{-5} \le$ **DTMIN** $\le 10^3$. Optional, default is 20. The HEGADAS-T output time algorithm will increase **DTMIN** by repeatedly multiplying with **OTFACT**, whenever the algorithm decides that the step size can be increased.
OTEPS	Tolerance in automatic output time algorithm (-). $10^{-5} \le$ **OTEPS** ≤ 100. Optional, default is 0.05.
OTFACT	Multiplication factor for **DTMIN** in output time algorithm (-). $0.01 \le$ **OTFACT** ≤ 100. Optional, default is 1.5. Every time the algorithm decides that the step between output times can be increased, it multiplies the current step with **OTFACT**.

The **POOL** block applies only to HEGADAS-S with gas-blanket calculations (evaporating pool scenario). It specifies the pool dimensions.

PLL	Pool length (m). $10^{-3} \leq$ **PLL** $\leq 10^6$. Mandatory if **POOL** block is used.
PLHW	Pool *half*-width (m). $10^{-3} \leq$ **PLHW** $\leq 10^6$. Mandatory if **POOL** block is used. N.B. The pool is also called the 'primary source' in HEGADAS documentation. If more gas evaporates than can be taken up into the atmosphere, a 'secondary source' or vapour blanket will form. See HEGADAS description in Technical Reference Manual.

The **TIMEDATA** block applies to HEGADAS-T only. This block specifies either the time-dependent source data (evaporating pool scenario, **SOURCE** records) or time-dependent data at a breakpoint (post-AEROPLUME/HFPLUME scenario, **BRKDATA** records). Not relevant for a post-HEGABOX run.

The block keyword **TIMEDATA** itself has two parameters: **INCRT** and **ITYPBR**:

INCRT Every (**INCRT** + 1)th record is read (-).
$0 \leq$ **PLL** ≤ 99.
Optional, default is 0 (read all records). Do not normally change this parameter.

ITYPBR Type of data. (-).
$0 \leq$ **ITYPBR** ≤ 3.
Optional, default is 0.
ITYPBR = 0 for evaporating pool scenario with gas-blanket calculation. **SOURCE** records need to be specified.
ITYPBR > 0 for full breakpoint at specified downwind location. Value of **ITYPBR** indicates type of data in **BRKDATA** records.

TSTPOOL Start time at which source (pool or breakpoint) becomes active (s).
$-10^4 \leq$ **TSTPOOL** $\leq 10^5$
Optional, default is 0.
Zero data (no source) assumed for times less than **TSTPOOL**.

TSTEPR Size of time step and bund size. This keyword has two parameters: **TSTEP** and **RBUND**.

TSTEP Size of time step between records (s).
$0 \leq$ **TSTEP** $\leq 10^3$
Mandatory.

RBUND Radius of bund/dike (m).
$0 \leq$ **RBUND** $\leq 10^4$.
Optional, no default.

SOURCE Source data for evaporating pool scenario (**ITYPBR** = 0). The **SOURCE** keyword has three parameters: pool radius **R**, evaporation rate **E** and (optional, for bunds only) vapour height **H**.

R radius of pool at current time (m).
$0 \leq$ **R** $\leq 10^4$
Mandatory.

E (evaporation) release rate of dry gas (kg/s).
$0 \leq$ **E** $\leq 10^6$
Mandatory.

H height of vapour (m).
$0 \leq$ **H** $\leq 10^6$
Optional, for bunds only.

The **SOURCE** records may occur up to 100 times. The i-th occurrence corresponds to time i·**TSETP**. The pool is assumed to be cylindrical.
SOURCE data records will be generated by LPOOL when it creates a link file for HEGADAS-T.

BRKDATA Source data for post-AEROPLUME/HFPLUME (full breakpoint) scenario (**ITYPBR** > 0). The **BRKDATA** keyword has three mandatory parameters: cloud half-width **BEFF**, **DATA2** and **DATA3**, where the type of the latter two depends on the value of **ITYPBR**.

BEFF cloud half-width (m).
$0 \leq \textbf{BEFF} \leq 10^6$
Mandatory.

DATA2 ground level wet-gas molar fraction (-) (**ITYPBR**=1,2) or cloud height (m) (**ITYPBR**=3).
$0 \leq \textbf{DATA2} \leq 10^6$
Mandatory.

DATA3 cloud height (m) (**ITYPBR**=1) or dry-gas flow (kg/s) (**ITYPBR**=2,3).
$0 \leq \textbf{DATA3} \leq 10^6$
Mandatory.

The **BRKDATA** records may occur up to 100 times. The i-th occurrence corresponds to time i·**TSETP**.
BRKDATA will be generated by the jet models (AEROPLUME or HFPLUME) when they create a link file to HEGADAS-T.

Either the **SOURCE** keyword (**ITYPBR** = 0) or the **BRKDATA** keyword (**ITYPBR** > 0) *must* be specified, but *not both.*

The optional **TRANSIT** block is used to specify a (full or partial) breakpoint. Apart from **DISTS**, the only keyword that applies to HEGADAS-T is **ZRS**. All keywords can be used for HEGADAS-S.

DISTS	Downwind (x) location of breakpoint (m). $0 \leq$ **DISTS** $\leq 10^5$ Mandatory.
WS	Effective cloud half-width at breakpoint (m). $-10^5 \leq$ **WS** $\leq 10^5$ Optional. HEGADAS-S only. A negative value indicates that only calculations downwind of the breakpoint should be carried out.
HS	Effective cloud height at breakpoint (m). $0 \leq$ **HS** $\leq 10^5$ Optional. HEGADAS-S only.
CONCS	Ground level mole fraction wet-gas at breakpoint (m). $0 \leq$ **CONCS** ≤ 1.0 Optional. HEGADAS-S only.
ZRS	Surface roughness downwind of breakpoint (m). $10^{-5} \leq$ **ZRS** ≤ 1.0 Optional.
TMPS	Cloud temperature at breakpoint (°C). $-270 \leq$ **TMPS** ≤ 50 Optional. HEGADAS-S only.
MSFLOW	Total flow (pollutant plus entrained air) at breakpoint (kg/s). $10^{-6} \leq$ **MSFLOW** $\leq 10^5$ Optional. HEGADAS-S only.
AVCONC	Cloud-averaged concentration at breakpoint (kg/m^3). $10^{-7} \leq$ **AVCONC** ≤ 5.0 Optional. HEGADAS-S only.

For HEGADAS-S, at least one of the keywords **CONCS**, **HS**, **MSFLOW**, **AVCONC** or **ZRS** should be given. This data will normally be generated by AEROPLUME or HFPLUME.
For HEGADAS-T only a full breakpoint can be specified or a partial surface roughness breakpoint. For a full breakpoint only the **DISTS** parameter needs to be specified, all other

data must be given in a **TIMEDATA** block. For a partial surface roughness breakpoint **DISTS** and **ZRS** must be given. The data for a full breakpoint will normally be generated by AEROPLUME or HFPLUME.

The **TRANSIT** block can occur more than once (multiple *partial* breakpoints). They must be given in increasing order of **DISTS**. This applies to both HEGADAS-S and HEGADAS-T.

The **MMESOPT** block contains the 'switches' which indicate the use of the extra options developed by Earth Technology and sponsored by Martin Marietta Energy Systems. An indicator value of 1 means that the corresponding option is used, a value of 0 means that the option is inactive.

IMETP	Indicator for use of meteorological pre-processor (-). **IMETP** = 0 or 1. Optional, default is 0. For **IMETP** = 1, an additional file 'casename.MET' *must* be supplied. See Chapter 18 for a description of the data which must be given in this file.
IDEP	Indicator for use of wet and dry deposition model (-). **IDEP** = 0 or 1. Optional, default is 0. HEGADAS-S only. For **IDEP** = 1, an additional file 'casename.DEP' *must* be supplied. See Chapter 18 for a description of the data which must be given in this file.
ICANY	Indicator for calculation of canyon effects (-). **ICANY** = 0 or 1. Optional, default is 0. HEGADAS-S only. For **ICANY** = 1, an additional file 'casename.CNY' *must* be supplied. See Chapter 18 for a description of the data which must be given in this file.
IFLUC	Indicator for calculation of centre-line concentration fluctuations (-). **IFLUC** = 0 or 1. Optional, default is 0. HEGADAS-S only. For **IFLUC** = 1, an additional file 'casename.PTL' *must* be supplied. See Chapter 18 for a description of the data which must be given in this file.
ILIFT	Indicator for use of plume lift-off description (-). **ILIFT** = 0 or 1. Optional, default is 0. HEGADAS-S only. No additional data needed. When **ILIFT** = 0, HEGADAS will stop program execution when plume lift-off is detected. When **ILIFT** = 1, lift-off is taken into account. See Chapter 9 in the HGSYSTEM 3.0 Technical Reference Manual for details.
IAVG	Indicator for calculation of variation of concentration with averaging time (-). **IAVG** = 0 or 1.

Optional. default is 0.
HEGADAS-S only.
No additional data is needed.
For **IAVG** = 1, an additional file 'casename.PTL' *must* be supplied. See Chapter 18 for a description of the data which must be given in this file.

14. PGPLUME

General introduction

The PGPLUME model is a far-field plume dispersion model for passive dispersion.
The high-momentum jet models AEROPLUME and HFPLUME are quite suitable to model near-field plume dispersion, but the entrainment relations used in these models will not accurately describe the (far-field) dispersion behaviour when the jet momentum no longer dominates the entrainment process. That is why AEROPLUME/HFPLUME will automatically make a transition to the PGPLUME passive dispersion model when this is necessary.
PGPLUME is a Gaussian plume model using well-known standard (Pasquill-Gifford) correlations to find the standard deviations.

PGPLUME will almost always be run *after* the near-field jet models (AEROPLUME and HFPLUME) have been used.

The downwind location where AEROPLUME/HFPLUME make a transition to PGPLUME is also indicated by the location of the 'matching' plane.

Range of applications and limitations

PGPLUME applies to passive dispersion: momentum and density excess with respect to the ambient atmosphere must be small. It assumes that the influence of chemical reactions (HF) has become negligible. It is not suitable for dense plumes: HEGADAS should be used for those cases.

Guidance for use

Normally the jet models AEROPLUME and HFPLUME decide to what far-field model a transition, if any, should be made. The user can use the link files prepared by AEROPLUME or HFPLUME to run PGPLUME.

If PGPLUME results have to be used later by the PROFILE program, then the averaging time AVTIMC in the DISP input block *must* be set to 18.75 s or less. In other words, PGPLUME must calculate 'instantaneous' results.

PGPLUME INPUT PARAMETERS

A description of all the input parameters that can occur in an PGPLUME input file will be given.

The PGPLUME input file has the DOS filename 'casename.PGI' where 'casename' is the user-supplied name of the problem.

In the following, actual keywords are given in *capitals* and in *bold*. The descriptions of less important parameters or parameters that need not normally be set by the user, are given in a *smaller font*.
All parameters, except **TITLE**, occur in blocks preceded by a specific block keyword. For PGPLUME these block keywords are: **GEOMETRY**, **GASDATA**, **STATE**, **AMBIENT**, **DISP** and **TERMINAT**.

The **TITLE** keyword does *not* occur in a parameter block.

TITLE	The title of the current problem to be run with PGPLUME. At most 50 alphanumeric characters. Optional. no default.

The **GEOMETRY** block gives the plume geometry at the transition point.

DXPLUME	Horizontal downwind distance of transition location (m). $0 \leq$ **DXPLUME** $\leq 10^4$ (10 km). Mandatory. Actual source is assumed to be at 0 m downwind.
ZPLUME	Plume centroid height at transition location (m) $0 \leq$ **ZPLUME** ≤ 500. Mandatory. **ZPLUME** can be less than **DPLUME**/2 for a touch-down or slumped plume.
DPLUME	Plume effective diameter at transition location (m) $0.1 \leq$ **DPLUME** ≤ 500. Mandatory. Valid for airborne, touch-down or slumped plumes.
PHIPLUME	Plume inclination (relative to horizontal) at transition location (°) $-10 \leq$ **PHIPLUME** ≤ 10. Mandatory. **PHIPLUME** should, by definition of a 'passive' plume, be small.

The **GASDATA** block contains the gas composition and thermodynamic data. The released gas is assumed to consist of water and a (dry) pollutant.

CPGAS	Specific heat at constant pressure of the *dry* gas (J/(mole K)). $5 \leq$ **CPGAS** ≤ 300. Mandatory.
MWGAS	Molar mass of *dry* gas (kg/kmole). $2 \leq$ **MWGAS** ≤ 200. Mandatory.
WATGAS	Mole fraction of water in released gas at release point (-). $0 \leq$ **WATGAS** ≤ 1 Optional, default is 0.
GASFRAC	Mole fraction of dry component in released gas at release point (-). $0 \leq$ **GASFRAC** ≤ 1 Optional, default is 1.

The **STATE** input block contains parameters describing the plume dynamic and thermodynamic state at the transition point.

UREL	Plume excess velocity at transition point (m/s). $-2 \leq$ **UREL** ≤ 2 Mandatory. Excess velocity is difference between the ambient wind-speed and the plume speed, both at plume centroid height. Must necessarily be small for a passive plume.
RREL	Plume excess density at transition point (kg/m^3). $-1 \leq$ **RREL** ≤ 1 Mandatory. Excess density is difference between the ambient density and the plume density, both at plume centroid height. Must necessarily be small for a passive plume.
CMASS	Concentration of released plume gas at transition point (kg/m^3). $10^{-15} \leq$ **CMASS** ≤ 1 Mandatory.
DURATION	Release duration (s). $-10^6 \leq$ **DURATION** $\leq 10^6$ Optional, default is steady-state release (**DURATION** < 0). Negative for steady-state releases, positive for finite-duration, constant releases. Using a positive value invokes finite-duration correction in PGPLUME.

The **AMBIENT** block contains parameters describing the conditions of the ambient atmosphere *at plume centroid height* at the transition point.

DENSITY	Ambient density at centroid height (kg/m^3). $0.5 <$ **DENSITY** ≤ 2.0. Mandatory.
UATM	Ambient wind velocity at centroid height (m/s). $1.0 <$ **UATM** ≤ 20. Mandatory.
AIRTEMP	Ambient air temperature at centroid height (°C). $-50 \leq$ **AIRTEMP** ≤ 50. Mandatory.
AIRPRESS	Ambient air pressure (atm). $0.7 \leq$ **AIRPRESS** ≤ 1.1. Optional, default is 1.0 atm.
RHPERC	Relative air humidity at centroid height (%). $0.0 \leq$ **RHPERC** ≤ 100. Mandatory.

The **DISP** block contains parameters describing the dispersion characteristics.

ZR	Land surface roughness (m). $10^{-5} \leq$ **ZR** ≤ 1. Mandatory.
PQSTAB	Pasquill/Gifford stability class. **PQSTAB** = A, B, C, D, E or F (character). Mandatory.
AVTIMC	Concentration measurement averaging time (s). $18.75 \leq$ **AVTIMC** ≤ 3600. Mandatory. 'Instantaneous' limit is 18.75 s.

Note: If the PROFILE program will be using results of a PGPLUME run, then **AVTIMC** *must* be 18.75 s or less in the PGPLUME calculations. In other words, PROFILE expects PGPLUME to have calculated results for an 'instantaneous' plume.

The **TERMINAT** block sets PGPLUME calculation termination criteria.

XFIRST	First output distance (m). 0 ≤ **XFIRST** ≤ 10^4 (10 km). Mandatory. **XFIRST** must exceed the downwind position of the transition point.
STEP	Arithmetic progression step-size (m). 0 ≤ **STEP** ≤ $5 \cdot 10^4$ (50 km). Mandatory. Output is at distance **XFIRST** and then at (arithmetic) intervals of **STEP** , until **NSTEP** steps have been taken or until **XLAST** has been reached or if gas concentration drops below **VFLAST**.
NSTEP	Maximum number of arithmetic steps to be taken (-). 0 ≤ **NSTEP** ≤ 500. Mandatory. See description **STEP**. **XLAST** will never be exceeded
FACTOR	Geometric progression scale factor (-). 1 ≤ **XFIRST** ≤ 100. Mandatory. Output is generated at distances (**XFIRST**+ISTEP·**STEP**)·**FACTOR**, where ISTEP goes from 1 to **NSTEP**. After this the distances are multiplied per output step by **FACTOR** until **XLAST** has been reached. **FACTOR** must be greater than 1.0 to be effective.
XLAST	Last output distance (m). 0 ≤ **XLAST** ≤ $5 \cdot 10^4$(50 km). Mandatory. **XLAST** must exceed **XFIRST**.
VFLAST	Last required mole fraction gas (ppm). 10^{-5} ≤ **VFLAST** ≤ $5 \cdot 10^4$. Mandatory. PGPLUME will halt if concentration of gas falls below **VFLAST**.

15. POSTHS AND POSTHT

The heavy gas dispersion models HEGADAS-S and HEGADAS-T (steady state and transient version respectively), are among the more complex HGSYSTEM models. In order to help the user to interpret the HEGADAS (-S and -T) results, in HGSYSTEM version 1.0 (NOV90), two 'interactive' post-processors were available, called HSPOST and HTPOST.

These two post-process utilities have been completely revised for HGSYSTEM version 3.0 and they are now called POSTHS and POSTHT respectively. POSTHS and POSTHT now can be run in 'batch' mode, that is they can be used as all other main HGSYSTEM modules, and they read their input data from an input file having the same structure as all other HGSYSTEM input files.

Data from HEGADAS (-S and -T) is communicated to POSTHS and POSTHT using a so-called *'model data file'*. These data files have a file name with extension HSM and HTM respectively. The first part of the model data file name is the user-specified case name. This name should be used when calling POSTHS and POSTHT.

Chapter 15.A of this User's Manual describes input parameters for POSTHS which processes HEGADAS-S results. Chapter 15.B deals with POSTHT, the HEGADAS-T post-processor.

15.A. POSTHS

General introduction

POSTHS is a utility for post-processing the model data files produced by HEGADAS-S, creating output files for submission to suitable user-selected plotting packages.

Range of applications and limitations

The post-processor can handle any HEGADAS-S model data file having a DOS filename 'casename.HSM', where 'casename' is the user-supplied name of the problem.

As well as being able to create all output previously produced by HSPOST (the post-processor available in HGSYSTEM 1.0), additional functionality is available, iso-concentration contour plots now being an option.

Guidance for use

When first used to post-process the HEGADAS-S output for a new case, it is strongly recommended that most of the data for each input block is not specified by the user, but allowed to take default values. Such usage has the advantage of requiring little if any data analysis by the user, enabling automatic running of the post-processor and the rapid production of an initial set of useful output files. Further refinement of the input data can then be made in a meaningful manner and the exact output requirements finalised for the current case.

This does not of course apply where the user is interested in exact values, such as when producing iso-concentration plots at lower and upper flammability limits, where it would obviously make sense to specify the required values in the contour input block immediately.

Whether values are specified by the user or the defaults taken, within the program most values will be adjusted if necessary to take account of the actual data in the input model file. This particularly applies to ranges of downwind x-values and contour values which are not allowed outside the ranges computed by HEGADAS-S.

Note that restraint should be shown when specifying long downwind x-ranges with small step-sizes. The resulting output files can be very large indeed for steady-state simulations terminating several kilometres downwind and a step-size such as 1 meter.
In such cases it is recommended that the user looks at the full x-range using a large step-size, or looks in detail at a section of the x-range using a small step-size. Such usage also avoids the danger of exceeding size limitations in the user's preferred plotting package.

A standard report file 'casename.PSR' containing a summary of the input from HEGADAS-S, is always produced. If the user-requested output files contain little or no (useful) data because of parameters being specified out of the relevant range, reference to the 'casename.PSR' file should enable the user to alter the required parameter values so as to obtain useful results.

POSTHS INPUT FILE PARAMETERS

A description of all the input parameters that can occur in a POSTHS input file will be given.

The POSTHS input file has the DOS filename 'casename.PSI', where 'casename' is the user-supplied name of the problem and *must match that used for the original HEGADAS-S run* which produced the model data file 'casename.HSM'.

When creating an input file the user should ensure that each specified output file has a unique filename, and that existing files having such names *are deleted or renamed before POSTHS is run* as POSTHS assumes that files with the specified names do not yet exist. An error will occur if the file does exist.

In the following, actual keywords are given in *capitals* and in *bold*. The descriptions of less important parameters or parameters that need not normally be set by the user, are given in a *smaller font*.

All parameters, except **TITLE**, occur in blocks preceded by a specific block keyword. For POSTHS these block keywords are: **GRAPH2**, **CONCBOX**, **CONTOUR**, **PARMSX**, **CONCXYZ** and **ERRORFUN**.

The three co-ordinate directions used in all input blocks are:

x	down wind
y	lateral (sideways)
z	vertical (height)

The *horizontal and vertical axis parameter type* described below may take values in the range 1 to 9, where each value has the following meaning:

1	downwind distance X to pool (m)
2	vol%. (dry) gas fraction CAV at $y = z = 0$
3	vertical dispersion coefficient SZ (m)
4	crosswind dispersion coefficient SY (m)
5	half-width b of middle part of crosswind concentration profile (m)
6	temperature TMP (°C)
7	effective cloud half-width B_{eff} (m)
8	effective cloud height H_{eff} (m)
9	cloud half-width (normal definition) (m)

The **TITLE** keyword does *not* occur in a parameter block.

TITLE	The title of the current problem to be run with POSTHS. At most 50 alphanumeric characters. Optional, no default.

The **GRAPH2** block, which may occur up to 6 times, specifies the parameters to produce output files containing values to generate graphs *relating any two types of data*. The first type of data is given by **HORAX2** (using the horizontal axis) and the second one by **VERAX2** (using the vertical axis).

OUT2

Filename of the required output file 'filename.ext' (full pathname if required).
At most 40 alphanumeric characters.
Mandatory.

XRANGE2

Range of values for down wind distance x.
Optional, defaults as given below.
Following the **XRANGE2** keyword, a block of 3 parameters (#1 to #3) *must* be specified:

#1 minimum value for x (m).
$-10^6 \le \#1 \le 10^6$.
(default is 0.0)

#2 maximum value for x (m).
$-10^6 \le \#2 \le 10^6$.
(default 1000.0)

#3 step size for x (m).
$10^{-6} \le \#3 \le 10^6$.
(default 10.0).

HORAX2

Horizontal axis parameter type (-).
1 ≤ **HORAX2** ≤ 9.
Mandatory.

VERAX2

Vertical axis parameter type (-).
1 ≤ **VERAX2** ≤ 9.
Mandatory.

The **CONCBOX** block, which may occur up to 6 times, specifies the parameters to produce 4-column output files containing *co-ordinates and concentrations* in box-shaped regions (3D). It is also possible to produce similar output files for planes (2D) by fixing one axis range while varying the other two axes, or lines parallel to an axis (1D) by only varying the required axis. Note that these latter two types of output must have range values supplied for the non-varying axes in which the minimum and maximum values are identical and the step-sizes are positive and non-zero.

OUTB		Filename of the required output file 'filename.ext' (full pathname if required). At most 40 alphanumeric characters. Mandatory.
XRANGEB		Range of values for x. Optional, defaults as given below. Following the **XRANGEB** keyword, a block of 3 parameters (#1 to #3) *must* be specified:
	#1	minimum value for x (m). $-10^6 \le \#1 \le 10^6$. (default 0.0)
	#2	maximum value for x (m). $-10^6 \le \#2 \le 10^6$. (default 1000.0)
	#3	step size for x (m). $10^{-6} \le \#3 \le 10^6$. (default 100.0)
YRANGEB		Range of values for y. Optional, defaults as given below. Following the **YRANGEB** keyword, a block of 3 parameters (#1 to #3) *must* be specified:
	#1	minimum value for y (m). $-10^6 \le \#1 \le 10^6$. (default 0.0).
	#2	maximum value for y (m). $-10^6 \le \#2 \le 10^6$. (default 20.0).
	#3	step size for y (m). $10^{-6} \le \#3 \le 10^6$. (default 10.0).
ZRANGEB		Range of values for z. Optional, defaults as given below. Following the **ZRANGEB** keyword, a block of 3 parameters (#1 to #3) *must* be specified:
	#1	minimum value for z (m). $0.0 \le \#1 \le 10^6$. (default 0.0).

#2 maximum value for z (m).
$0.0 \leq \#2 \leq 10^6$.
(default 10.0).

#3 step size for z (m).
$10^{-6} \leq \#3 \leq 10^6$.
(default 5.0).

The **CONTOUR** block, which may occur up to 6 times, specifies the parameters to produce 2-column output files containing data to generate *iso-concentration* contour plots.

OUTC

Filename of the required output file 'filename.ext' (full pathname if required).
At most 40 alphanumeric characters.
Mandatory.

RANGEC

Range of contour values.
Optional, defaults as given below.
Following the **RANGEC** keyword, a block of 3 parameters (#1 to #3) *must* be specified:

#1 minimum contour value (%).
$10^{-6} \le \#1 \le 100.0$.
(default set from actual model file data).

#2 maximum contour value (%).
$10^{-6} \le \#2 \le 100.0$.
(default set from actual model file data).
Limited to 90% of maximum concentration in the model file for the requested plane.

#3 number of contours (-).
$1 \le \#3 \le 6$.
(default 6).

XC

Constant value x for contour plane yz (m).
$-10^6 \le \mathbf{XC} \le 10^6$.
Optional, no default.

YC

Constant value y for contour plane xz (m).
$-10^6 \le \mathbf{YC} \le 10^6$.
Optional, if none of **XC**, **YC** or **ZC** are specified, default is taken to be **YC** = 0.

ZC

Constant value z for contour plane xy (m).
$0.0 \le \mathbf{ZC} \le 10^6$.
Optional, no default.

The **PARMSX** block specifies the parameters to produce a multi-column output file containing the value of each model file variable for a series of x-values.

OUTSX Filename of the required output file 'filename.ext' (full pathname if required).
At most 40 alphanumeric characters.
Mandatory.

XRANGESX Range of values for x.
Optional, defaults as given below.
Following the **XRANGESX** keyword, a block of 3 parameters (#1 to #3) *must* be specified:

#1 minimum value for x (m).
$-10^6 \leq \#1 \leq 10^6$.
(default 0.0).

#2 maximum value for x (m).
$-10^6 \leq \#2 \leq 10^6$.
(default 1000.0).

#3 step size for x (m).
$10^{-6} \leq \#3 \leq 10^6$.
(default 10.0).

The **CONCXYZ** block specifies the parameters to produce a 4-column output file containing the *co-ordinates and concentrations* at a set of up to 20 specified x, y, z co-ordinate positions.

OUTXYZ		Filename of the required output file 'filename.ext' (full pathname if required). At most 40 alphanumeric characters. Mandatory.
XYZ		Co-ordinate position which may occur up to 20 times, but which *must occur at least once.* Following the **XYZ** keyword, a block of 3 parameters (#1 to #3) *must* be specified:
	#1	x-co-ordinate (m). $-10^6 \leq \#1 \leq 10^6$. No default.
	#2	y-co-ordinate (m). $-10^6 \leq \#2 \leq 10^6$. No default.
	#3	z-co-ordinate (m). $0.0 \leq \#3 \leq 10^6$. No default.

The **ERRORFUN** block applies the *finite duration* error function *correction* to the model file input data. Any such correction takes place before the processing of other data blocks and affects the results written to the output files.

DURATION	Duration of release (s). 1 ≤ **DURATION** ≤ 3600. Optional, *must* be specified if **ERRORFUN** block is used..
AVTIMC	Averaging time for concentrations (s). 0 ≤ **AVTIMC** ≤ 3600. Optional, default is the value used in the corresponding HEGADAS-S run. Should *not* normally be set by the user, value will be read from the model data file 'casename.HSM'. Any value set in POSTHS will override the value used in the corresponding HEGADAS-S run. If the user has specified **DELTA** in the HEGADAS-S **DISP** input block then **AVTIMC** in HEGADAS-S has no value and **AVTIMC** *must* be specified here. **AVTIMC** is only ised in HEGADAS-S for the finite duration correction.

15.B. POSTHT

General introduction

POSTHT is a utility for post-processing the model data files produced by HEGADAS-T, creating output files for submission to suitable user-selected plotting packages.

Range of applications and limitations

The post-processor can handle any HEGADAS-T model file having a DOS filename 'casename.HTM', where 'casename' is the user-supplied name of the problem.

As well as being able to create all output previously produced by HTPOST (the post-processor available in HGSYSTEM 1.0), additional functionality is also available, iso-concentration contour plots being one of several new options.

Guidance for use

When first used to post-process the HEGADAS-T output for a new case, it is strongly recommended that most of the data for each input block is not specified by the user, but allowed to take default values. Such usage has the advantage of requiring little if any data analysis by the user, enabling automatic running of the post-processor and the rapid production of an initial set of useful output files. Further refinement of the input data can then be made in a meaningful manner and the exact output requirements finalised for the current case.

This does not of course apply where the user is interested in exact values, such as when producing iso-concentration plots at lower and upper flammability limits, where it would obviously make sense to specify the required values in the contour input block immediately.

Whether values are specified by the user or the defaults taken, within the program most values will be adjusted if necessary to take account of the actual data in the input model file. This particularly applies to ranges of downwind x-values and contour values which are not allowed outside the ranges computed by HEGADAS.

Note that restraint should be shown when specifying long downwind x-ranges with short step-sizes. The resulting output files can be very large indeed for simulations terminating several kilometres downwind and a step-size such as 1 meter.
In such cases it is recommended that the user looks at the full x-range using a large step-size, or looks in detail at a section of the x-range using a small step-size. Such usage also avoids the danger of exceeding size limitations in the user's preferred plotting package. This is not such a problem for POSTHT as it sometimes is for POSTHS, because of the nature of the output criteria in HEGADAS.

A standard report file 'casename.PTR' containing a summary of the input from HEGADAS-T, is always produced. If the user-requested output files contain little or no (useful) data because of parameters being specified out of the relevant range, reference to the 'casename.PTR' file should enable the user to alter the required parameter values so as to obtain useful results.

POSTHT INPUT FILE PARAMETERS

A description of all the input parameters that can occur in a POSTHT input file will be given.

The following information is valid for **POSTHT version 2.0**.

The POSTHT input file has the DOS filename 'casename.PTI', where 'casename' is the user-supplied name of the problem and *must match that used for the original HEGADAS-T run* which produced the model data file 'casename.HTM'.

When creating an input file the user should ensure that each specified output file has a unique filename, and that existing files having such names *are deleted or renamed before POSTHT is run*, as POSTHT assumes that files with the specified names do not yet exist. An error will occur if the file does exist.

In the following, actual keywords are given in *capitals* and in *bold*. The descriptions of less important parameters or parameters that need not normally be set by the user, are given in a *smaller font*.

All parameters, except **TITLE**, occur in blocks preceded by a specific block keyword. For POSTHT these block keywords are: **GRAPHDX**, **CONCBOX**, **CONTOUR**, **PARMSX**, **CONCXYZ**, **GRAPHDT**, **CONCXYZT**, **DOSAGE**, **GRAPHMX**, **ENVCURVE** and **AVTIMC**.

The three co-ordinate directions used in all input blocks are:

x	down wind
y	lateral (sideways)
z	vertical (height)

The *dispersion data type* described below may take values in the range 1 to 7 where each value has the following meaning:

1	vol% (dry) gas fraction CAV at $y = z = 0$
2	vertical dispersion coefficient SZ (m)
3	crosswind dispersion coefficient SY (m)
4	half-width b of middle part of crosswind concentration profile (m)
5	effective cloud half-width B_{eff} (m)
6	effective cloud height H_{eff} (m)
7	concentration at $y = z = 0$ (kg/m^3)

The **TITLE** keyword does *not* occur in a parameter block.

TITLE	The title of the current problem to be run with POSTHT. At most 50 alphanumeric characters. Optional, no default.

The **GRAPHDX** block, which may occur up to 6 times, specifies the parameters to produce 2-column output files containing values to generate graphs of dispersion data (indicated by **TYPEDX**) against x.

OUTDX		Filename of the required output file 'filename.ext' (full pathname if required). At most 40 alphanumeric characters. Mandatory.
TIMEDX		Required time for output (s). $0 \leq$ **TIMEDX** ≤ 3600. (default set to first time in model file data).
TYPEDX		Dispersion data type (-). $1 \leq$ **TYPEDX** ≤ 7. Mandatory.
XRANGEDX		Range of values for x. Optional. Following the **XRANGEDX** keyword, a block of 3 parameters (#1 to #3) *must* be specified:
	#1	minimum value for x (m). $-10^6 \leq \#1 \leq 10^6$. (default 0.0).
	#2	maximum value for x (m). $-10^6 \leq \#2 \leq 10^6$. (default 1000.0).
	#3	step size for x (m). $10^{-6} \leq \#3 \leq 10^6$. (default 10.0).

The **CONCBOX** block, which may occur up to 6 times. specifies the parameters to produce 4-column output files containing *co-ordinates and concentrations* in box-shaped regions (3D). It is also possible to produce similar output files for planes (2D) by fixing one axis range while varying the other two axes, or lines parallel to an axis (1D) by only varying the required axis. Note that these latter two types of output must have range values supplied for the non-varying axes in which the minimum and maximum values are identical and the step-sizes are positive and non-zero.

OUTB

Filename of the required output file 'filename.ext' (full pathname if required).
At most 40 alphanumeric characters.
Mandatory.

TIMEB

Required time for output (s).
0 ≤ **TIMEB** ≤ 3600.
(default set to first output time in model file data).

XRANGEB

Range of values for x.
Optional.
Following the **XRANGEB** keyword, a block of 3 parameters (#1 to #3) *must* be specified:

#1 minimum value for x (m).
$-10^6 \leq \#1 \leq 10^6$.
(default 0.0).

#2 maximum value for x (m).
$-10^6 \leq \#2 \leq 10^6$.
(default 1000.0).

#3 step size for x (m).
$10^{-6} \leq \#3 \leq 10^6$.
(default 100.0).

YRANGEB

Range of values for y.
Optional.
Following the **YRANGEB** keyword, a block of 3 parameters (#1 to #3) *must* be specified:

#1 minimum value for y (m).
$-10^6 \leq \#1 \leq 10^6$.
(default 0.0).

#2 maximum value for y (m).
$-10^6 \leq \#2 \leq 10^6$.
(default 20.0).

#3 step size for y (m).
$10^{-6} \leq \#3 \leq 10^6$.
(default 10.0).

ZRANGEB		Range of values for z. Optional. Following the **ZRANGEB** keyword, a block of 3 parameters (#1 to #3) *must* be specified:
	#1	minimum value for z (m). $0.0 \le \#1 \le 10^6$. (default 0.0).
	#2	maximum value for z (m). $0.0 \le \#2 \le 10^6$. (default 10.0).
	#3	step size for z (m). $10^{-6} \le \#3 \le 10^6$. (default 5.0).

The **CONTOUR** block, which may occur up to 6 times, specifies the parameters to produce 2-column output files containing data to generate *iso-concentration* contour plots.

OUTC		Filename of the required output file 'filename.ext' (full pathname if required). At most 40 alphanumeric characters. Mandatory.
TIMEC		Required time for output (s). $0 \leq$ **TIMEC** ≤ 3600. (default set to first time in model file data).
RANGEC		Range of contour values. Optional. Following the **RANGEC** keyword, a block of 3 parameters (#1 to #3) *must* be specified:
	#1	minimum contour value (%). $10^{-6} \leq \#1 \leq 100.0$. (default set from actual model file data).
	#2	maximum contour value (%). $10^{-6} \leq \#2 \leq 100.0$. (default set from actual model file data).
	#3	number of contours (-). $1 \leq \#3 \leq 6$. (default 6).
XC		Constant value x for contour plane yz (m). $-10^6 \leq$ **XC** $\leq 10^6$. Optional, no default.
YC		Constant value y for contour plane xz (m). $-10^6 \leq$ **YC** $\leq 10^6$. Optional. If none of **XC**, **YC** or **ZC** are specified, default taken as y=0.
ZC		Constant value z for contour plane xy (m). $0.0 \leq$ **ZC** $\leq 10^6$. Optional, no default.

The **PARMSX** block specifies the parameters to produce a multi-column output file containing the value of each model data file variable for a series of x-values.

OUTSX	Filename of the required output file 'filename.ext' (full pathname if required). At most 40 alphanumeric characters. Mandatory.

TIMESX		Required time for output (s). $0 \le$ **TIMESX** ≤ 3600. (default set to first time in model file data).
XRANGESX		Range of values for x. Optional. Following the **XRANGESX** keyword, a block of 3 parameters (#1 to #3) *must* be specified:
	#1	minimum value for x (m). $-10^6 \le \#1 \le 10^6$. (default 0.0).
	#2	maximum value for x (m). $-10^6 \le \#2 \le 10^6$. (default 1000.0).
	#3	step size for x (m). $10^{-6} \le \#3 \le 10^6$. (default 10.0).

The **CONCXYZ** block specifies the parameters to produce a 4-column output file containing the co-ordinates and concentrations at a set of up to 20 specified x, y, z co-ordinate positions.

OUTXYZ		Filename of the required output file 'filename.ext' (full pathname if required). At most 40 alphanumeric characters. Mandatory.
TIMEXYZ		Required time for output (s). $0 \le$ **TIMEXYZ** ≤ 3600. (default set to first time in model file data).
XYZ		Co-ordinate position which may occur up to 20 times, but which *must* occur at least once. Mandatory. Following the **XYZ** keyword, a block of 3 parameters (#1 to #3) *must* be specified:
	#1	x-co-ordinate (m). $-10^6 \le \#1 \le 10^6$. No default.
	#2	y-co-ordinate (m). $-10^6 \le \#2 \le 10^6$. No default.
	#3	z-co-ordinate (m). $0.0 \le \#3 \le 10^6$. No default.

The **GRAPHDT** block, which may occur up to 6 times, specifies the parameters to produce 2-column output files containing values to generate graphs of dispersion data against time.

OUTDT		Filename of the required output file 'filename.ext' (full pathname if required). At most 40 alphanumeric characters. Mandatory.
TRANGEDT		Range of values for time. Optional. Following the **TRANGEDT** keyword, a block of 3 parameters (#1 to #3) *must* be specified:
	#1	minimum value for time (s). $0 \leq \#1 \leq 3600$. (default set to first time in model file data).
	#2	maximum value for time (s). $0 \leq \#2 \leq 3600$. (default 3600.0).
	#3	step size for time (s). $10^{-6} \leq \#3 \leq 3600$. (default 10.0).
TYPEDT		Dispersion data type (-). 1 ≤ **TYPEDT** ≤ 7. Mandatory.
XVALDT		Value for x (m). $-10^6 \leq$ **XVALDT** $\leq 10^6$. Mandatory.

The **CONCXYZT** block specifies the parameters to produce a 2-column output file containing the *concentrations against time* at each co-ordinate in a set of up to 20 specified x, y, z co-ordinate positions.

OUTXYZT
Filename of the required output file 'filename.ext' (full pathname if required).
At most 40 alphanumeric characters.
Mandatory.

TRXYZT
Range of values for time.
Optional.
Following the **TRXYZT** keyword, a block of 3 parameters (#1 to #3) *must* be specified:
#1 minimum value for time (s).
$0 \leq \#1 \leq 3600$.
(default set to first time in model file data).
#2 maximum value for time (s).
$0 \leq \#2 \leq 3600$.
(default 3600.0).
#3 step size for time (s).
$10^{-6} \leq \#3 \leq 3600$.
(default 10.0).

XYZT
Co-ordinate position which may occur up to 20 times, but which *must occur at least once*.
Mandatory.
Following the **XYZT** keyword, a block of 3 parameters (#1 to #3) *must* be specified:
#1 x-co-ordinate (m).
$-10^6 \leq \#1 \leq 10^6$.
No default.
#2 y-co-ordinate (m).
$-10^6 \leq \#2 \leq 10^6$.
No default.
#3 z-co-ordinate (m).
$0.0 \leq \#3 \leq 10^6$.
No default.

The **DOSAGE** block specifies the parameters to produce a 4-column output file containing the *co-ordinates and dosages* at a set of up to 20 specified x, y, z co-ordinate positions. For a given position (x,y,z), the dosage at time t is given by $\int_{-\infty}^{t} c(x,y,z,\tau)\,d\tau$. In POSTHT the calculated value is $\int_{t_0}^{t} c(x,y,z,\tau)\,d\tau$, where t_0 is the first output time. If the dosage calculation is unreliable because x is too far upwind compared to the available data at time t_0, a warning is given.

OUTD		Filename of the required output file 'filename.ext' (full pathname if required). At most 40 alphanumeric characters. Mandatory.
TIMED		Required time for output (s). $0 \le$ **TIMED** ≤ 3600. Mandatory.
XYZD		Co-ordinate position which may occur up to 20 times, but which *must occur at least once*. Mandatory. Following the **XYZD** keyword, a block of 3 parameters (#1 to #3) *must* be specified:
	#1	x-co-ordinate (m). $-10^6 \le \#1 \le 10^6$. No default.
	#2	y-co-ordinate (m). $-10^6 \le \#2 \le 10^6$. No default.
	#3	z-co-ordinate (m). $0.0 \le \#3 \le 10^6$. No default.

The **ENVCURVE** block specifies the parameters to produce a 3-column output file containing the maximum concentration and its position for a series of output times. The resulting curve is an 'envelope' curve of the concentration profiles per output time.

OUTE	Filename of the required output file 'filename.ext' (full pathname if required). At most 40 alphanumeric characters. Mandatory.
TMINE	Minimum time for output (s). 0 ≤ **TMINE** ≤ 3600. Optional (default set to first output time in model file data).
TMAXE	Maximum time for output (s). 0 ≤ **TMAXE** ≤ 3600. Optional (default 3600.0).

The **GRAPHMX** block, which may occur up to 6 times, specifies the parameters to produce 2-column output files containing the maximum values of selected types of dispersion data (indicated by **TYPEMX**) over all times, for a series of x-values.

OUTMX
Filename of the required output file 'filename.ext' (full pathname if required).
At most 40 alphanumeric characters.
Mandatory.

TYPEMX
Dispersion data type (-).
1 ≤ **TYPEMX** ≤ 7.
Mandatory.

XRANGEMX
Range of values for x.
Optional.
Following the **XRANGEMX** keyword, a block of 3 parameters (#1 to #3) *must* be specified:

#1 minimum value for x (m).
$-10^6 \leq \#1 \leq 10^6$.
(default 0.0).

#2 maximum value for x (m).
$-10^6 \leq \#2 \leq 10^6$.
(default 1000.0).

#3 step size for x (m).
$10^{-6} \leq \#3 \leq 10^6$.
(default 10.0).

The **AVTIMC** keyword does not occur in a parameter block. If the keyword is used a time-averaging correction is applied to the model data file input data. Any such correction takes place before the processing of other data blocks and affects the results written to the output files.

AVTIMC	Averaging time for concentrations (s). $0 \leq$ **AVTIMC** ≤ 3600. Optional, default is the value used in the corresponding HEGADAS-T run. Should *not* normally be set by the user, value will be read from the model data file 'casename.HTM'. Any value set in POSTHT will override the value used in the corresponding HEGADAS-T run. If the user has specified **DELTA** in the HEGADAS-T **DISP** input block then **AVTIMC** in HEGADAS-T has no value and **AVTIMC** *must* be specified here.

AVTIMC in POSTHT is (only) used for time-averaging (or time-smoothing) of calculated concentrations $c(t)$ to obtain (average) concentrations $c_{av}(t)$ where

$$c_{av}(t) = \frac{1}{\mathbf{AVTIMC}} \int_{t-\mathrm{AVTIMC}/2}^{t+\mathrm{AVTIMC}/2} c(\tau)d\tau.$$

16. PROFILE

General introduction

PROFILE is a utility for post-processing the results files produced by AEROPLUME and PGPLUME, creating output files for submission to suitable user-selected plotting packages. PROFILE creates data to plot *concentration contours* assuming a Gaussian concentration profile perpendicular to the plume-axis.

PROFILE was not available in versions of HGSYSTEM previous to version 3.0.

PROFILE is run in an identical manner to other HGSYSTEM programs using the batch file PROFILE.BAT.

Range of applications and limitations

The post-processor can handle any AEROPLUME report file, having a DOS filename 'casename.APR', and any PGPLUME report file, having a DOS filename 'casename.PG1', where 'casename' is the user-supplied name of the problem. If only one of the files 'casename.APR' or 'casename.PG1' exists, this is taken as the sole input for post-processing purposes, while if both exist, both are used.

Note that if AEROPLUME and PGPLUME have been run separately using the *same* 'casename', the utility will combine the data of both result files even if there is no meaningful connection between the two simulations.

PROFILE will only produce contours for that part of the plume which is airborne.

As the program considers slices through a plume, if the axis inclination changes rapidly the slices may overlap relatively near to the centroid, the result being contours that cross each other.

Guidance for use

When first used to post-process AEROPLUME and/or PGPLUME output for a new case, it is recommended that most of the input data is not specified by the user, but allowed to take default values. Such usage has the advantage of requiring little if any data analysis by the user, enabling automatic running of the post-processor and the rapid production of an initial set of output files. Further refinement of the input data can then be made in a meaningful manner and the exact output requirements finalised for the current case.

This does not of course apply where the user is interested in exact values, such as when producing iso-concentration plots at lower and upper flammability limits, where it would obviously make sense to specify the required values in the contour input block.

PROFILE INPUT FILE PARAMETERS

A description of all the input parameters that can occur in a PROFILE input file will be given.

The PROFILE input file has the DOS filename 'casename.PRI', where 'casename' is the user-supplied name of the problem and *must* match that used for the original AEROPLUME run which produced the result file 'casename.APR', and/or the original PGPLUME run which produced the result file 'casename.PG1'.

A standard report file 'casename.PRR' containing a summary of the input from AEROPLUME and/or PGPLUME is always produced. If the other two output files contain little or no data, reference to the '.PRR' file should enable the user to alter the required contour value or horizontal height so as to obtain useful results.

In the following, actual keywords are given in *capitals* and in *bold*. The descriptions of less important parameters or parameters that need not normally be set by the user, are given in a *smaller font.*

All parameters, except **TITLE**, occur in blocks preceded by a specific block keyword. For PROFILE these block keywords are: **CONTOUR** and **AVTIMC**.

The **TITLE** keyword does *not* occur in a parameter block.

TITLE	The title of the current problem to be run with PROFILE. At most 50 alphanumeric characters. Optional, no default.

The **CONTOUR** block specifies the parameters to produce 2 output files containing data to generate iso-concentration contour plots at a user-specified concentration.
The file 'casename.PRH' gives downwind distance versus lateral displacement for a *horizontal plane* at a user-specified height.
The file 'casename.PRV' gives 2 pairs of downwind distance versus height values for a *vertical centre-line plane*.

CMINC	Required contour value (%). 1.0E-05 ≤ **CMINC** ≤ 100.0. Mandatory, no default.
ZC	Constant value z for horizontal contour plane xy (m). 0.0 ≤ **ZC** ≤ 1.0E06. Optional (default 0.0).

The **AVTIMC** keyword does not occur in a parameter block. If the keyword is used a time-averaging correction is applied to the results file input data. Any such correction takes place before the processing of other data blocks and affects the results written to the output files.

AVTIMC	Averaging time for concentrations (s). $18.75 \le$ **AVTIMC** ≤ 600. Optional, default is 18.75 (no time averaging). Note: it is assumed by PROFILE that all PGPLUME generated results are for an 'instantaneous' plume, that is for an averaging time of 18.75 s or less. If the user wants to apply time-averaging during the PROFILE run then the appropriate value of **AVTIMC** should be set here but *not* in the PGPLUME input file.

17. GET2COL

General introduction

GET2COL is a utility for post-processing standard results files produced by the models within HGSYSTEM, creating output files for submission to suitable user-selected plotting packages. The GET2COL program selects any two columns from a multi-column HGSYSTEM results file and puts these two columns in a new file. These two columns can then be plotted. GET2COL can in fact be used for *any* multi-column input file.

The GET2COL utility has been completely revised for HGSYSTEM version 3.0. It can now be run in 'batch' mode, that is it can be used as all other main HGSYSTEM modules, and GET2COL reads its input data from an input file having the same structure as all other HGSYSTEM input files.

Range of applications and limitations

As well as HGSYSTEM result files the post-processor can handle any file as long as the format is standard ASCII and not binary.

Guidance for use

When first used to post-process the HGSYSTEM output for a new case, it is recommended that the row numbers are not specified by the user, but allowed to take default values. Such usage has the advantage of requiring no data analysis by the user, enabling automatic running of the post-processor and the production of an initial useful output file, assuming the output column requirements are already known and specified. If needed, further refinement of the row requirements can then be made in a meaningful manner.

Despite the above recommendation, restraint should be shown if the result file to be post-processed is likely to be very large. This may happen, for example, where very small output steps or very stringent termination criteria were selected when running the model to produce the result file. In such cases, it is recommended that the user looks at the full range of data using a large row extraction frequency, or looks in detail at a section of the data using a small row extraction frequency. Such usage also avoids the danger of exceeding size limitations in the user's preferred plotting package.

Care should be taken when using GET2COL with files which have so called problem columns containing blank or non-numeric values. Such files are post-processed successfully if both columns selected by the user lie to the left of any problem columns, otherwise incorrect values are obtained. Such a situation should *not* arise for existing HGSYSTEM 3.0 result files.

A standard report file 'casename.G2R' containing the number of data-pairs read from the multi-column input file and written to the 2-column output file, is always produced.

GET2COL INPUT FILE PARAMETERS

A description of all the input parameters that can occur in a GET2COL input file will be given.

The GET2COL input file has the DOS filename 'casename.G2I', where 'casename' is the user-supplied name of the problem.

When creating an input file the user should ensure that each specified output file has a unique filename, and that existing files having such names *are deleted or renamed* before GET2COL is run, because GET2COL assumes that files with the specified names do not yet exist. An error will occur if the file does exist.

In the following, actual keywords are given in *capitals* and in *bold*. The descriptions of less important parameters or parameters that need not normally be set by the user, are given in a *smaller font*.

All parameters occur in blocks preceded by a specific block keyword. For GET2COL these block keywords are: **FILES**, **COLUMNS** and **ROWS**.

The **FILES** block is mandatory and specifies the filenames of the input and output files.

INFILE	Filename of the multi-column input file 'filename.ext' (full pathname if required). At most 40 alphanumeric characters. Mandatory.
OUTFILE	Filename of the two-column output file 'filename.ext' (full pathname if required). At most 40 alphanumeric characters. Mandatory.

The **COLUMNS** block is mandatory and specifies the two column numbers from the multi-column input file required to produce the two-column output file.

COLUMN1	First column required (-). $1 \leq$ **COLUMN1** ≤ 19. Mandatory.
COLUMN2	Second column required (-). $2 \leq$ **COLUMN2** ≤ 20. Mandatory. Must be greater than **COLUMN1**.

The **ROWS** block is optional and may be used to specify the row numbers from the multi-column input file required to produce the two-column output file. If this block is not used, the default is to include all rows from the input file, up to a maximum of 100000 rows.

ROWMIN	First row required (-). 1 ≤ **ROWMIN** ≤ 99999. Optional, default 1.
ROWMAX	Last row required (-). 2 ≤ **ROWMAX** ≤ 100000. Optional, default 100000. **ROWMAX** must be greater than **ROWMIN**.
FREQ	Frequency for extracting data (-). 1 ≤ **FREQ** ≤ 10000. Optional, default 1.

18. EXTRA 'MMES' OPTIONS

18.1. Introduction

There are six additional general HGSYSTEM Modeling enhancements developed by EARTH TECH under the sponsorship of Martin Marietta Energy Systems. These six enhancements. which do not refer to any specific chemical, include:

(1) Meteorological processor,
(2) Calculation of dry and wet deposition fluxes,
(3) Effects of street canyon,
(4) Fluctuation of centreline concentration,
(5) Plume lift-off, and
(6) Variation of centreline concentration with averaging time.

The reader is referred to Chapter 9 of the HGSYSTEM 3.0 Technical Reference Manual for detailed descriptions of various enhancements. The following table summarises the applicability of each enhancement to various HGSYSTEM modules (Y = yes and N = no):

	AEROPLUME	HEGADAS-S	HEGADAS-T	HEGABOX
Meteorological Processor	Y	Y	Y	Y
Deposition	Y	Y	N	Y
Canyon	Y	Y	N	Y
Centreline Concentration Fluctuation	Y	Y	N	Y
Plume Lift-off	Y	Y	N	N
Variation of Concentration with Averaging Time	N	Y	N	N

Note that most of the enhancements are not used in HEGADAS-T, because each 'observer', used to describe the transient nature of the source, sees the plume differently. Consequently, the results for several modeling enhancements cannot be merged in a straightforward manner. Also, the plume lift-off scenario does not apply to HEGABOX, since that module is used to describe the gravity-dominated phase (i.e., cloud density always exceeds ambient density) of an instantaneous release. The algorithm describing the variation of concentration with averaging time does not apply to the AEROPLUME and HEGABOX models, since both modules predict instantaneous concentrations.

The user can select any of the above enhancements (assuming that they are applicable to a particular scenario) via the specification of various control flags in the main input files for the modules (i.e., the API file for AEROPLUME, the HSI file for HEGADAS-S, the HTI file for HEGADAS-T, and the HBI file for HEGABOX) as described in the corresponding chapters of the User's Manual. These control flags include:

IMETP	for the meteorological processor
IDEP	for the deposition calculations
ICANY	for the canyon effects
IFLUC	for then centreline concentration fluctuations
ILIFT	for plume lift-off
IAVG	for the variation of concentrations with averaging time

A value of 1 for the control flag indicates that the enhancement should be used, a value of 0 indicates otherwise. Once an enhancement is selected by the user, that enhancement may or may not require the input of additional parameters. If an enhancement requires additional input, it expects all necessary parameters to be contained in a file whose name is the same as the run name ('casename'), and whose extension is specified as follows:

	Extension of Input file
Meteorological Processor	MET
Deposition	DEP
Canyon	CNY
Centreline Concentration Fluctuation	PTL
Plume Lift-off	no additional data needed
Variation of Concentration with Averaging Time	no additional data needed

The required additional input parameters for each enhancement are discussed in the following sections. Note that once an enhancement is selected, all corresponding input parameters are mandatory and must be specified by the user. There are *no default values* assumed by the model.

18.2. Input Parameters for the MET File

The following parameters in the 'casename'.MET file are required if the user decides to use the meteorological processor to calculate the Monin-Obukhov length and the friction velocity, and the equivalent Pasquill/Gifford stability class. The procedure overrides the stability class specified in the main input files for various modules (see Chapter 9 of the HGSYSTEM 3.0 Technical Reference Manual). The file is read with free-format. There must be one entry per line. All data must be given *in the specified order*. There are *no default values* assumed by the model for the parameters.

Line No.	Real/ Integer	Remarks
1	R	Site latitude in degrees (positive for north)
2	R	Site longitude in degrees (positive for east)
3	R	Time zone (e.g., 5.0 for EST, 8.0 for PST)
4	I	Year (e.g., 1994)
5	I	Month (e.g., 10 for October)
6	I	Day
7	R	Hour (e.g., 1.5 = 1:30 AM)
8	R	Albedo with sun directly overhead, see below for more instructions
9	R	Moisture availability of the soil, see below for more instructions
10	R	The lower limit in meters for the Monin-Obukhov length during stable conditions, see below for more instructions
11	R	Anthropogenic heat flux, W/m^2, (usually 0.0 for rural areas)
12	R	Ratio of ground heat flux to net radiation, see below for more instructions
13	R	Fractional cloud cover (0. = clear, 1. = overcast)

The reader is referred to Hanna and Chang (1991, 1992) for a detailed description of the choice of site characteristics (i.e., albedo, moisture availability, the lower limit on the Monin-Obukhov length, anthropogenic heat flux, and ratio of ground heat flux to net radiation). Some instructions are repeated below.

Suggested input values for albedo (Iqbal, 1983) as a function of land use type and season are given in the following table. Further information regarding albedo for specific ground covers is given by Iqbal (1983).

Land Use Type	Spring[1]	Summer[2]	Autumn[3]	Winter[4]
Water (fresh water and sea water)	0.12	0.10	0.14	0.20
Deciduous forest	0.12	0.12	0.12	0.50
Coniferous forest	0.12	0.12	0.12	0.35
Swamp	0.12	0.14	0.16	0.30
Cultivated land	0.14	0.20	0.18	0.60
Grassland	0.18	0.18	0.20	0.60
Urban	0.14	0.16	0.18	0.35
Desert shrubland	0.30	0.28	0.28	0.45

[1] Spring: Periods when vegetation is emerging or partially green. This is a transitional situation that applies to one to two months after the last killing frost in spring.

[2] Summer: Periods when vegetation is lush and healthy, typical of mid-summer, but also of other seasons where frost is less common.

[3] Autumn: Periods when freezing conditions are common, deciduous trees are leafless, crops are not yet planted or are already harvested (bare soil exposed), grass surfaces are brown, and no snow is present.

[4] Winter: Periods when surfaces are covered by snow, and when temperatures are sub-freezing. Winter albedo also depends on whether a snow cover is present continuously, intermittently, or seldom. Albedo ranges from about 0.30 for bare snow cover to about 0.65 for continuous cover.

The moisture availability, α, describes the wetness of the ground on a scale from 0.0 (dry) to 1.4 (saturated). The parameter α is preferred to the commonly-used Bowen ratio, Br, because α is not a function of temperature. However, there have only been a few observations of α while the textbooks are full of tables of observed Br. Note that although a relation between α and Br can be derived, that relation depends greatly on time of day and the magnitude of the sensible heat flux (Hanna and Chang, 1991). Holtslag and van Ulden (1983) found that $\alpha \sim 0.4$ to 0.6 over dry agricultural fields with vegetation, and $\alpha \sim 0.9$ over these same fields when the soil was wet. The following ranges of values of α are proposed (Hanna and Chang, 1992), based on information presented by Beljaars and Holtslag (1989 and 1991):

$\alpha = 0.0 - 0.2$ dry desert with no rain for months
$\alpha = 0.2 - 0.4$ arid rural area
$\alpha = 0.4 - 0.6$ crops and fields, mid-summer during periods when rain has not fallen for several days
$\alpha = 0.5 - 1.0$ urban environment, some parks
$\alpha = 0.8 - 1.2$ crops, fields, or forests with sufficient soil moisture
$\alpha = 1.2 - 1.4$ large lake or ocean with land more than 10 km away

The meteorological processor recognises that the stability of the atmosphere at night is limited by the presence of the mechanically well-mixed layer. Since the depth of the mechanically well-mixed layer is about two or three times the representative building height (Uno at al., 1988), and the Monin-Obukhov length, L, can be thought of as the depth of the mechanically-mixed layer, the meteorological processor uses a minimum L during stable conditions. The following subjective scheme for minimum L is based on the EPA/Auer (1978) land use classification system, and can be refined as the user gains experience with the system. Note that, as shown in the table below, the effects of minimum L are more important for urban areas.

Land Use Type	Minimum L
Commercial, > 40 story buildings	150 m
Commercial, 10 - 40 story buildings	100 m
Commercial, < 10 story buildings	50 m
Industrial	50 m
Compact residential	50 m
Residential	50 m
Agricultural	2 m

When using the meteorological processor, the user also needs to specify the ratio of the ground heat flux to the net radiation flux. A value of 0.1 for the ratio is recommended as default. This value is characteristic of an agricultural crop or a field. A value of 0.3 for the ratio is recommended for urban areas because of the associated heat-island effects.

18.3. Input Parameters for the DEP File

The following parameters in the DEP file are required if the user decides to calculate the dry and wet deposition fluxes (Chapter 9 of the HGSYSTEM 3.0 Technical Reference Manual). The file is read with free-format. There must be one entry per line. All data must be given *in the specified order*. There are *no default values* assumed by the model for the parameters.

Line No.	Real/ Integer	Remarks
1	R	Reference height in meters for computing atmospheric resistance (usually 2.0 m)
2	R	Molecular diffusivity, cm^2/s, for the particles
3	R	Particle diameter, µm; = 0. for gas
4	R	particle density, kg/m^3 (5053.14 for UF_6, 6381.86 for UO_2F_2)
5	R	Precipitation rate, mm/hr; < 0. indicates that raining but rate unknown, = 0. indicates no precipitation
6	I	Form of precipitation; 0 = liquid, 1 = frozen

18.4. Input Parameters for the CNY File

The following parameters in the CNY file are required if the user decides to estimate the effects of canyons on the concentrations (Chapter 9 of the HGSYSTEM 3.0 Technical Reference Manual). The file is read with free-format. There must be one entry per line. All data must be given *in the specified order*. There are *no default values* assumed by the model for the parameters.

Line No.	Real/ Integer	Remarks
1	R	Building height, m
2	R	Canyon width, m

18.5. Input Parameters for the PTL File

The following parameter in the PTL file is required if the user decides to estimate the effects of centreline concentration fluctuation (Chapter 9 of the HGSYSTEM 3.0 Technical Reference Manual). The file is read with free-format. There is *no default value* assumed by the model for the parameter.

Line No.	Real/ Integer	Remarks
1	R	Percentile (in fractions) on the cumulative distribution curve at which the centreline concentrations are to be estimated

18.6. Output for Additional Modeling Enhancements

The meteorological processor is used to calculate the values of the Monin-Obukhov length, L, and the friction velocity, u_*. It is called only once prior to the dispersion calculations. Therefore, the meteorological processor does not have any special output, except for the values of L and u_* printed in the regular model output file.

The effects of plume lift-off are included in the regular APR and HSR report files.

The results for the remaining four enhancements are listed in the additional 'casename'.MMO output file (i.e., a file whose file name is the same as the run name, and whose extension is MMO), as detailed in the following.

The effects of (1) canyon, (2) concentration fluctuation, and (3) variation of concentration with averaging time were parameterised as correction factors to the original concentration field. For example, if the model originally predicts the pollutant centreline concentration at a given downwind distance to be 0.0010 kg/m^3, and if the existence of a canyon causes the concentration to increase to 0.0012 kg/m^3, then a correction factor of 1.2 is assigned to the canyon effects. As another example, if the model originally predicts the pollutant centreline concentration at a given downwind distance to be 0.0010 kg/m^3, and according to the concentration fluctuation module the 99th percentile of that concentration is found to be 0.0025 kg/m^3, then a correction factor of 2.5 is assigned to the concentration fluctuation effects. If more than one process would influence the predicted concentrations, it is assumed that these processes are independent, and that their associated correction factors can be multiplied to obtain the final results.

The plume thermodynamic and chemistry algorithms in HGSYSTEM assume that no mass is removed from the plume. Consequently, it is assumed that gas or particle deposition fluxes due to dry and wet deposition are small compared to the total flux of material in the plume, which is assumed to remain unchanged. The local gas or particle deposition flux to the ground is calculated as the product of the ground-level concentration (already given by the model) and the deposition velocity. Therefore, as long as the deposition velocity is known, the deposition flux can be estimated. The dry deposition velocity is a constant for any model run and does not vary with space. The wet deposition velocity, on the other hand, varies with downwind distance since it involves an integration over the depth of the plume as it grows vertically with downwind distance.

The correction factors for the effects of (1) canyons, (2) concentration fluctuations, and (3) variations of concentrations with averaging time, together with the dry and wet deposition velocities, are listed in the MMO file for each reported downwind distance of the model.

18.7. References

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