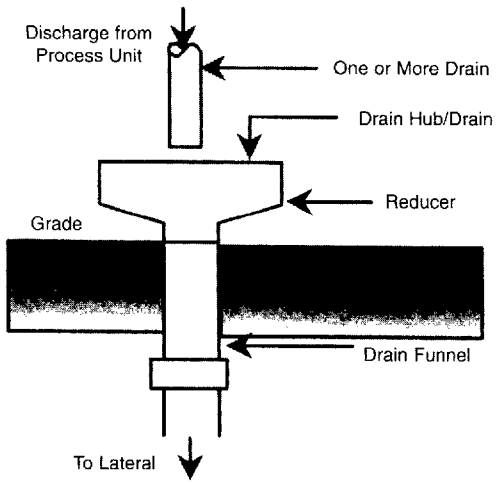
American Petroleum Institute

STEP Strategies for Today's Environmental Partnership

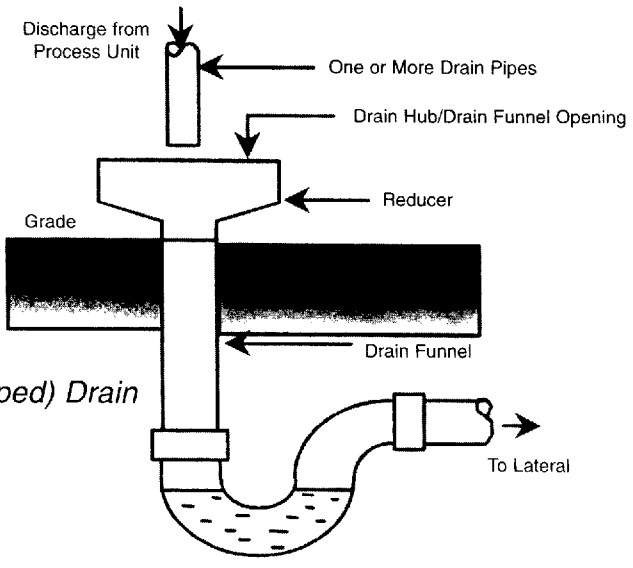
FUGITIVE EMISSIONS FROM REFINERY PROCESS DRAINS VOLUME III

PROCESS DRAIN EMISSION CALCULATOR

APIDRAIN VERSION 1.0 USER'S GUIDE



Unsealed Drain



Sealed (Trapped) Drain

HEALTH AND ENVIRONMENTAL SCIENCES DEPARTMENT
PUBLICATION NUMBER 4681
APRIL 1999

For Technical Support:

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Record the APIDRAIN Registration Number
from the enclosed registration form:
I46810 - _ _ _

Fugitive Emissions From Refinery Process Drains Volume III

Process Drain Emission Calculator

APIDRAIN Version 1.0 User's Guide

Health and Environmental Sciences Department

API PUBLICATION NUMBER 4681

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PREFACE

The results of this study are presented in three separate reports.

- Volume I entitled "*Fugitive Emission Factors for Refinery Process Drains*" (API Publication Number 4677) contains simplified emission factors that can be used to quickly estimate total volatile organic compound (VOC) emissions from refinery process drains.

- Volume II entitled "*Fundamentals of Fugitive Emissions from Refinery Process Drains*" (API Publication Number 4678) describes theoretical concepts and equations that may be used in a model (APIDRAIN) to estimate speciated VOC emissions. The model can provide insight on how to change process drain variables (flow rate, temperature, etc.) to reduce emissions.

- Volume III entitled "*APIDRAIN Version 1.0, Process Drain Emission Calculator*" (API Publication Number 4681) is the computer model with user's guide to estimate emissions from refinery process drains. The software allows users to calculate VOC emissions based on the emission factors in Volume I and equations for speciated emissions in Volume II.

All three volumes of this study can be purchased separately; however, it is suggested that the user consider purchase of the entire set to gain a complete understanding of fugitive emissions from refinery process drains.

ABSTRACT

Emissions from refinery process drains are under increasing regulatory scrutiny, particularly with respect to volatile organic compounds (VOCs) and hazardous air pollutants (HAPs). Drain emissions are currently estimated using EPA's AP-42 factor for non-methane hydrocarbons. The factor is now considered obsolete because it does not reflect design modifications that have resulted in significant reductions in emissions. As a result, the AP-42 factor over-predicts emission rates in many cases. API has recently sponsored projects that investigate emissions from process drains and that develop mechanistic models to predict VOC and HAP emission rates based on mass transfer fundamentals and conservation of mass. In this project, API has funded the development of a user-friendly model called APIDRAIN that incorporates a suite of procedures for estimating emission rates from refinery process drains. In addition to the mass transfer model, APIDRAIN also provides an option to estimate emission rates using emission factors, correlation equations, and a stripping efficiency estimation procedure. Users may create process units, and within each process unit, specify the drain estimation procedure used. The level of detail in reports generated ranges from a simple facility overview to a detailed categorization of emission rates of specific chemical compounds from individual drains within each process unit. The APIDRAIN model will enable users to easily categorize drains and report drain emission rates in various process units based on the quality of collected analytical data of contaminants in process liquid or gas phase streams.

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TABLE OF CONTENTS

Section Page

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LIST OF FIGURES

LIST OF TABLES

Section 1

INTRODUCTION

1.1 BACKGROUND

Emissions from refinery process drains are under increased regulatory scrutiny, particularly with respect to volatile organic compounds (VOCs) and hazardous air pollutants (HAPs), pursuant to the Clean Air Act Amendments of 1990. Emissions from refinery process drains are currently estimated in the industry using EPA's AP-42 factor of 0.070 lb/hr of total non-methane hydrocarbons. There have been significant design modifications to refinery process drains over the years since the AP-42 factor was first developed. The design changes have resulted in significant emission reductions from process drains, and the AP-42 factor is now considered obsolete because it over-predicts emission rates in many cases.

The American Petroleum Institute (API) funded a project to develop a mathematical model that predicts acceptably accurate emissions from refinery process drains. A mechanistic model was developed to predict VOC and HAP emission rates from process drains based on mass transfer fundamentals and conservation of mass. The mechanistic model accounts for emissions that may occur as the process wastewater is discharged from a pipe nozzle to the drain hub, emissions from the surface of a water seal, if present, and emissions from wastewater falling from the leg of the process drain into water conveyed in the underlying collection channel.

API initiated a project to incorporate the mechanistic model for refinery process drains into a suite of procedures for estimating emissions from refinery process drains resulting in a user-friendly software tool called APIDRAIN. In addition to the mass transfer mechanistic model, APIDRAIN also offers two other options for estimating emissions from process drains. They include (1) emission factors, and (2) correlation equations. Each calculation option requires considerably different input information. Thus, the user can choose the appropriate estimation method based on the level of detailed information available. APIDRAIN enables the user to sum up the emissions from drains within a refinery process unit, or from the entire refinery. The model user can quickly and easily predict the contribution of process drain emissions to the total emission inventory of a refinery.

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The estimation procedures provided by APIDRAIN are generally applicable across the petroleum industry (exploration and production, refining and marketing terminals), as indicated in Table 1-1. The screening value correlation developed for the South Coast Air Quality Management District (SCAQMD) applies only to petroleum refineries in southern California, and only to inactive drains in those refineries. The stripping efficiency procedure and University of Texas model may be used to estimate process drain emissions in other industrial sectors. The stripping efficiency procedure applies only to sealed drains, while the UT model can be used to estimate emission rates from both sealed and unsealed drains.

Table 1-1 Applicability of Drain Emission Estimation Procedures in APIDRAIN Model

Estimation Procedure	Applicable to		
	South. California Petroleum Refineries	Petroleum Industry	Other Industries
AP-42 Zero/Pegged Factors		X	
OVA Screening (EPA)		X	
OVA Screening (SCAQMD)*	X		
Stripping Efficiency Factors†		X	X
University of Texas Model		X	X

* for inactive drains †for sealed drains only

1.2 PRINCIPLES OF USE AND SYSTEM REQUIREMENTS

APIDRAIN operates as a workbook under the PC-based Microsoft® Excel™ for Windows™ environment, and therefore requires a PC system with the capacity to run Excel™ and the Windows™ operating system. (At a minimum, a 486DX2 Windows™ 3.11 platform with 8 Mbyte RAM is needed to operate the APIDRAIN workbook.) The user must complete independent installations of Windows™ and Excel™ to begin using the software. The APIDRAIN workbook is enhanced with automatic functions that enable the user to summarize easily important reporting information and to generate tabular emission totals for both specific refinery process units and for the entire refinery. Therefore, it is not necessary for the user to possess a rigorous understanding of Excel™ to use APIDRAIN; only a few common principles of the Windows™

operating environment are needed (such as point-and-click, and navigation of tab and arrow keys). APIDRAIN is also designed such that the user has a great deal of discretion in the selection of emission estimation procedures.

1.3 INSTALLATION

APIDRAIN comes with an installation program to assist a user in transferring the model to the user's computer hard drive. **Users must employ the SETUP.EXE program to install APIDRAIN**. To begin the installation program from MS-Windows™ '95, the user first clicks with the mouse pointer on the Windows™ Explorer icon, and then on the floppy disk drive (usually A:). From Windows™ 3.1, use the file manager to access the floppy drive (usually A:). The floppy disk contains four files:

- apid.001
- apidc.inf
- disk.id
- setup.exe

Double-click on the setup.exe file to activate the installation program. A dialog box appears with development information, with a prompt to continue; click OK to proceed. A second dialog box next appears offering the user two choices, either to proceed with the installation or to exit the installation. The user should click on the install option and OK to proceed. The installation next prompts the user to declare the drive on which to install the model; this will usually be the local hard drive root directory (C:). Click on OK to accept the selected drive. The installation program then prompts the user to define the directory name for the APIDRAIN files. By default, the installation will create a directory called "APIDRAIN" at the root directory. The user may accept this by clicking on the OK box, or if desired, modify the name of the directory, using up to eight characters, prior to accepting. At the completion of the installation, a dialog box appears with address and contact information about the developer (Enviromega Inc.) regarding technical assistance or bug reporting.

The user will now have a program group box with an icon on the computer screen. The icon is:

- APIDrain 1.0

1.4 SAVING APIDRAIN FILES

To ensure the model runs properly, it is recommended that users retain the original master Excel™ file without any modifications, and that all configured facilities be renamed as separate files. Any saved, renamed files should be kept in the same directory as the master Excel™ file so that links in the macros may be maintained.

1.5 EXITING FROM APIDRAIN

To exit from the APIDRAIN model, users should use the menu item *File/Exit Drain Model*. This will leave the program in Excel™, but will remove the APIDRAIN model toolbar from the worksheet. The user may then exit from Excel™ if so desired. If a user closes the model using the MS- Windows™ close icon (box with X in the upper right corner of Windows™ programs), the model and Excel™ will close, but the model toolbar will be left active in Excel™ the next time it is opened. To remove the drain model toolbar from Excel™ in this case, use the menu item *View/Toolbars*, and click off the Drain toolbar.

1.6 TECHNICAL SUPPORT

API has retained Enviromega Inc., the contractors who developed the APIDRAIN model, to provide technical support for registered users of the modeling software. Technical questions arising from use of the model may be addressed to

Enviromega Inc.
7 Innovation Drive, Ste 245
Flamborough, ON, Canada
L9H 7H9

Tel: (905) 689-4410
FAX: (905) 689-7040
Email: eng@enviromega.com

Please have your registration number available when requesting technical support, as only registered users will be eligible for this service.

Section 2

USING APIDRAIN

2.1 START-UP

Reminder: Excel™ does not have an automatic back-up feature. Periodic saving of the spreadsheet is recommended after data entry, either by clicking the save icon on the tool bar, or clicking on the *File/Save* menu items.

To initiate the APIDRAIN model, the user double-clicks on the APIDRAIN 1.0 icon. If operating in MS Office 97, a dialog box will appear with a button that shows "Enable Macros" (Figure 2.1). Click on this button to generate the macros used in the APIDRAIN model. If operating in Excel™ Version 5, this dialog box will not appear.

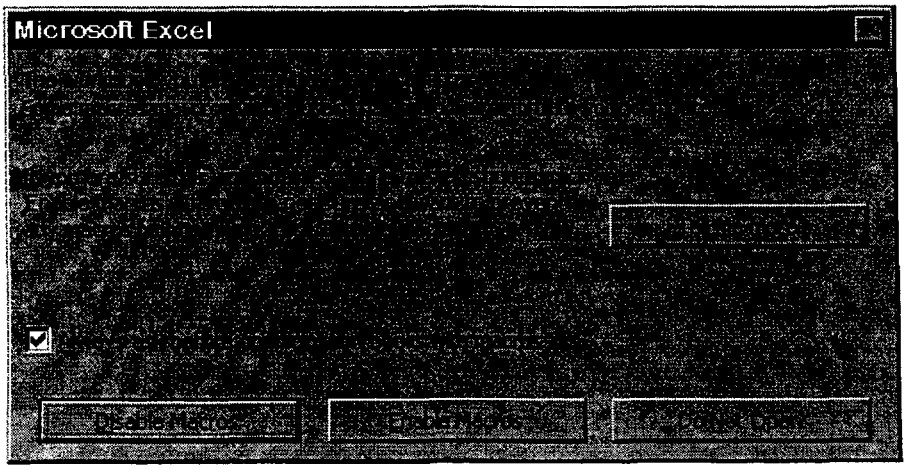


Figure 2.1 Enable Macro Dialog Box

Three initial start-up screens will appear sequentially. These describe the model ownership, copyright and development.

Following the last start-up screen, the user is presented with three options (Figure 2.2):

- create a new facility workbook;
- open an existing facility workbook;
- exit the APIDRAIN program.

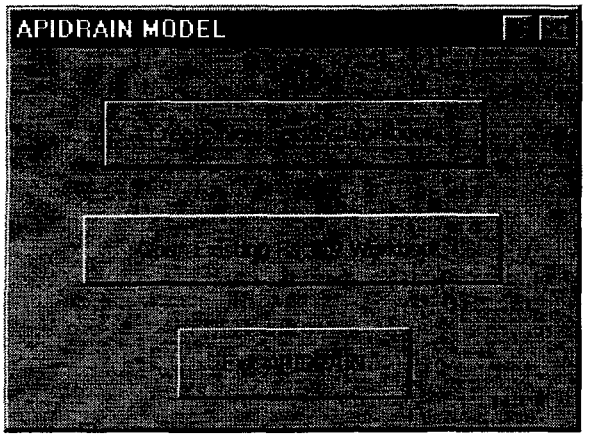


Figure 2.2 APIDRAIN Start-Up Dialog

When the user clicks on the *Create New Facility Workbook* button, the summary facility page will appear (Figure 2.3). At this point in the program, the facility summary is empty, showing no process units or facility total emissions. All estimation methods are shown on this summary, so that emissions from different units may be characterized by different estimation methods (AP-42 factors, OVA screening correlations, stripping efficiency factors or the UT drain model).

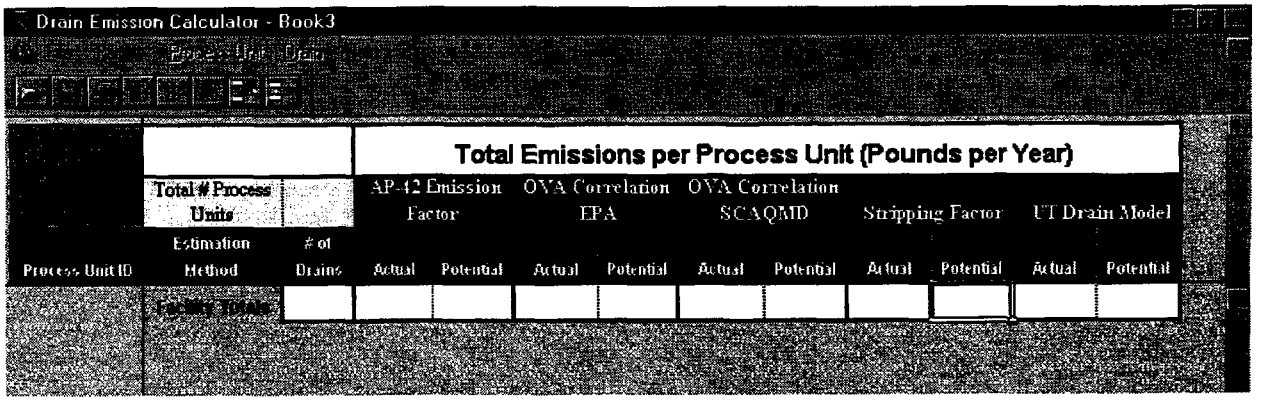


Figure 2.3 New Facility Worksheet

If the user has previously created a facility workbook, by clicking on the *Open Existing Facility Workbook* button, a dialog box appears that allows the user to select the directory and file name of the previously created facility.

2.2 *FACILITY DESCRIPTION*

The next step for a user starting to work with the spreadsheet will be to characterize the facility (refinery, distribution terminal, other). Point the mouse to the menu at the top of the screen to the item ***Facility*** and click. A drop-down box will appear with the following items:

- ***Add New Process Unit***
- ***Edit Selected Process Unit***
- ***Delete Selected Process Unit***
- ***Author Info***
- ***General Info***
- ***Operating Info***
- ***Contact Info***

Click on the *Author Info* item to enter information regarding the facility and corporate name, and the person preparing the model (Figure 2.4).

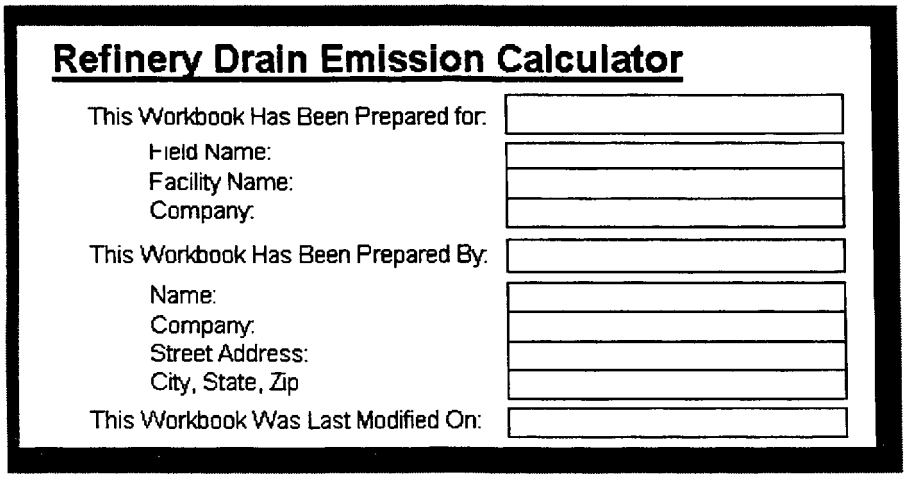


Figure 2.4 Author Information

When entry is finished, click on the *Facility/General Info* menu item to characterize the facility site information, permit and regulatory data (Figure 2.5).

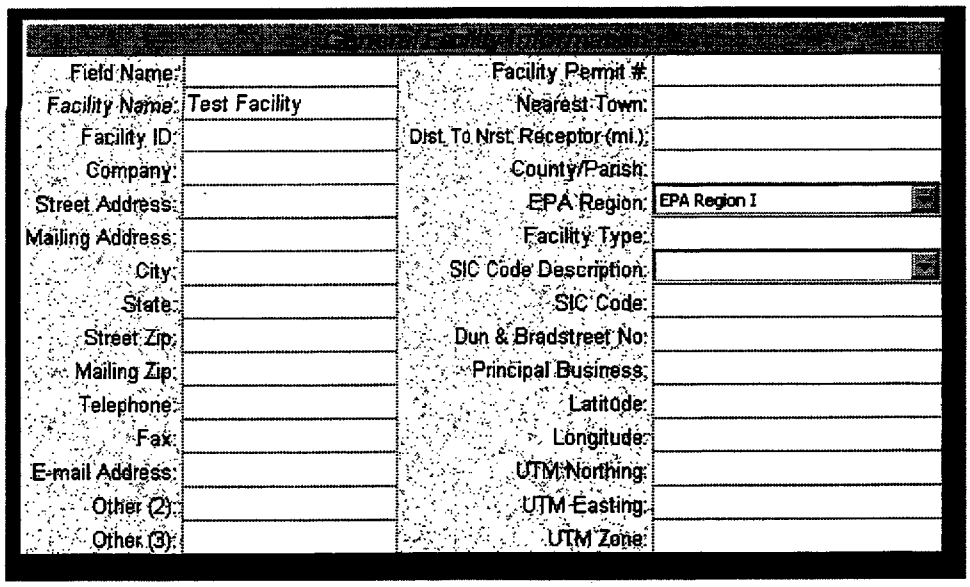


Figure 2.5 General Facility Information Sheet

When entry is finished, click on the *Facility/Operating Info* menu item (Figure 2.6). This describes the schedule of the facility that is used in estimating the monthly, quarterly and annual emission rates. Note the number of hours per year is a calculated value based on the hours/day, days/week and weeks/year. As a calculated number (protected cell), the value appears in red. Atmospheric pressure at the specified elevation is calculated according to the formula (ASCE, 1992):

$$P_{el} = 14.7*(1 - 3.5*10^{-5}*h)$$

where: P_{el} = atmospheric pressure in psia at elevation h (feet) above mean sea level.

When entry is finished, click on the *Facility/Contact Info* menu item to enter the information (Figure 2.7). At the completion of this entry, all the preliminary facility site information has been entered. It is recommended that the user save the information to a working file if not already done.

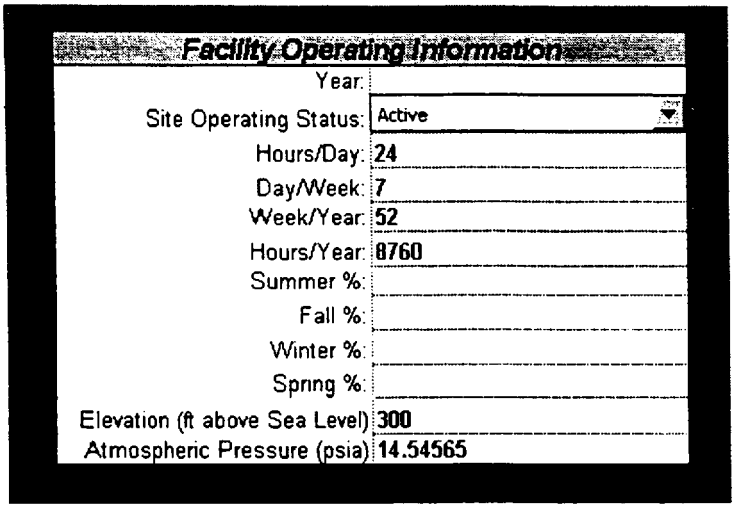


Figure 2.6 Facility Operation Sheet

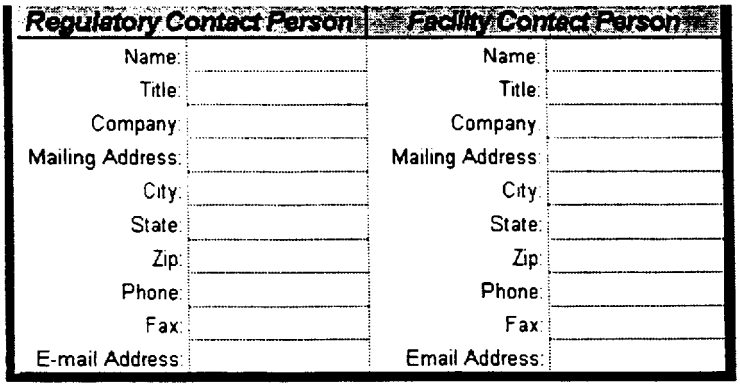


Figure 2.7 Contact Information Sheet

2.3 APIDRAIN TOOLBAR ICONS

At the top of the APIDRAIN model is a toolbar with a series of icons that can be used to speed the characterization of the process units and drains. A brief identification of the toolbar icons follows.

Open Facility. This icon is used to retrieve an existing facility file, and is equivalent to the menu selection *File/Open Facility*.

Save Facility. This icon is equivalent to the menu selection *File/Save Facility*.

Print Facility. This icon is equivalent to the menu selection *File/Print*.

Go to Facility View. This icon duplicates the menu selection items *Process Unit/Return to Facility Emissions* and *Drain /Return to Facility Emissions*.

Edit Process Unit. Either of these icons is equivalent to the menu selection *Facility/Edit Selected Process Unit*.

Edit Drain. This icon is equivalent to the menu selection *Process Unit/Edit Selected Drain*.

Insert New Unit/Drain. In the Facility Summary worksheet, this icon is equivalent to the menu selection *Facility/Add New Process Unit*, or, in the Process Unit worksheet, it is equivalent to the menu selection *Process Unit/Add New Drain*.

Delete Selected Unit/Drain. In the Facility Summary worksheet, this icon is equivalent to the menu selection *Facility/Delete Selected Process Unit*, or, in the Process Unit worksheet, it is equivalent to the menu selection *Process Unit/Delete Selected Drain*.

2.4 PROCESS DATA ENTRY

2.4.1 Creating Process Units and Drains

Once the facility information has been entered, characterization of the process units and the drains within those units may proceed. Click on the *Facility/Add Process Unit* menu item to reveal a dialog box that enables the user to label a new unit (crude, catalytic reforming, etc.) (Figure 2.8). The dialog box will show the number of the next unit to be added. This may either be overwritten or extended by users according to their preference. Beneath the unit I.D. box is the list of available estimation procedures. For the current unit to be modeled, click on the estimation procedure to be used for estimating emissions from drains in the current process unit. For this illustrative discussion, select the *AP-42 emission factors*. Following this selection, click on the *Add* button of the dialog box.

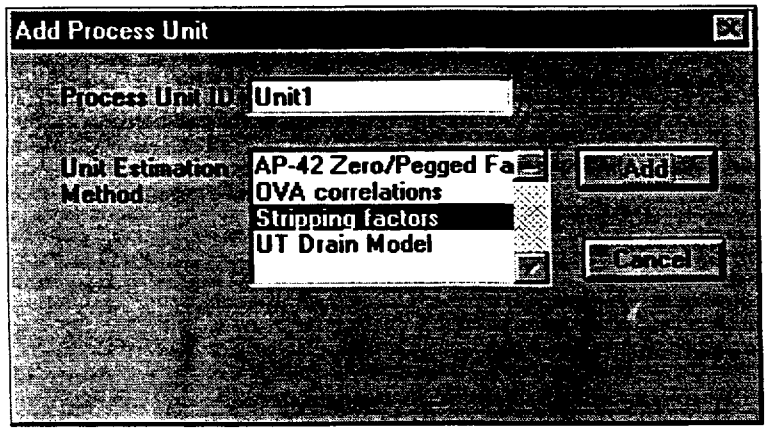


Figure 2.8 Add Process Unit Dialog

At this time, the process unit emission worksheet will appear (Figure 2.9). This sheet identifies the process unit in the upper left hand corner. Then moving to the right, along the worksheet is the unit estimation method, and finally the total emission rate summary for the different estimation procedures selected. Note that the emission rate is provided in units of pounds/year **per drain** in this summary sheet.

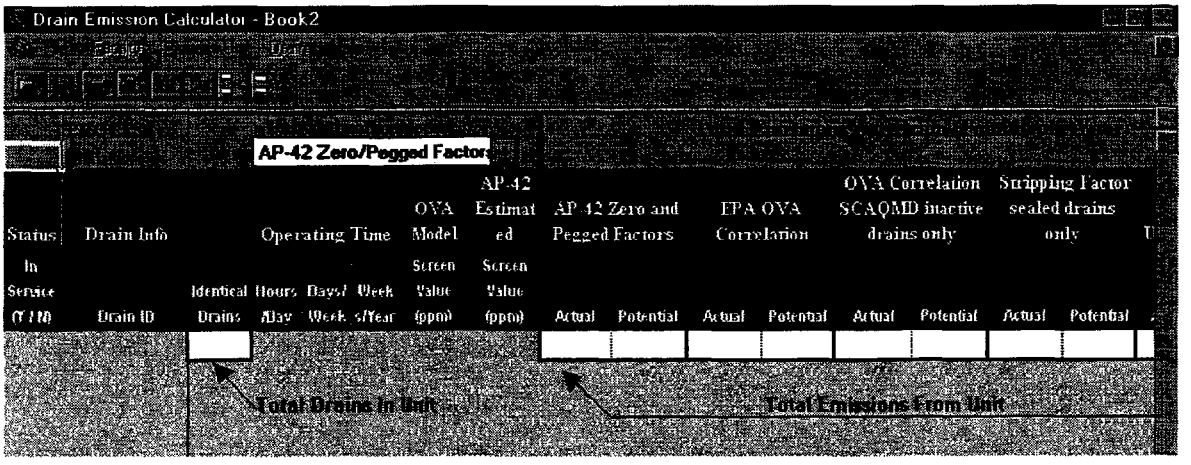


Figure 2.9 Process Unit Worksheet Prior to Drain Entry

Below the unit estimation method, running in the background are the hours, days and weeks of operation. These values are not linked to the hours, days and weeks entered in the Facility Operation dialog box to provide greater modeling flexibility. While the whole facility may operate continuously on a year-round basis, certain process units may only be operated for part of the year. Separate identification of the time of operation of each process unit provides a more realistic estimation of chemical emissions.

To begin entry to the Process Unit sheet, click on the *Process Unit* menu item to see the available options. These include:

- *Change the unit name;*
- *Add a new drain;*
- *Edit a selected drain;*
- *Delete a selected drain;*
- *Rename a selected drain;*
- *Return to Facility Emissions summary.*

If this is the initial characterization of the process units, click on the *Add a new drain* item for designation of the drain (Figure 2.10). At the bottom of the dialog box, the unit name previously specified and the sequential drain number appears. This name can be accepted as is, or a user designation (1a, crude-1a, 01-1-1-1, etc.) can be entered.

If a user edits the drain name using the keyboard arrow keys, a cell reference may show in the entry box as indicated in Figure 2.11. This is a function of the programming code and may be overcome by highlighting the characters to be deleted with the left mouse button, then pressing the delete key. The drain name may then be correctly entered.

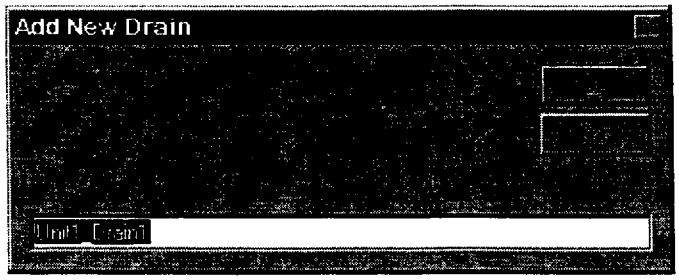


Figure 2.10 Add New Drain Dialog Box

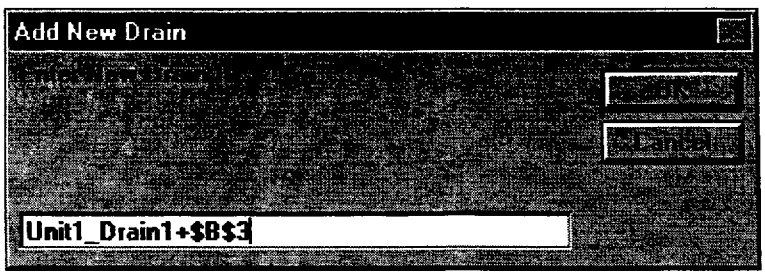


Figure 2.11 Example of Drain I.D. After Use of Arrow Key to Edit Name

Click on OK to accept the drain name. The screen returns to the process unit summary, showing that the first drain has been entered (Figure 2.12). The current emission estimation procedure is displayed to the right of the process unit description. If the estimation method procedure has been entered incorrectly, or needs to be changed, click on the estimation procedure showing, and a drop-down box appears showing the available estimation procedures. Click on the desired procedure, and the spreadsheet will update the estimation procedure for the drains in that process unit. Save the file again if necessary.

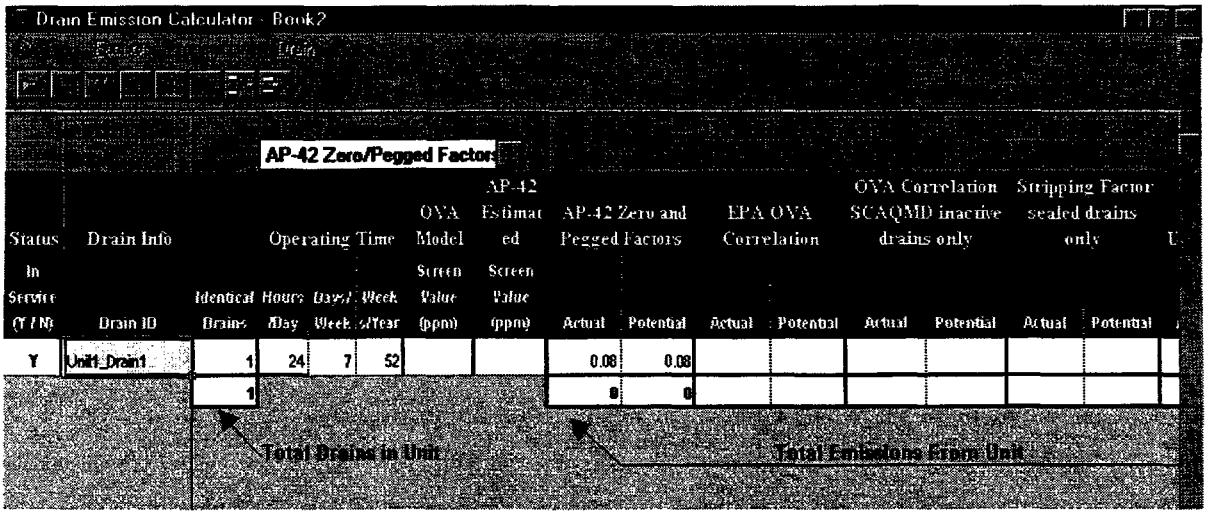


Figure 2.12 Process Unit Worksheet After Drain Emission (Zero Default Value)

Note that with the selected AP-42 emission method, there is no value to edit in the drain entry, so the item ***Edit a Selected drain*** is not enabled. If the drain identifier needs to be changed, use the menu item ***Rename a selected drain***.

Should a drain be entered by mistake (a double entry for example), it is possible to delete the drain by first clicking on the drain identifier in the Process Unit column, then clicking on the menu item *Process Unit/Delete Selected Drain*. A dialog box will prompt the user whether the drain is to be deleted permanently or not. If yes, the drain is removed from the spreadsheet; otherwise the model returns to data entry mode.

During different times of the year when modeling of emission rates can take place, various drains may be in or out of service. The APIDRAIN model allows a user to select whether the drain is active or not. At the far-left column of the Process Unit worksheet is a column heading called "Status". This column is used to indicate if the drain is active or not. By default, if a drain is entered, the model considers the drain to be active. If a drain is out of service, the user types N for not in service. The result is that the drain will continue to show a potential emission rate, but the actual emission rate will disappear. This feature gives the user some flexibility in the number of drains that may be in service in a unit at the time of modeling.

2.4.2 Use of AP-42 Zero/Pegged Factors

AP-42 emission factors used in the APIDRAIN model are those specified by the US EPA (1995) for the zero and pegged factors for "other" equipment in the petroleum industry, as shown in Table 2-1. In the AP-42 Zero/Pegged Factor estimation procedure, when a new drain has been entered, the emission rate will show as 0.08 lb/year initially. The APIDRAIN model uses a zero default value (0 ppm) in the Screen Value data entry box upon initiation, resulting in the emission rate of 0.08 lb/year. The other potential entries for this data box are 10,000 and100,000 ppm. The units in the EPA report have been converted from kg/hr to lb/yr.

The calculated emission rate for zero emission default rate is 0.08 lb/year **per drain**. [If either of the pegged emission rates for screening values of 10,000 ppm or 100,000 ppm is to be used, those values are entered in the column under the heading Screening Value]. If no value is entered for the pegged screening value, the model assumes a default zero value, resulting in a displayed emission rate of 0.08 lb/year. The emission rate output is provided in a summary row beneath the Emissions Output. The summary row rounds to the nearest whole integer.

Table 2-1 AP-42 Zero and Pegged Emission Factors

Factor	Emission Rate (lb/hour)	Emission Rate (lb/year)
Default Zero	8.8E-06	0.08
Pegged 10,000 ppm Screening Value	0.16	1410
Pegged 100,000 ppm Screening Value	0.24	2125

APIDRAIN has a short-cut data entry procedure if many identical drains are to be entered. Under the Unit Estimation Procedure heading is a prompt for the number of identical drains. If the drain being entered is unique, the value entered for number of identical drains is 1. If there should happen to be, say 10 identical drains, however, then the value 10 may be entered, and the model will calculate the total emissions for 10 identical drains.

If this short-cut procedure is used, it is possible to use only three drain entries as indicated in Figure 2.13. Because this estimation procedure uses zero default and pegged factors, the drains in this method will result in three distinct emission rates, corresponding to the zero default, 10,000 and 100,000 pegged factors. Note that 0 does not appear as a cell entry.

Note also that in this figure the model accounts for differences in potential and actual emission rates if the time of operation is less than year-round, day-in and day-out. Drain I.D.#3 has listed 40 weeks of operation rather than 52, so the model estimates that the actual emission rate is proportionately less than the potential emission rate.

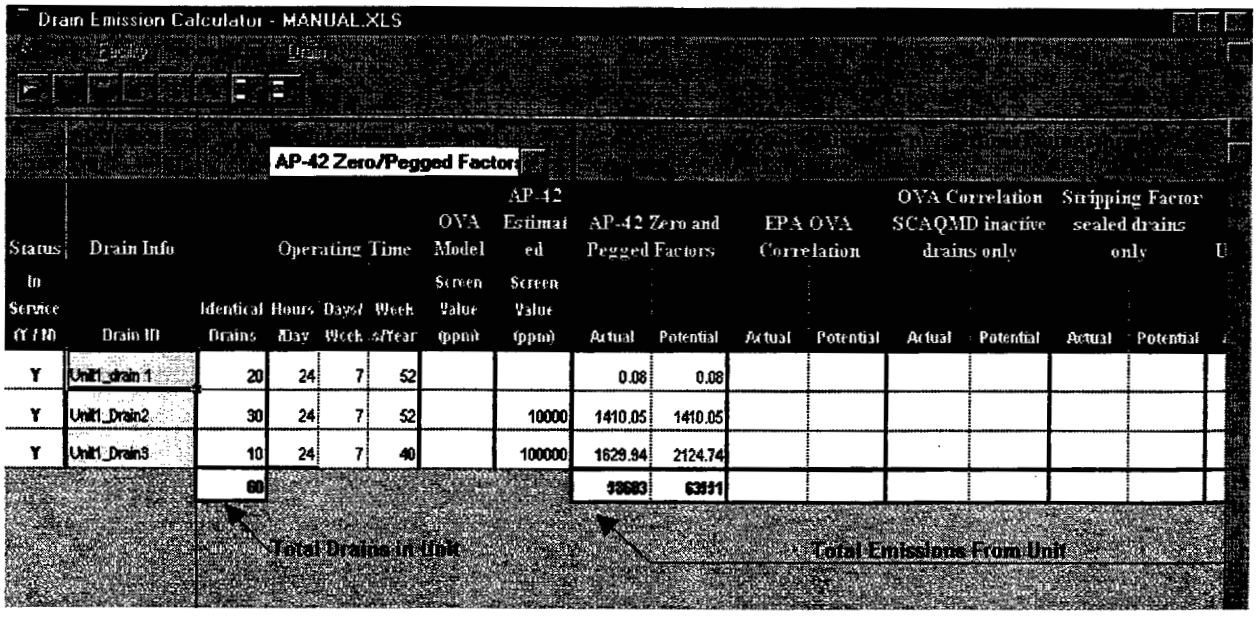


Figure 2.13 Process Unit Characterized by 3 AP-42 Zero/Pegged Factors

Once all the drains for this process unit have been entered, the user may return to the facility summary by clicking on the menu item *Process Unit/Return to Facility Emissions.*

In the Facility summary workbook, the total number of process units included in the emission estimates is then updated, as shown in Figure 2.14. The Facility summary also includes the emission estimation method and number of drains included in the emission estimate for the process unit.

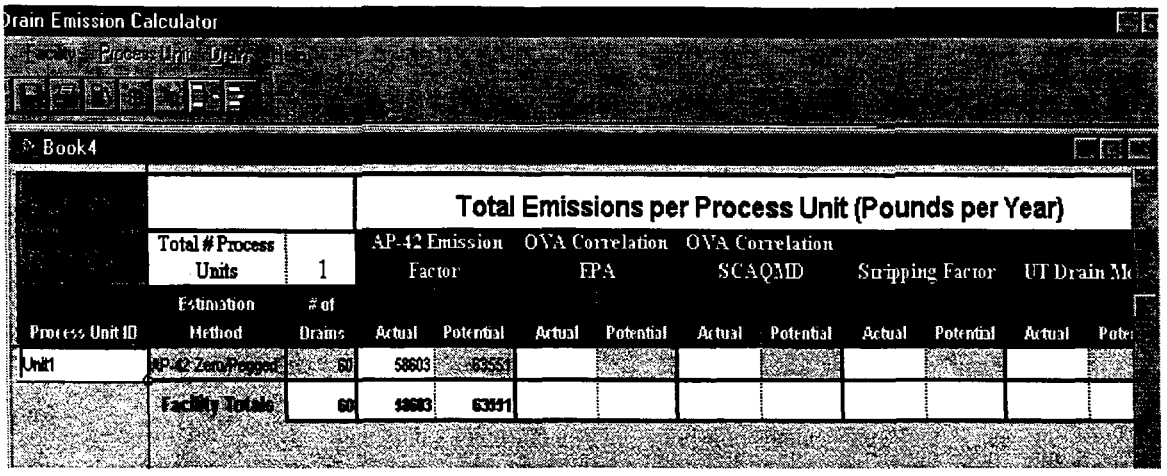


Figure 2.14 Facility Sheet after a Drain Has Been Added

2.4.3 Use of OVA Screening Values

APIDRAIN enables the user to estimate emissions of total non-methane hydrocarbons based on screening value readings taken with an organic vapor analyzer (OVA) instrument. Two correlations are provided in the estimator. One is a correlation developed by the U.S. EPA (EPA, 1995) for emissions from "other" equipment in the petroleum industry:

$$Leak\ Rate = 3.00*10^{-5}\ (SV)^{0.589} \qquad \textbf{(Equation 2-1)}$$

where: Leak Rate is in lb/hour

SV = screening value in ppm

A second correlation provided in the APIDRAIN model, similar in form to the EPA correlation, was developed for application **to inactive drains** by refineries within California's South Coast Air Quality Management District (SCAQMD). In this case, the correlation is of the form (SCAQMD, 1995):

$$Leak\ Rate = 3.147*10^{-4}\ (SV)^{1.02} \qquad \textbf{(Equation 2-2)}$$

with the emission rate in lb/hour and the screening value measured in ppm.

For SCAQMD users, note that the District has specified for screening values of 10 ppm or less, the default zero for the drain emission rate is 28.87 lb/yr. Users of the SCAQMD procedure should enter a screening value of 10 ppm as the default zero value.

The values for the emission rates in the row designated for the drain being characterized is in lb/year (i.e., the model converts the correlations from lb/hour to lb/year) **per drain**. The total emission rate for all drains appears in the row beneath the last characterized drain. As with the other estimation procedures, the number of identical drains may be entered as a short-cut. The total emission rate from these similar drains will be included in the total emission rate in the summary row beneath the final characterized drain in the process unit summary (Figure 2.15). Features of the model including actual vs. potential emissions (drain #2), identical drains (drain #4), and inactive drain status (drain #5) are all illustrated in Figure 2.15. The user may then return to the Facility Worksheet to see the addition of the second process unit to the total facility (Figure 2.16).

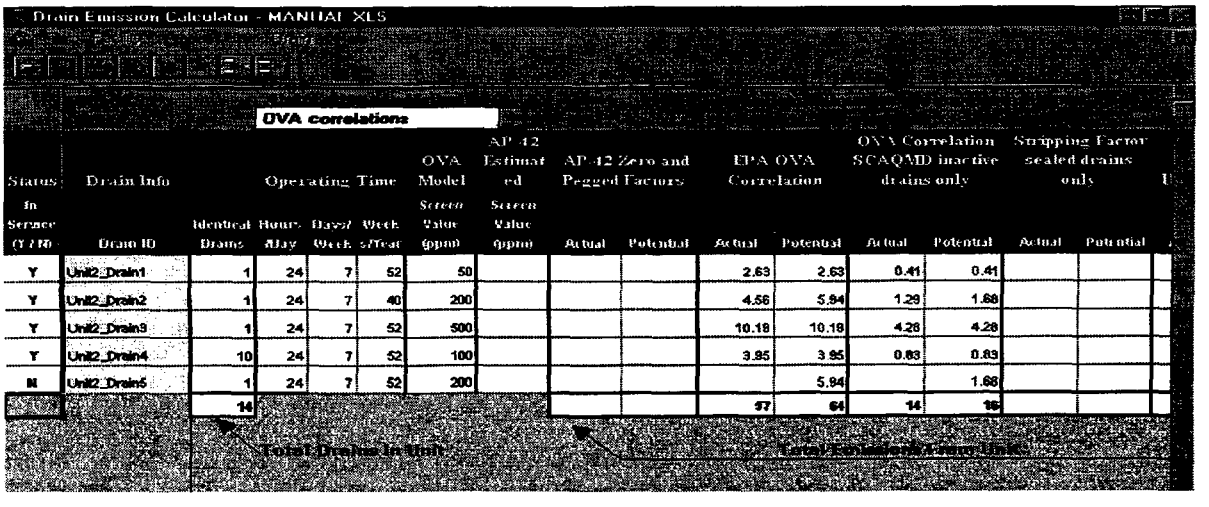


Figure 2.15 Drain Emissions from AP-42 and OVA Methods

2.4.4 Use of Stripping Efficiency Factor Estimation Method

The stripping efficiency method calculates total VOC emissions, and is based on a study of refinery process drain emissions completed for API by Brown and Caldwell, Enviromega Inc. and Dr. R. Corsi of the University of Texas. This report, Publication Number 4677, "Fugitive Emission Factors for Refinery Process Drains", has been published by API. The factors were established based on many test experiments with a pilot-scale drain. Emissions from a drain can

be estimated using these factors when the discharge flow to the drain and the concentrations of specific organic compounds within the discharge are known. **This procedure is applicable to sealed drains only**.

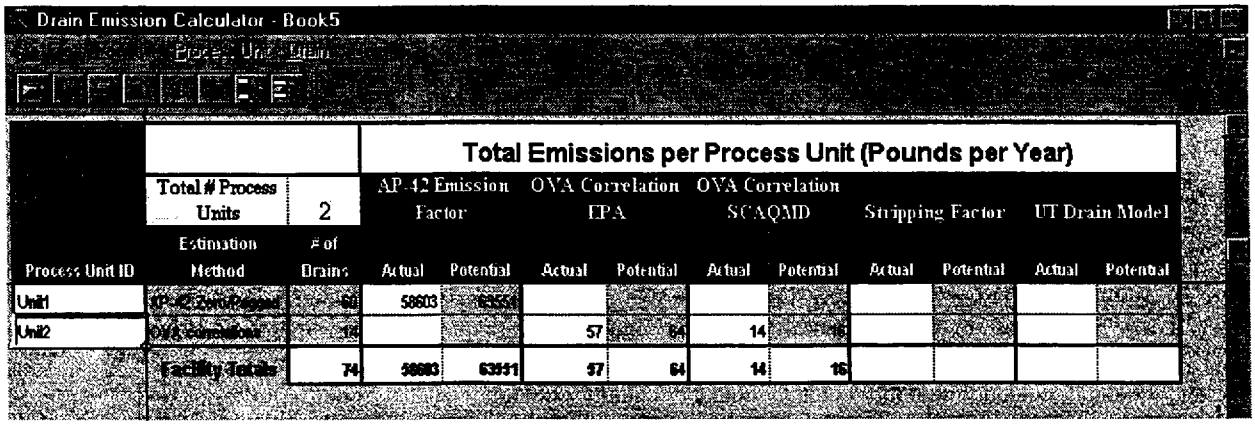


Figure 2.16 Facility Worksheet Summary with OVA Correlation Method Added

The following steps are needed to implement the stripping efficiency estimation procedure. Click with the mouse on the *Process Unit* menu item, then *Add a new drain.* Title the drain as appropriate, and enter it to the worksheet. The Process Unit worksheet shows that a drain has been added. Click on the drain to be characterized, then move to the menu item *Process Unit/Edit Selected Drain.* The inputs needed for the stripping efficiency method are displayed (Figure 2.17). Note that because of the number of influents and chemical compounds permitted by the model, the worksheet extends off the screen. The scroll bars at the bottom and right hand side of the screen may be used to scroll more of the workbook onto the screen. [After initial opening of this model, certain cell references in this estimation procedure may show as "#NAME". This is an artifact of the Excel™ spreadsheet. Section 4.2 of the manual describes how to correct this problem.]

The modeling parameters that are used to establish the stripping efficiency emission rate are indicated in the influent discharge streams to the drain. Inputs needed by the stripping efficiency model, with their corresponding default values, include:

- water flow (2 gpm)
- nozzle diameter (1 inches)

- height of the nozzle above the drain (4 inches), and
- liquid (wastewater) temperature (85 °F).

Mathematical derivations of the emission rate by the stripping efficiency procedure are discussed in detail in Section 3.

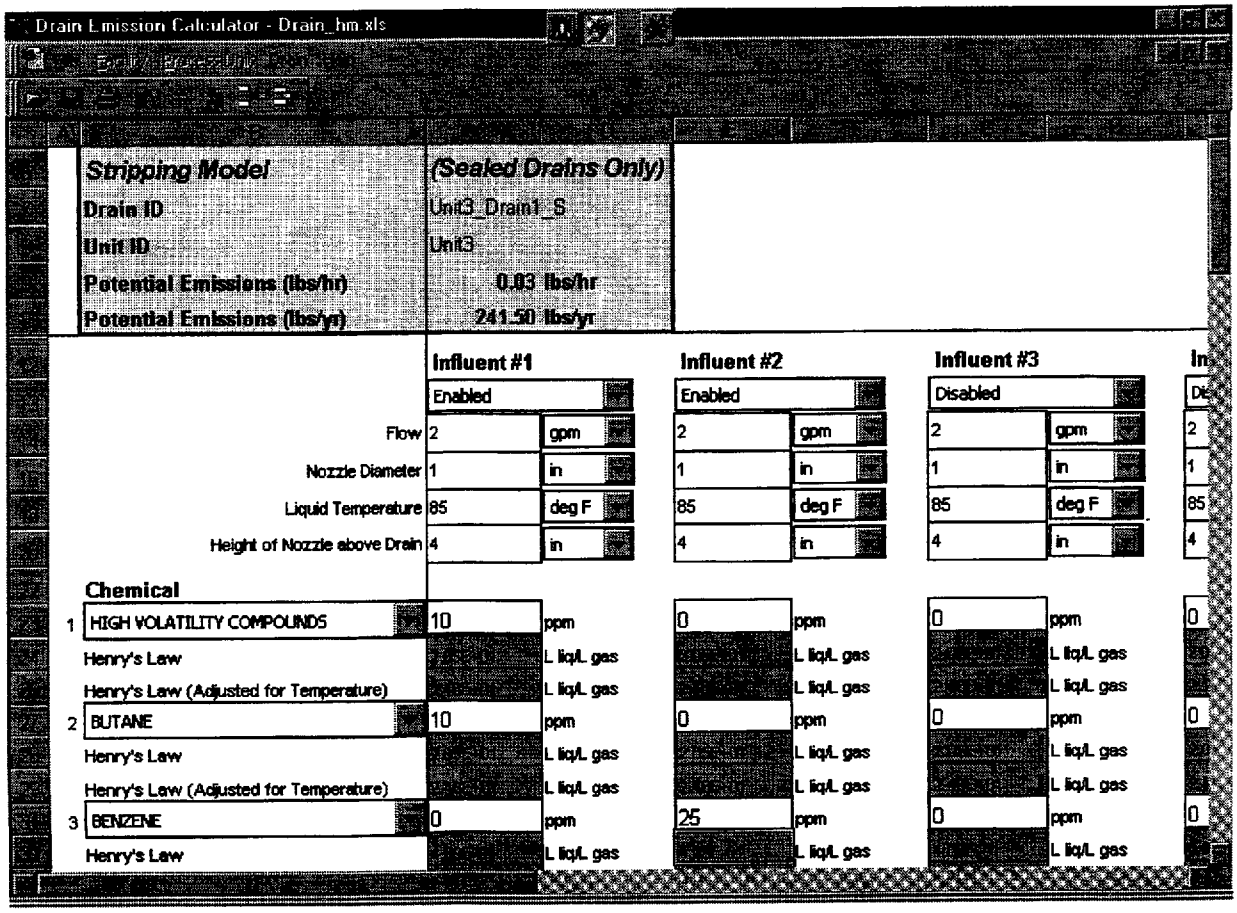


Figure 2.17 Stripping Efficiency Model Data Entry Screen

The model allows up to six influent streams per drain to be characterized. To activate an influent discharge to the drain, the user must click on the drop-down box to the right of Influent waste stream number, and select *Enabled*. At any time once the model is configured, if the influent stream discharged to the drain stops, the user may remove that influent stream from the drain by clicking on the drop-down box and selecting the *Disabled* item.

Allowable data entry values in the worksheet are highlighted in blue, while required parameter values, which are converted from the data entry values, are noted in red. [Values appearing in red are protected cells, and can not be altered by the user]. To the right of each data entry cell is a units drop-down box. By toggling this box between US and metric units, the user may select the preferred units for data entry. The workbook is programmed to convert the units to those required in the emission models.

In the stripping efficiency model, users may estimate emissions of unspeciated compounds depending on the perceived volatility of the compounds, classified generically as high, moderate and low volatility compounds. The classes of compounds, based on the pilot study referenced above, are differentiated by Henry's law coefficient (H_c), as follows:

high volatility:	$H_c > 0.72\ m^3_{liq}/m^3_{gas}$
moderate volatility:	$0.13 \leq H_c \leq 0.72\ m^3/m^3$
low volatility:	$H_c < 0.13\ m^3/m^3$

The user may select up to 15 chemical compounds for which to estimate emission rates from each drain. The user clicks on the drop-down box to the right of name of Chemical #1-15 (Figure 2.17). The first compound entry is listed as "None", followed by all of the compounds listed in AP-42 in alphabetical order. The user can scroll down through the list, partially displayed in Figure 2.18, and then select the compound. The concentration of the chemical is next entered below the chemical name. The default concentration of individual chemical compounds or classes of compounds is set to 0 ppm.

The generic compound classes are located at the top of each list of chemicals, in alphabetical order, that fall within these classes. For example, hexane is grouped with compounds under high volatility, while benzene is classed with compounds of moderate volatility. Individually speciated compounds use the same Henry's law coefficient as the generic class compound under which they are categorized. For example, in Figure 2.17, the displayed Henry's law coefficients for the highly volatile (generic) compound, and butane, which is categorized as a highly volatile compound, are the same. Only the UT model makes use of the Henry's law coefficient for each speciated compound.

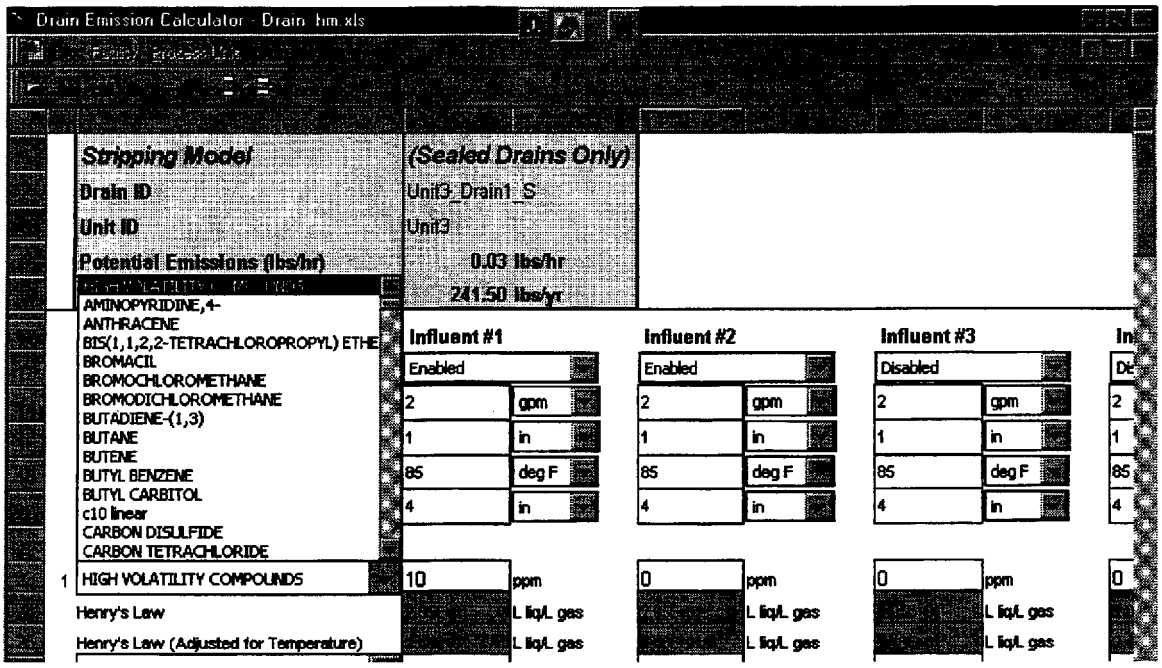


Figure 2.18 Drain Worksheet Displaying Scroll List of Chemicals

The stripping efficiency model uses temperature-corrected Henry's law coefficients to select the proper stripping factor for estimating the emission rate. Both the H_c at 25 °C and the temperature-corrected coefficient are displayed for each compound. The Henry's law coefficients may be removed from the display by using the menu item *Drain/Hide Drain Calculations* so that more compounds may be viewed simultaneously. The coefficients may be restored to the display by the menu item *Drain/Unhide Drain Calculations*.

Emission rates are summarized in several ways in this worksheet. Total emissions from the drain in units of lb/hr and lb/year are provided in the yellow-shaded box at the top of the worksheet (Figure 2.17). These emission rates in lb/year are then linked back to the process unit summary sheet, and the facility summary sheet. Beneath the row designating the 15th chemical for the drain is a summary row that lists the emission rate for each of the six potential influent streams to the drain. This row is depicted in Figure 2.19. The emission rates in the summary row correspond to the chemicals and concentrations indicated in Figure 2.17.

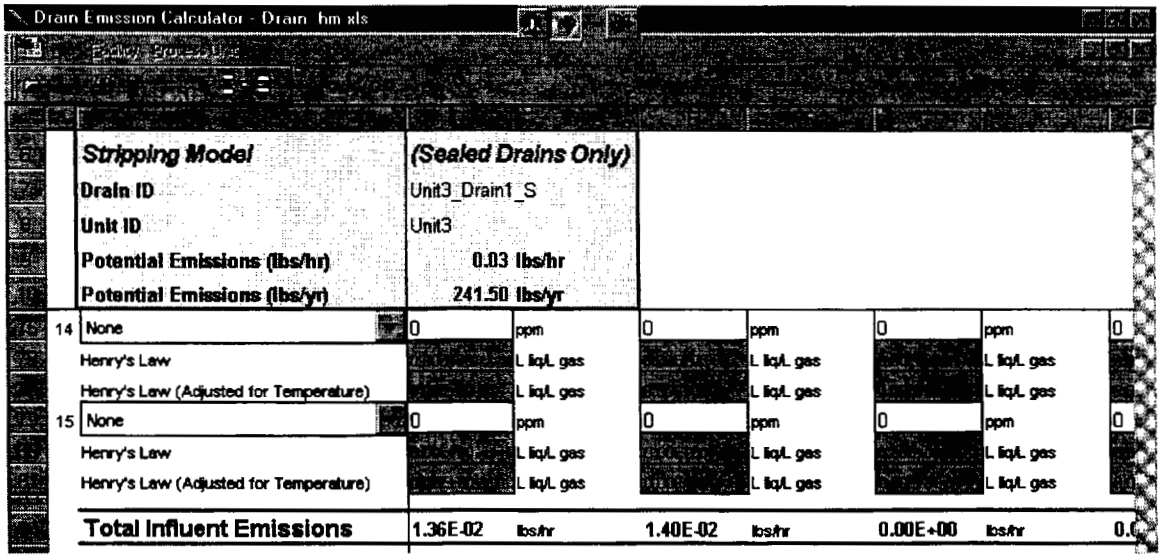


Figure 2.19 Drain Worksheet Showing Summary of Emission Rates from Each Influent

Emissions from inactive drains were investigated in the pilot study. APIDRAIN allows a user to estimate emission rates from inactive drains. The procedure required is to select the specific compounds or class of compounds, and enter the concentration in the drain seal. With the drain enabled, the discharge flow rate is set to zero. The emission rate then is indicated for the chemical(s) or class of chemicals selected.

When the user has completed characterizing the influent streams to this drain, and the emission rate(s) has been estimated, the user may then either return to the process unit to characterize another drain, or return to the facility summary sheet. To execute either of these decisions, the user clicks on the menu item *Drain*, and then either selects *Return to Process Unit*, or *Return to Facility Emissions*.

2.4.5 Use of the UT Drain Model

The UT model was developed by Dr. R. Corsi at the University of Texas, and is based on sophisticated mass transfer processes. The model enables the user to calculate speciated compound emissions, and requires more input values characterizing the drains than the other estimation methods. The inputs required for the UT model, with the default values, include:

- water flow (2 gpm)
- nozzle diameter (1 inch)
- liquid (wastewater) temperature (85 °F)
- ambient air temperature (70 °F)

To characterize the emissions from a process drain using the UT model, complete the preliminary steps of identifying a new process unit [*Facility/Add Process Unit*], naming the unit, and selecting the UT Drain Model as the estimation method. Next, return to the menu bar and click on *Process Unit/Add New Drain*. Enter the drain identification and accept it. The process unit worksheet shows the drain has been added. The data entry screen for the UT model is provided in Figure 2.20.

To characterize the inputs to the drain, click on the drain identifier (appearing in the first worksheet column as a pale yellow entry), then return to the menu toolbar, and click on *Process Unit/Edit Selected Drain*. This set of commands results in display of the UT model worksheet.

Because of the potentially large quantity of information that may be used to characterize discharges to the drain, the entire worksheet is not displayed on the screen. The user must use the vertical and horizontal scroll bars to view all the possible data entry points in this model.

The first characterization step for a drain in the UT model is to specify whether it is a sealed (trapped) or open (unsealed) drain. This entry appears in the upper left corner of the worksheet as a Yes (Y) or No (N) response. To the right of this entry are the characterization data for elevation (user-entered as previously specified in the Operating Info worksheet (thus a blue cell entry), and the ventilation rate in the channel connected to an unsealed drain.

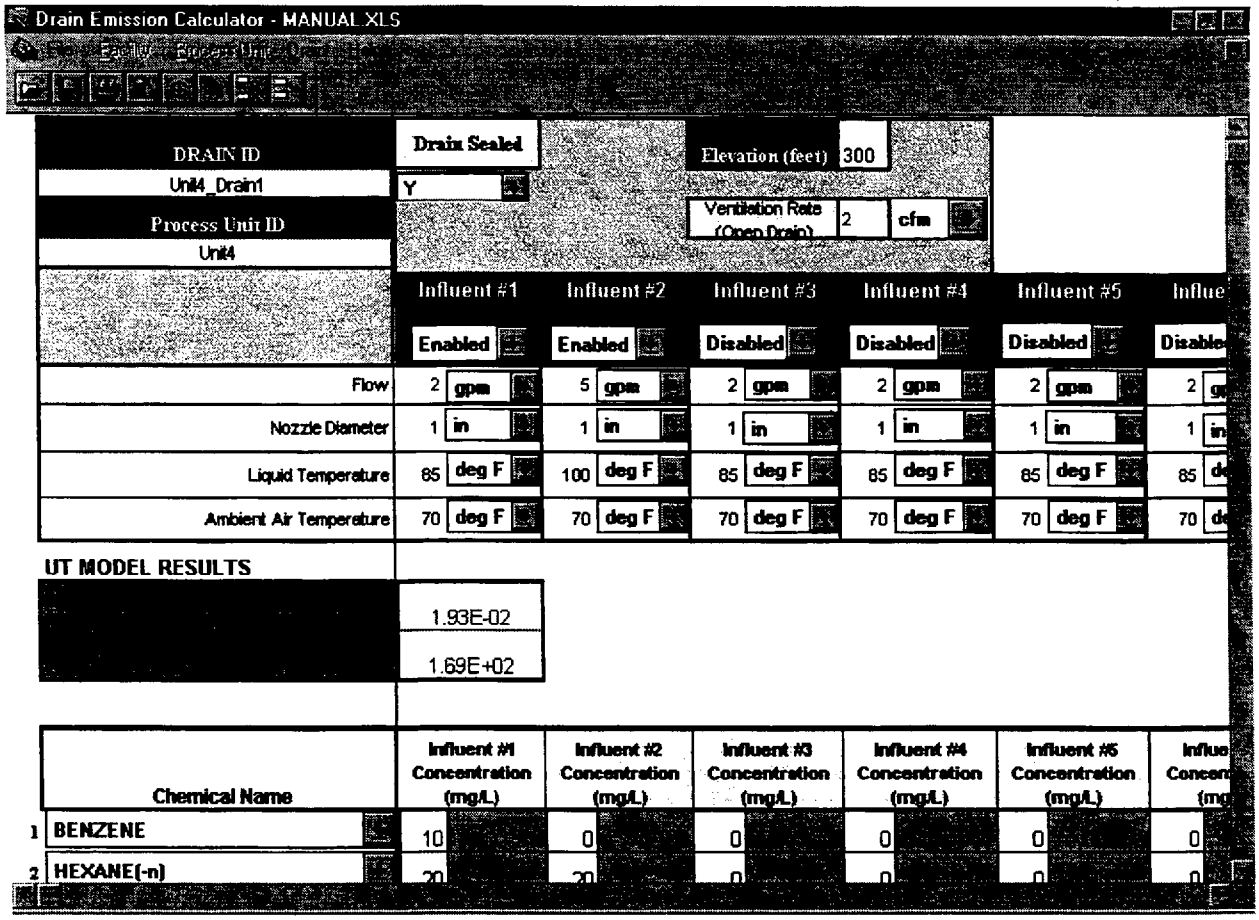


Figure 2.20 UT Model Drain Characterization Worksheet

The user next characterizes the individual influent discharges (nozzles) to the current drain. At the top of each influent stream is a drop-down box to indicate whether the influent is active or not. An influent may be characterized, but if it is shut down for a period of time, by selecting the *Disabled* status, it may be removed temporarily from the estimation of emissions from the drain. If, at a later date, the discharge resumes, it may be included again by selecting the *Enabled* status. To ensure that the influent is included in the emission estimate, the stream must be *Enabled*. The model allows for characterization of up to six influents to each drain.

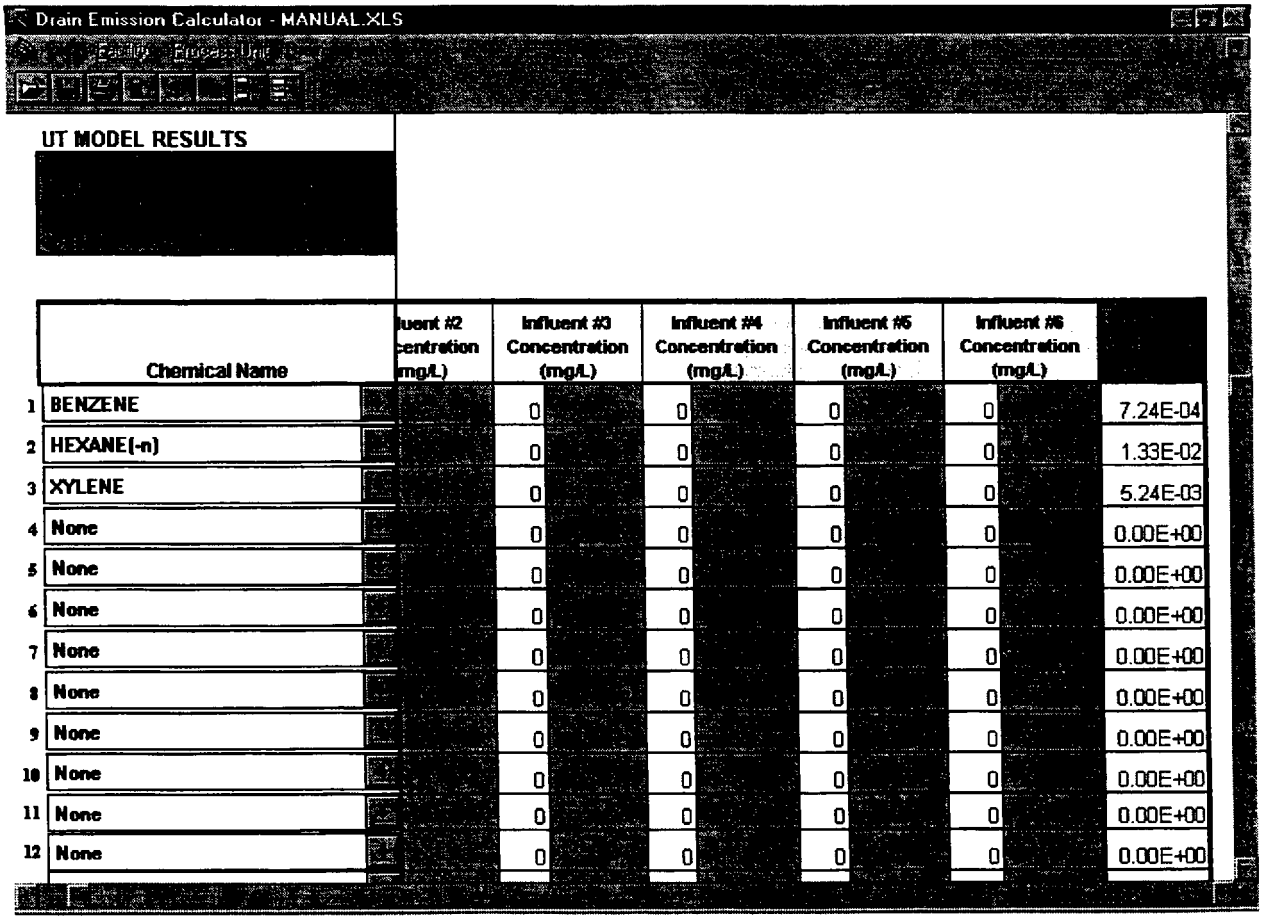
Data entry for inputs to the UT model influents (discharge flow, nozzle diameter, liquid temperature, ambient air temperature) can either be in U.S. or metric units. Following entry of the drain characterization parameters, specific chemicals found in the influent stream are selected and the corresponding concentration specified. All the chemicals listed in EPA's AP-42 documentation are provided in APIDRAIN and are available for selection. Click on the drop-down

box listed to the right of the cell identified as *Chemical #1 Name*. The first item in the list is "None", with the remaining chemicals following in alphabetical order. Scroll down through the list until the chemical of interest is found, then click on it. The chemical name appears in the cell. Then, enter the concentration of the chemical, in units of ppm (equal to mg/L), in each of the discharge streams in which it is detected. In a summary column to the right of the chemical concentrations, the model calculates the total emission rate for each chemical in units of lb/hr.

The user may continue to select up to 15 chemicals in the same influent discharge. Once the chemicals have been selected and concentrations entered, a summary box above the list of chemicals displays the total emission rate of all compounds from the drain. The rates are provided in units of lb/hr and lb/year.

The predicted emission rate by the UT model may read as "#Div/0!" if a compound name is selected before the concentration is entered. The correct emission rate will be displayed as soon as a concentration value is entered for the selected compound in a discharge that is enabled. If for any reason discharges that have been previously activated are all set to the disabled status, the total emission rate may show as "#Value!". To return to display of an actual emission rate, at least one of the characterized discharges must be returned to enabled status.

The total emission rate for each chemical compound specified in the discharges to the drain is tabulated in the column to the right of the sixth influent stream, as indicated by Figure 2.21. The ventilation rate is a user-entered number used in the unsealed drain model at present. Many factors affect the ventilation rate, including the number of openings in the system, wind eduction over the drain openings, buoyancy effects of the gas phase in the sewer, and liquid drag. The ventilation rate may be estimated from the liquid flow rate through the sewer beneath the drain, using a gas phase-to-liquid phase flow ratio (Qg/Ql). For "closed" systems with few opportunities for exchange of the sewer gas phase with the ambient atmosphere, a ratio of 0.2 is appropriate, while for an "open" system, a ratio of 2 is appropriate.



	Chemical Name	luent #2 centration mg/L)	Influent #3 Concentration (mg/L)	Influent #4 Concentration (mg/L)	Influent #5 Concentration (mg/L)	Influent #6 Concentration (mg/L)	
1	BENZENE		0	0	0	0	7.24E-04
2	HEXANE(-n)		0	0	0	0	1.33E-02
3	XYLENE		0	0	0	0	5.24E-03
4	None		0	0	0	0	0.00E+00
5	None		0	0	0	0	0.00E+00
6	None		0	0	0	0	0.00E+00
7	None		0	0	0	0	0.00E+00
8	None		0	0	0	0	0.00E+00
9	None		0	0	0	0	0.00E+00
10	None		0	0	0	0	0.00E+00
11	None		0	0	0	0	0.00E+00
12	None		0	0	0	0	0.00E+00

Figure 2.21 UT Drain Worksheet Showing Emission Summary for Each Chemical Compound

To add another drain, return to the Process Unit worksheet by clicking on *Drain/Return to Process Unit* in the menu toolbar, and then *Process Unit/Add New Drain.*

A number of chemical properties are used in the UT model to estimate the emission rates. It is possible in APIDRAIN for the user to view the chemical properties and derived mass transfer properties such as Schmidt numbers, diffusivities (identified as D_c) and mass transfer coefficients. Click on the menu toolbar *Drain/Unhide Drain Calculations* (Figure 2.22). For convenience they may be re-hidden by clicking on the menu toolbar *Drain/Hide Drain Calculations.*

If all the drains have been entered for this process unit, the user may return to the facility summary sheet by clicking on the menu toolbar *Drain/Return to Facility Emissions.*

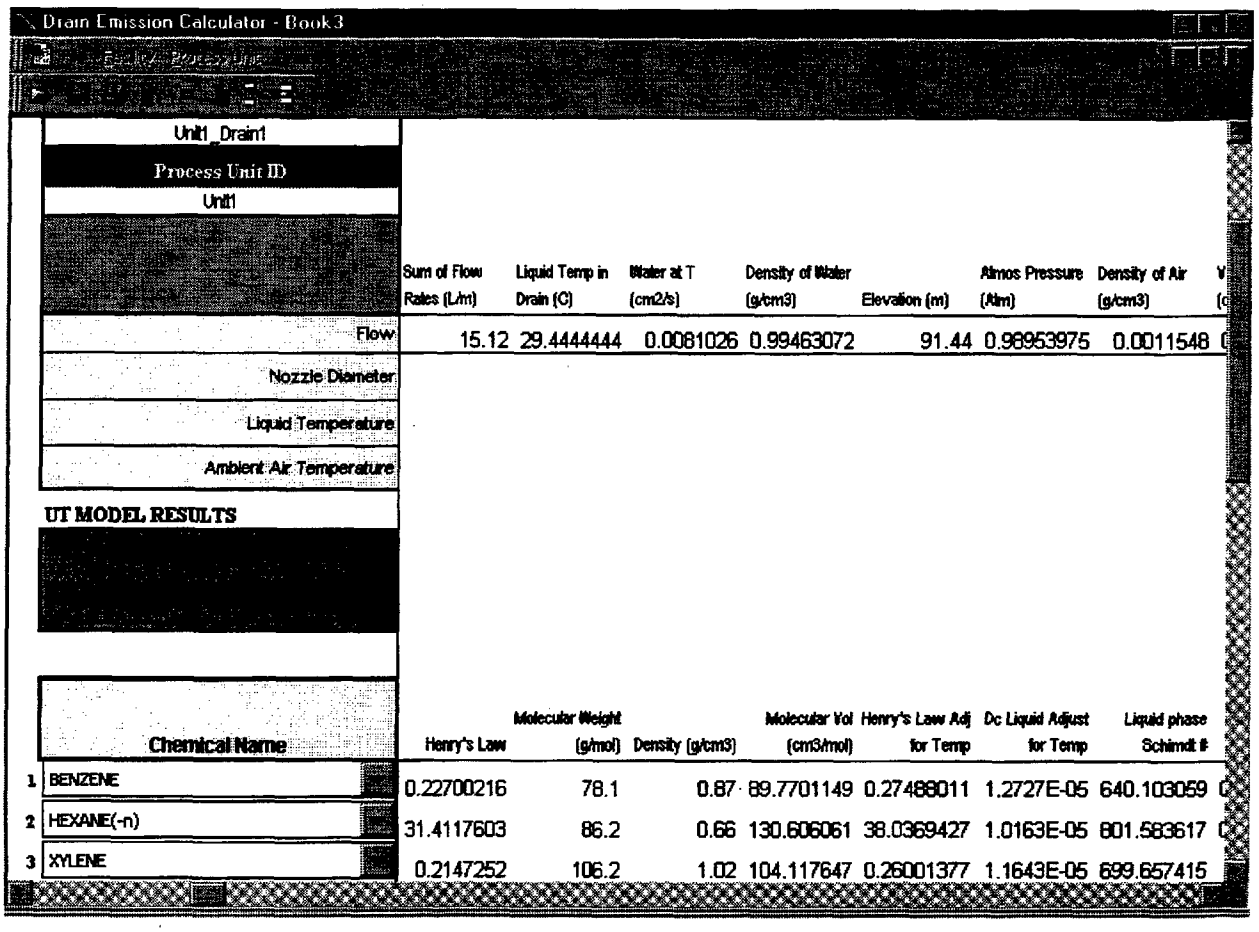


Figure 2.22 UT Model Worksheet with Unhidden Chemical Properties

2.5 REPORT SET-UP AND PRINTING

APIDRAIN includes options for customizing drain emission reports according to the level of detail required by the user. The simplest report summarizes emission rates from the whole facility calculated by the different estimation methods. The most complicated reporting level provides details of individual compound emission rates in each discharge to each drain in all process units.

The report feature has been designed when reporting emissions determined by the OVA Screening procedure to include either the EPA correlation or the South Coast Air Quality Management District (SCAQMD) correlation (for inactive drains) in the summary, but not both. The SCAQMD correlation is intended for use in the vicinity of Los Angeles, CA, and therefore has limited application elsewhere. When a user clicks on the *File/Report* menu item, the dialog

box shown in Figure 2.23 will appear, enabling the user to select the OVA correlation to be printed in the report. Most users can obtain an emissions summary report with the four main estimation procedures (AP-42 factors, EPA OVA screening correlations, stripping efficiency and UT drain model). Users requiring the SCAQMD OVA correlations in a report may print a second report, selecting the SCAQMD option as indicated in Figure 2.23.

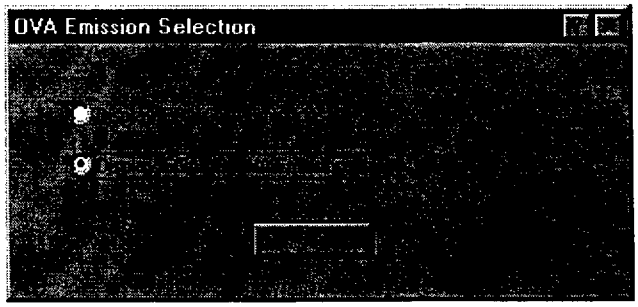


Figure 2.23 Dialog Box for Selection of OVA Correlation in Report Output

The level of reporting is controlled by a series of buttons that appear in the left-hand margin when the menu item *File/Report* is activated. The left-to-right order of the buttons in the left-hand margin corresponds to the reporting level from overall facility, through process units, to individual drains in the process units. The buttons appear with a "+" or "-", indicating whether they are in collapsed or expanded mode, respectively. By using the mouse to click on a button labeled by a "+", more detailed information on drain emission rates will be displayed. Alternatively, by clicking on a button with a "-" displayed, detailed information will be removed from display, leaving only summary data. An example report is displayed as Figure 2.24.

A report summarizing only the total facility emissions estimated by the different modeling procedures is generated if only a single "+" button appears in the left margin. The most detailed report is produced when all buttons in the left margin display the "-" notation. To exit the report, click on the Facility View icon.

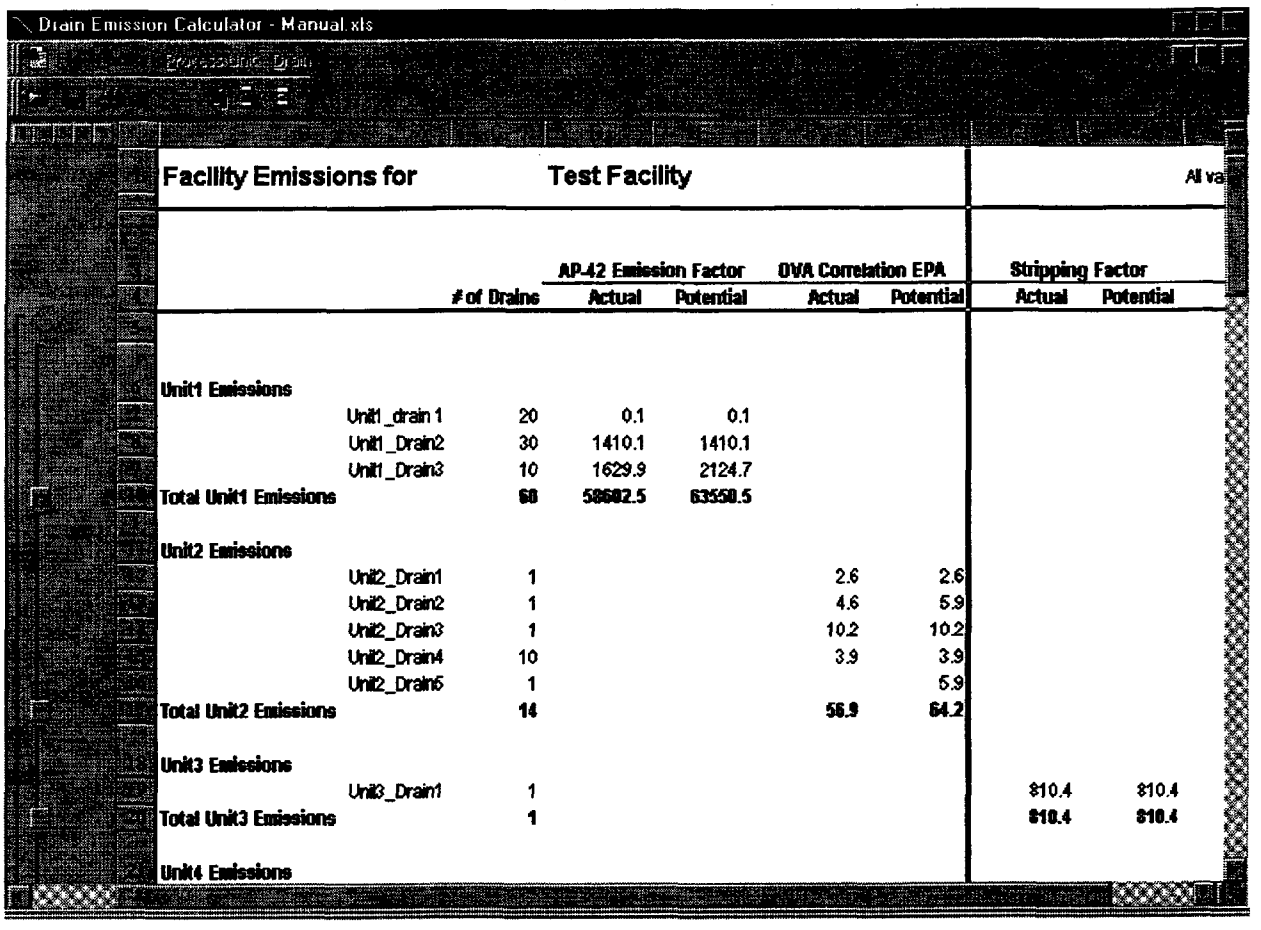


Figure 2.24 Example of Emission Report Screen in APIDRAIN

Due to the detailed information presented in the report, the user may be required to adjust the printer output to fit the report on one (or more) pages. To begin the print operation, the printer button in the toolbar is activated (or use the File/Print menu item); a series of printer option buttons will appear (see Figure 2.25). The "Setup" button is used to size the report. In the report setup (Figure 2.26), the orientation should be set to Landscape to optimize the size of the font used in printing the report. If the report is short in length, as in a facility summary sheet, the user can click on the dialog box item fitting the report to one page wide by one page high. Alternatively, in longer reports, the user can adjust the scaling (e.g. 90 %) to ensure the report falls within the right margin, with the output displayed over one or more pages. In long, detailed reports, using the option to fit the report to one page may result in a very small font being used by the printer.

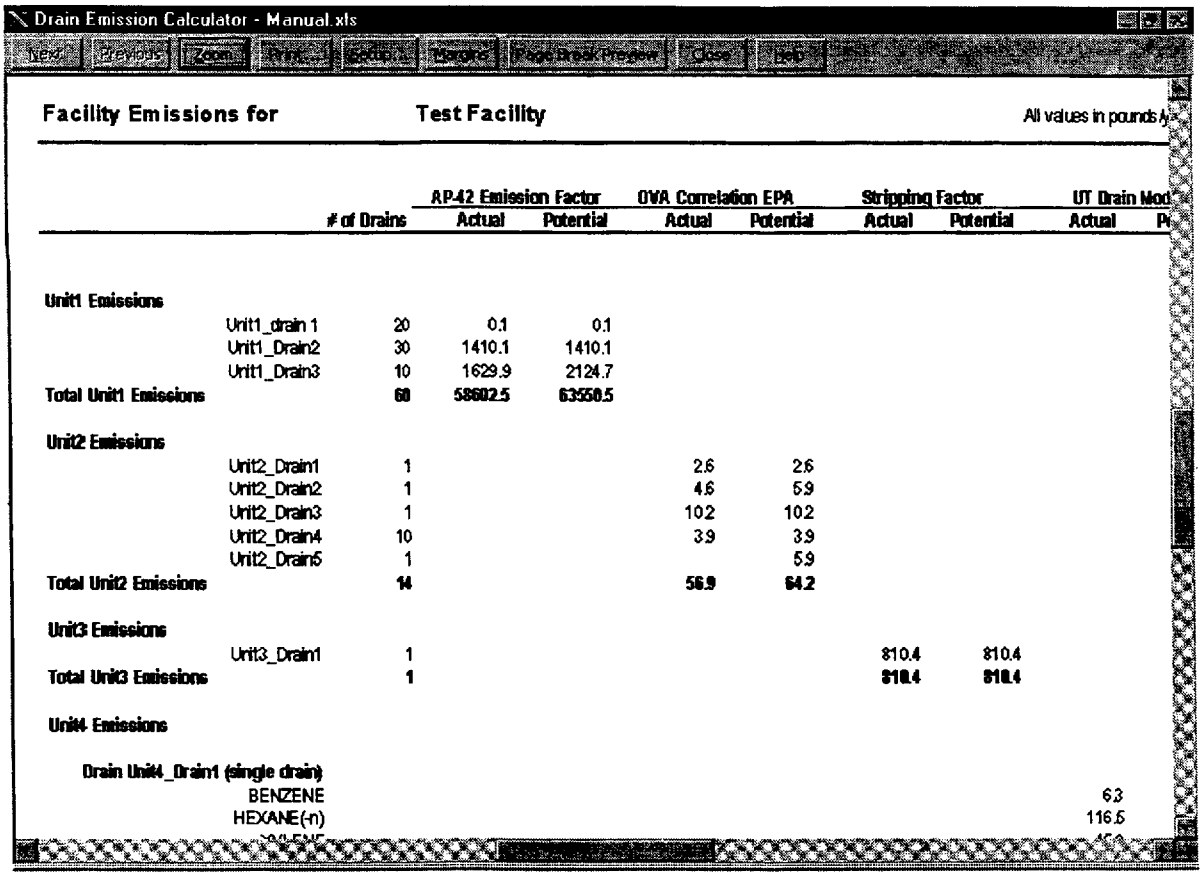


Figure 2.25 Printer Options Toolbar

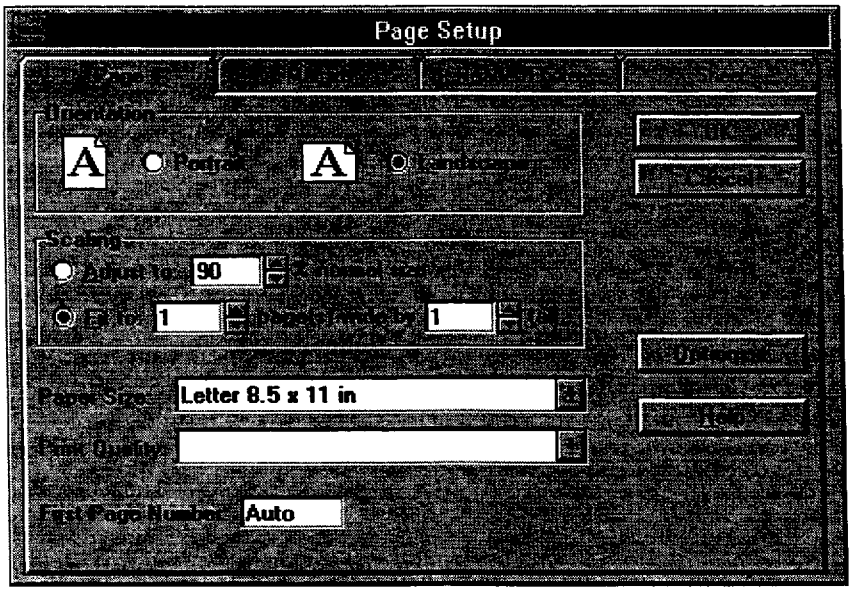


Figure 2.26 Page Set-Up Options

An example of a simple facility summary report is provided as Figure 2.27. An example of a Process Unit summary appears as Figure 2.28.

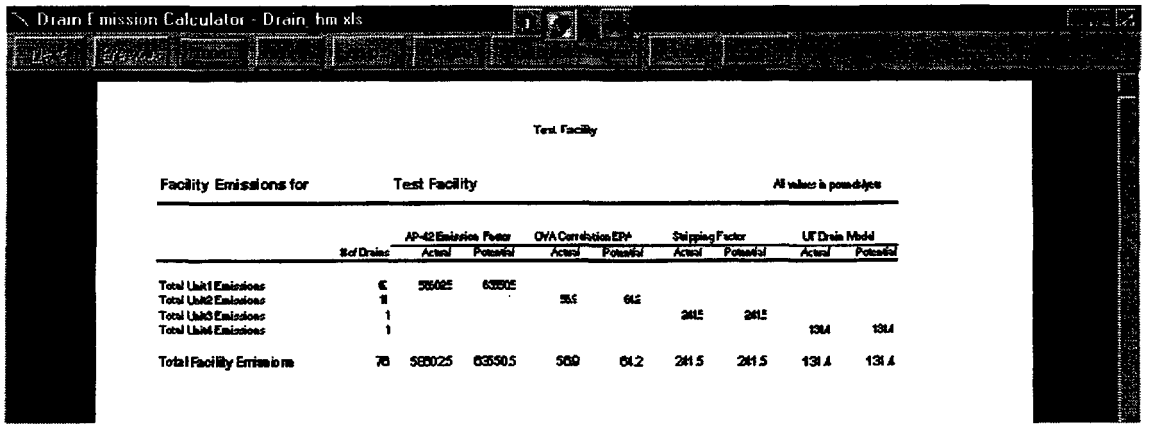


Figure 2.27 Example of Facility Emission Summary Report

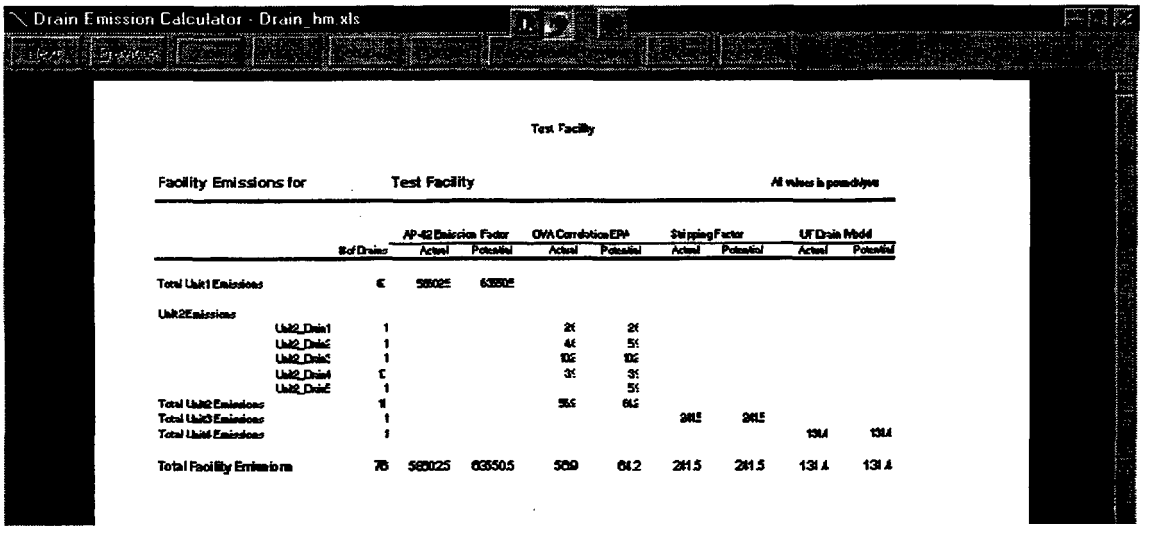


Figure 2.28 Process Unit Emission Report

The user can exit from the Report feature by clicking on the Facility Summary icon, for example, or by using another menu item under the "Facility" heading.

If detailed reports of emissions of specific organic compounds at each drain are required, the report option should not be used. Instead, the user should go to the specific drain in the UT

model, use the Print icon, set the appropriate margins with the "Set-up" button, and then print the page, as illustrated by Figure 2.29.

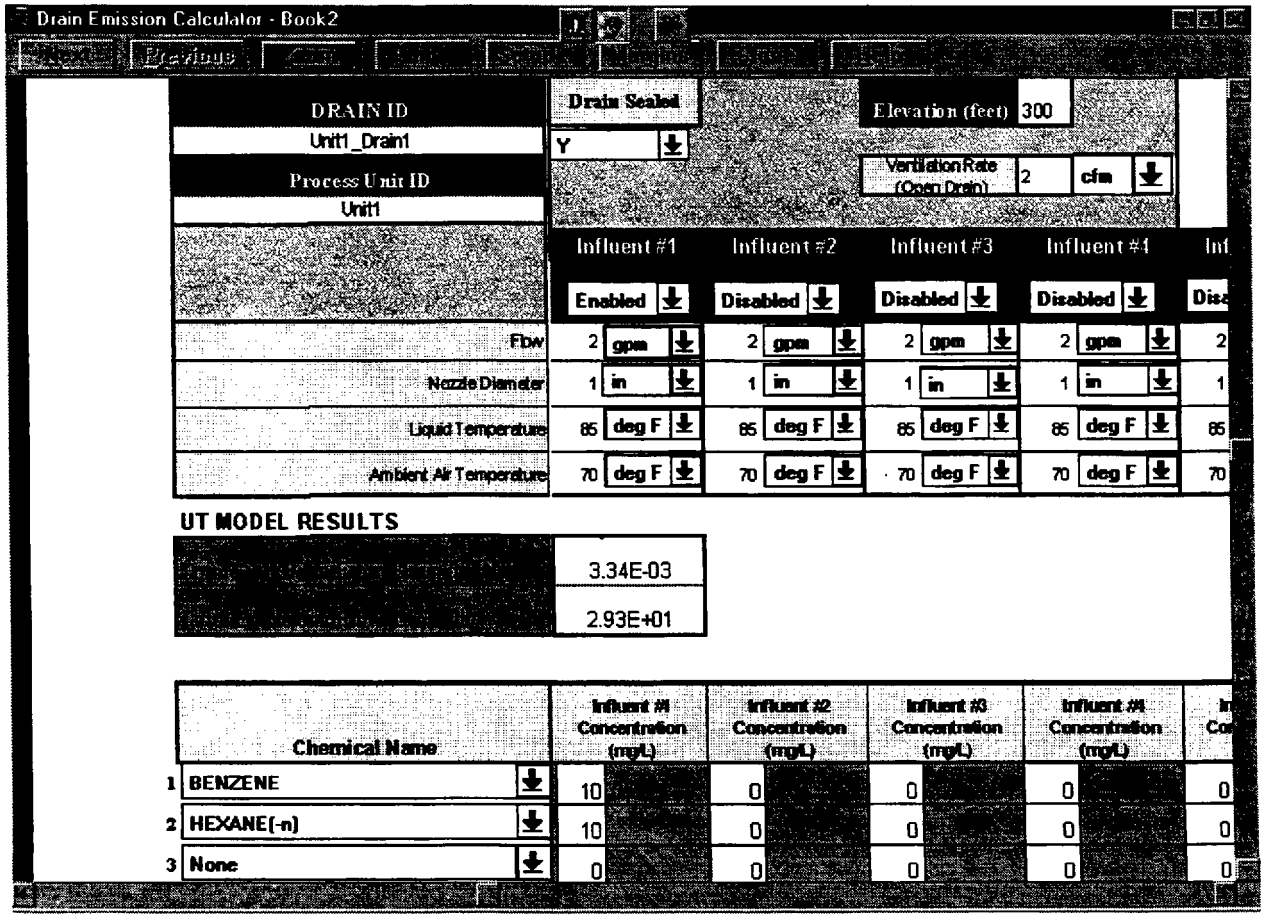


Figure 2.29 Drain Emission Summary Report

Section 3

MODEL EQUATIONS

3.1 USE OF STRIPPING EFFICIENCY FACTORS

A study initiated previously by API (Brown and Caldwell, 1998) included an investigation of emissions from a pilot-scale sealed drain. Stripping factors for specific organic compounds were calculated, expressed as a percentage of the influent mass discharged through a pipe nozzle to an open hub drain. Experimental factors included the height of the discharge from the nozzle above the plane of the drain hub, the rate of water flow, water temperature, and volatility of the target organic compounds, represented by the Henry's law coefficients of the compounds. Schematic depictions of the sealed and unsealed drains are provided in Figure 3.1.

To use this method, knowledge of the wastewater flow, temperature, and individual contaminant concentrations are required; these provide a compound mass discharged to the process drain. The Henry's law coefficient is linked to the compound database contained in another part of the workbook. Stripping efficiencies are provided for three ranges of compound volatility, based on the results of the pilot drain study. Compounds are considered of high volatility if H_c is greater than 0.72 m^3_{liq}/m^3_{gas}. Organics of moderate volatility fall in the range of H_c values between 0.13 and 0.72 m^3_{liq}/m^3_{gas}. Compounds are considered to be of low volatility if the H_c value is less than 0.13 m^3_{liq}/m^3_{gas}.

Because users may not always have concentrations of individual speciated compounds for use with this estimation procedure, compounds in the stripping efficiency model have been grouped according to their volatility as described in the paragraph above. Examples of the compounds that fall into the ranges of high, intermediate and low volatility are provided in Table 3-1.

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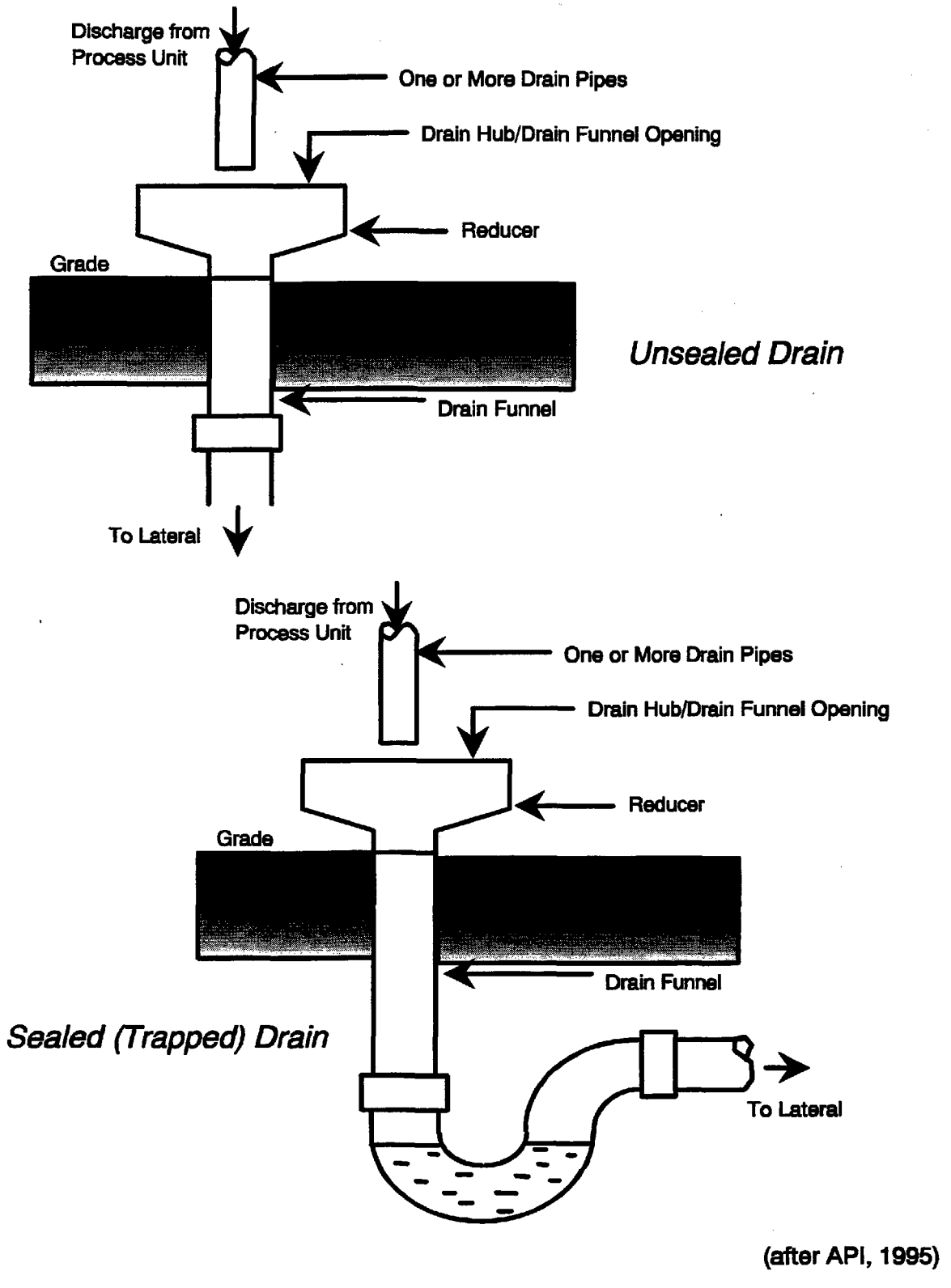

Figure 3.1 Schematic Representations of Unsealed and Sealed Drains

Table 3-1 Examples of Compound Volatility in Stripping Efficiency Model

Low Volatility	Moderate Volatility	High Volatility
Naphthalene	Benzene	Hexane
Phenol	Toluene	Cyclohexane
Styrene	Xylene	1,3-Butadiene
Mesitylene	Nonane	Butyl benzene

Concentrations of organic compounds in the discharges to the drains are most accurately determined by analytical procedures such as gas chromatography coupled to a mass spectrometer. If the concentration of a compound in the wastewater stream is not known, it may be possible to estimate a concentration by judgment of the fraction of compound mass lost during processing. Wastewater flow can be estimated relatively easily by collecting a known volume in a bucket or other container over a measured time period.

The experimental conditions of the pilot-scale tests define the wastewater temperature as low if less than or equal to 20 °C, or high if greater than 20 °C. The height of the discharge above the drain is similarly defined as low if the height is less than or equal to 4 inches, while a high drop height is defined as greater than 4 inches.

The velocity of the water, also needed in the stripping efficiency procedure, can be estimated from the calculated flow by dividing the flow in gallons per minute by the cross-sectional area of the discharge pipe in square inches. In this estimation method, the flow velocity needs to be defined as either a low or high velocity. Based on the experimental conditions of the pilot-scale study, a low velocity may be defined as less than 0.67 gpm/inch^2, while a high velocity is greater than or equal to 0.67 gpm/inch^2.

If means are not available to calculate the water velocity, a qualitative judgment can be made based on the appearance of the discharge from the nozzle. A low velocity flow has the appearance of a trickle or spray of water from the nozzle (also referred to as a disintegrated flow, while a high velocity flow has the appearance of a "glassy" column (also referred to as an intact discharge).

When the information defining the drain discharge characteristics is entered in the information panel, the model calculates the emission rate in lb/hour by multiplying the appropriate stripping efficiency factor, defined by the information entered in another part of the workbook, by the calculated mass discharged to the drain. The stripping efficiencies resulting from the experimental procedures are summarized in Tables 3-2 to 3-4 below. The factors provided in these tables generate emission rates in lb/hr when multiplied by the specified chemical concentration and liquid flow rate.

Table 3-2 Stripping Efficiency Factors for High Volatility Compounds

$H_c > 0.72\ m^3_{liq}/m^3_{gas}$			
Water Temperature (°C)	Drop Height (inches)	Mass Emission [(lb/hr)/(ppm_w·gpm)] Water Discharge Velocity (gpm/inch^2)	
		≤ 0.67	> 0.67
≤ 20	< 4	0.258×10^{-3}	0.130×10^{-3}
	≥ 4	0.298×10^{-3}	0.139×10^{-3}
> 20	< 4	0.340×10^{-3}	0.215×10^{-3}
	≥ 4	0.309×10^{-3}	0.194×10^{-3}
Inactive Drain		5.29×10^{-7} [(lb/hr)/ppm_w]	

Table 3-3 Stripping Efficiency Factors for Moderate Volatility Compounds

$0.13 \leq H_c \leq 0.72\ m^3_{liq}/m^3_{gas}$			
Water Temperature (°C)	Drop Height (inches)	Mass Emission [(lb/hr)/(ppm_w·gpm)] Water Discharge Velocity (gpm/inch^2)	
		≤ 0.67	> 0.67
≤ 20	< 4	0.189×10^{-3}	0.110×10^{-3}
	≥ 4	0.170×10^{-3}	0.0896×10^{-3}
> 20	< 4	0.279×10^{-3}	0.105×10^{-3}
	≥ 4	0.258×10^{-3}	0.139×10^{-3}
Inactive Drain		3.08×10^{-7} [(lb/hr)/ppm_w]	

Table 3-4 Stripping Efficiency Factors for Low Volatility Compounds

H_c < 0.13 m^3_{liq}/m^3_{gas}			
Water Temperature (°C)	Drop Height (inches)	Mass Emission [(lb/hr)/(ppm_w·gpm)]	
		Water Discharge Velocity ($gpm/inch^2$)	
		≤ 0.67	> 0.67
≤ 20	< 4	0.119×10^{-3}	0.0745×10^{-3}
	≥ 4	0.0158×10^{-3}	0.0783×10^{-3}
> 20	< 4	0.219×10^{-3}	0.0448×10^{-3}
	≥ 4	0.179×10^{-3}	0.0943×10^{-3}
Inactive Drain		4.40×10^{-7} [(lb/hr)/ppm_w]	

3.2 MODELING EQUATIONS FOR THE UT DRAIN MODEL

The UT model was developed from a laboratory study that investigated emissions from a single nozzle discharging to a drain. The UT model allows a user to estimate emissions from a drain with up to 6 different nozzles (influents). To allow for this extrapolation from a single nozzle, an assumption was made that the emission rate resulting from each discharge was independent of all the others. This assumption is the most conservative and is the most defensible, given the lack of knowledge of the interaction of multiple discharges on air entrainment in the drain seal.

The following section provides the derivation of the equations used in the UT drain model for both sealed (trapped) and unsealed (open) drains.

3.2.1 Sealed Drain

The concentration of a chemical in the drain trap, C_t is given by:

$$C_t = \frac{\sum_{i=1}^{n} (Q_d C_d)_i}{\sum_{i=1}^{n} (Q_{di}) + n(K_L A_s) + \gamma_t H_c \sum_{i=1}^{n} (Q_{ei})} \qquad \textbf{(Equation 3-1)}$$

where: Q_{di} = liquid flow rate from discharge pipe i (L/min)

C_{di} = concentration of target chemical in liquid discharged from pipe i (mg/L)

n = number of discharge pipes into drain (-)

$K_L A_s$ = overall mass transfer parameter associated with splashing at surface for target chemical (L/min)

H_c = Henry's law coefficient of target chemical at temperature T, (m^3_{liq}/m^3_{gas})

γ_t = degree of equilibrium for entrained gas bubbles (-)

Q_{ei} = bubble entrainment rate associated with discharge pipe i (L/min)

Many of the parameters used in this expression are themselves derived from other relationships. The derivation of these parameters follows.

The overall mass transfer rate ($K_L A_s$, L/min) associated with splashing at the water surface for a target chemical is given by:

$$K_L A_s = \frac{1}{\frac{1}{k_l A_s} + \frac{1}{k_g A_s H_c}} \qquad \textbf{(Equation 3-2)}$$

where:

$k_l A_s$ = liquid-phase mass transfer parameter associated with splashing at surface for chemical of interest (L/min)]

$k_g A_s$ = gas-phase mass transfer parameter associated with splashing at surface for target chemical (L/min)

H_c = Henry's law constant for target chemical at water temperature T_t (m^3_{liq}/m^3_{gas}).

The expression derived for the liquid-phase mass transfer parameter associated with splashing at the water surface for chemical of interest, $k_l A_s$ (L/min) is:

$$k_l A_s = 0.592 \left\{ \frac{D_{lj}}{D_{l,EB}} \right\}^{2/3} + \theta^{(T_t - 22)} \qquad \textbf{(Equation 3-3)}$$

where:

D_{lj} = liquid molecular diffusion coefficient for target chemical j at 25°C (cm^2/s)

$D_{l,EB}$ = liquid molecular diffusion coefficient for ethylbenzene at 25°C (cm^2/s)

Θ = empirical correction factor (= 1.024)

T_t = water temperature in trap (°C)

Equations 3-3 and 3-6 (below) incorporate temperature correction factors using a reference temperature (e.g. 25 °C in equation 3-3). Model users enter the actual operating water temperature. The model then accounts for the difference between the actual and reference temperatures in the emission rate calculations.

The water temperature in the trap T_t may be estimated using a heat balance of the form:

$$T_t = \frac{\sum_{i=1}^{n} (Q_d T_d)_i}{\sum_{i=1}^{n} Q_d} \qquad \textbf{(Equation 3-4)}$$

where: T_d = liquid temperature stemming from discharge pipe i (°C)

The expression for the gas-phase mass transfer parameter associated with splashing at surface for target chemical, $k_g A_s$ (L/min) is:

$$k_g A_s = 45 \{k_l A_s\} \left\{\frac{D_{l,ace}}{D_{l,j}}\right\}^{2/3} \left\{\frac{D_{g,j}}{D_{g,ace}}\right\}^{2/3} \qquad \textbf{(Equation 3-5)}$$

where: $D_{l,ace}$ = molecular diffusion coefficient for acetone in water at 25°C (cm^2/s)
$D_{g,ace}$ = molecular diffusion coefficient for acetone in air at 25°C (cm^2/s)
$D_{g,j}$ = molecular diffusion coefficient for target chemical j in air at 25°C (cm^2/s)
$D_{l,j}$ = molecular diffusion coefficient for target chemical j in water at 25°C (cm^2/s)

Henry's law coefficient is temperature dependent. The value specified in many databases is referenced to a specific temperature such as 25 °C. APIDRAIN has a built-in temperature dependence relationship for Henry's law coefficient. The relationship is given by:

$$H_c = H_{c,25} \Theta^{(T-25)} \qquad \textbf{(Equation 3-6)}$$

where: $H_{c,25}$ = Henry's law coefficient for target chemical at 25 °C (m^3_{liq}/m^3_{gas})
Θ = temperature correction factor, (-)
T = water temperature (°C)

Henry's law coefficient data for a group of 13 chlorinated organic compounds (Gossett, 1987) were examined to estimate the applicability of this relationship. A modified Van't Hoff relationship was linearly regressed with all of the Gossett data to estimate the value of Θ. The results of the regression provided an estimated value for Θ of 1.044 with 95 % confidence limits of 0.0035. From the narrow confidence limits, it is apparent this relationship can reasonably predict the temperature influence on Henry's law coefficient.

The validity of the relationship beyond the lower molecular weight chlorinated organic compounds investigated by Gossett (1987) was assessed by comparing Henry's law coefficients measured by Ashworth *et al.* (1988) for an additional 23 organic compounds of varying volatility. Henry's law coefficient (H_c) values were estimated by the relationship based on Gossett's data, and by a more traditional chemical engineering approach using Antoine's coefficients (retrieved from AP-42). The analysis showed that the errors computed for the relationship derived from Gossett's data, and for the Antoine relationship, relative to the measured values, were 16.4 % and 17.2 %, respectively. The spreadsheet analysis is provided in Appendix A. Thus, the relationship based on Gossett's data, proposed for APIDRAIN, was determined to be as accurate as the method using Antoine's coefficients. Because the relationship derived from Gossett's data is much simpler to use and required fewer data inputs, it was incorporated into the APIDRAIN model.

The liquid discharge velocity V_{oi} (m/s) for discharge pipe *i* is expressed as:

$$V_{oi} = \frac{4Q_{di}}{d_{oi}^2 \pi}(1m^3/1000L)(1\min/60s) \qquad \textbf{(Equation 3-7)}$$

where: d_{oi} = pipe diameter for discharge pipe i (m)

Q_{di} = liquid discharge flow rate for discharge pipe i (L/min)

For each discharge pipe i, the bubble entrainment rate Q_{ei} (L/min) in APIDRAIN is dependent on the discharge pipe velocity, V_{oi}. The different values of V_{oi} are used to differentiate between discharges that are intact or disintegrated upon leaving the nozzle. If V_{oi} is less than 0.38 m/s, then the discharge is modeled as disintegrated. Otherwise, the discharge is modeled as intact.

For a discharge pipe velocity V_{oi} < 0.38 m/s (disintegrated flow), the bubble entrainment rate is given by:

$$Q_{ei} = 135 V_{oi}^{0.63} d_{oi}$$ **(Equation 3-8)**

where: V_{oi} = liquid discharge velocity for discharge pipe i (m/s)

Otherwise, for intact flow,

$$Q_{ei} = 1210 V_{oi}^{5.09} d_{oi}$$ **(Equation 3-9)**

The degree of equilibrium for entrained bubbles γ_t (dimensionless) is needed in the expression for the concentration of the target chemical in the drain trap. The degree of equilibrium is also dependent on the liquid discharge velocity for a nozzle. The model considers two cases:

- all discharges have velocities greater than 0.38 m/s (all are intact);
- any one discharge is less than 0.38 m/s (assume all disintegrated).

For the first case, where all V_{oi} > 0.38 m/s, the degree of equilibrium of the entrained air bubbles γ_t, is given by:

$$\gamma_t = 1 - 0.956(2.718^{\frac{-0.123}{\Sigma Q_{ei} H_c}})$$ **(Equation 3-10)**

For the second case, where any one V_{oi} < 0.38 m/s,

$$\gamma_t = 1 - 0.979(2.718^{\frac{-0.309}{\Sigma Q_{ei} H_c}})$$ **(Equation 3-11)**

The stripping efficiency for a sealed drain η_T (dimensionless) is defined by:

$$\eta_T = 1 - \frac{C_t \sum_{i=1}^{n} Q_{di}}{\sum_{i=1}^{n} (Q_d C_d)_i} \qquad \textbf{(Equation 3-12)}$$

Now finally, the emission rate from the water in the drain seal, E_t (mg/min)

$$E_T = \eta_T \sum_{i=1}^{n} (Q_d C_d)_i \qquad \textbf{(Equation 3-13)}$$

The model stores η_T and E_T for each drain. The emission rate E_T may be converted from units of mg/min to lb/hr by the following expression:

$$E_T(lb/hr) = E_T(mg/min)(60min/hr)(2.2054lb/kg)(10^{-6} kg/mg) \qquad \textbf{(Equation 3-14)}$$

The sum of E_T values for all drains in a process unit is the total emission rate for the process unit. Emission rates for all process units are summed to provide the total facility emission rate.

3.2.2 Unsealed (Open) Drain

In an unsealed drain, emissions may result from wastewater flowing through the channel that connects the drains. The concentration of a target chemical in the connecting channel C_c (mg/L) may be estimated from the expression:

$$C_c = \frac{\sum_{i=1}^{n}(Q_d C_d)_i}{\left\{ \sum_{i=1}^{n} Q_{di} + \sum_{i=1}^{n}(K_L A_c)_i - \frac{\left(\sum_{i=1}^{n}(K_L A_c)_i\right)^2}{Q_v H_c + \sum_{i=1}^{n}(K_L A_c)_i} \right\}} \qquad \textbf{(Equation 3-15)}$$

where: Q_v = ventilation rate for drains (L/min)

$K_L A_c$ = overall mass transfer parameter in channel for discharge from pipe I (L/min)

and all other parameters are as previously defined.

The overall mass transfer parameter in the channel for a discharge from pipe i, $(K_L A_c)_i$ (L/min) is given by:

$$(K_L A_c)_i = \frac{1}{\frac{1}{(k_l A_c)_i} + \frac{1}{(k_g A_c)_i H_c}} \qquad \textbf{(Equation 3-16)}$$

where: $(k_l A_c)_i$ = liquid mass transfer parameter in channel for discharge from pipe i (L/min)

$(k_g A_c)_i$ = gas mass transfer parameter in channel for discharge from pipe i (L/min)

As with the sealed drain, the liquid phase mass transfer parameters are dependent on the velocity of the discharge V_{oi} from any nozzle above the drain. For the unsealed drain, the critical velocity has been experimentally determined as 0.50 m/s. For a velocity $V_{oi} < 0.50$ m/s, the liquid-phase mass transfer parameter $(k_l A_c)_i$ (L/min) in the channel for a discharge from pipe i is:

$$(k_l A_c)_i = \{-1350(V_{oi}-0.249)^2 + 149.5\}\, Sc_l^{-1/2} \qquad \textbf{(Equation 3-17)}$$

where: Sc_l = liquid-phase Schmidt number = ν/D_{lj}

ν = kinematic viscosity of water at temperature T_c (cm^2/s).

D_{lj} = liquid molecular diffusion coefficient for target chemical j at T_c (cm^2/s)

The temperature of the liquid in the channel T_c (°C) can be estimated from a heat balance on discharges to the channel, as per

$$T_c = \frac{\sum_{i=1}^{n} (Q_d T_d)_i}{\sum_{i=1}^{n} Q_d} \qquad \textbf{(Equation 3-18)}$$

For a discharge velocity V_{oi} > 0.50 m/s, the liquid-phase mass transfer parameter $(k_l A_c)_i$ (L/min) in the channel for a discharge from pipe i is:

$$(k_l A_c)_i = 64 * Sc_l^{-1/2} \qquad \textbf{(Equation 3-19)}$$

The gas-phase mass transfer parameter may be expressed as a function of the liquid-phase mass transfer parameter according to the following relationship:

$$(k_g A_c)_i = 17.2 * (k_l A_c)_i \qquad \textbf{(Equation 3-20)}$$

The stripping efficiency η_c, for an unsealed drain is:

$$\eta_c = 1 - \frac{c_c \sum_{i=1}^{n} Q_{d,i}}{\sum_{i=1}^{n} (Q_d C_d)_i} \qquad \textbf{(Equation 3-21)}$$

where: η_c =stripping efficiency of unsealed drain, (-)

The emission rate E_c (mg/min) from the channel beneath the unsealed drain is:

$$E_c = \eta_c \sum_{i=1}^{n} (Q_d C_d)_i \qquad \textbf{(Equation 3-22)}$$

As with the sealed drain, the emission rate can be converted from units of mg/min to lb/hr using equation 3-14.

3.3 TEMPERATURE-CORRECTED FACTORS

APIDRAIN incorporates a number of mathematical equations in the mechanistic mass transfer drain model that are temperature-dependent. The modeled parameters that vary with temperature are noted in the following section, with the references to the source of the relationships.

3.3.1 Diffusion Coefficients

3.3.1.1 Liquid Phase Diffusion Coefficient.

Liquid and gas phase diffusion coefficients (also called diffusivities) are used in the estimation of liquid and gas phase Schmidt numbers, which themselves are incorporated in liquid and gas phase mass transfer coefficients.

The equation for the liquid phase diffusion coefficient of an organic compound is (Wilke and Chang, 1955, from Perry and Chilton, 1973):

$$D_l = 7.4x10^{-6}\left(\frac{T(XM)^{0.5}}{\mu_w V_b^{0.6}}\right) \qquad \textbf{(Equation 3-23)}$$

where:
- D_l = liquid phase diffusion coefficient (cm^2/s)
- T = temperature (°K)
- μ_w = viscosity of water (g/cm-s)
- X = association number for water [value =2.6]
- M = molecular weight of solvent [water = 18.0 g/g-mole]
- V_b = molar volume of solute (L/g-mole)

In this expression and others following, the molar volume of a chemical compound has been approximated by dividing the molecular weight of the chemical compound in solution by the density at a reference temperature such as 25 °C. More rigorously, the molar volume is defined as the molecular weight divided by the density at the boiling point of the compound. Because

the densities of organic compounds at their boiling points may not be available in all cases, diffusion coefficients of selected organic compounds were calculated with molar volumes based on a reference temperature. These calculated coefficients were compared to diffusion coefficients calculated with molar volumes tabulated in the technical literature. The mean value of deviations between the coefficients using the approximated molar volume and coefficients using the published molar volumes was determined to be 5.1 % for 21 compounds, with a range of 1.1 % to 10.1 %. The comparison of calculated liquid phase diffusion coefficients is provided in a table in Appendix B. The mean deviation was deemed sufficiently small that the approximation of the molar volume could be used in the calculation of the liquid phase diffusion coefficient.

3.3.1.2 Gas Phase Diffusion Coefficient

The equation defining the gas phase diffusion coefficient in APIDRAIN is (Gilliland, 1934; from Perry et al. 1963):

$$D_g = 0.0043 \frac{T^{3/2}}{P(V_1^{1/3} + V_2^{1/3})^2} \sqrt{\frac{1}{M_1} + \frac{1}{M_2}} \qquad \textbf{(Equation 3-24)}$$

where:

D_g = gas phase diffusion coefficient (cm^2/s)

T = temperature (°K)

P = absolute pressure (atm)

V_1 , V_2 = molar volumes of components 1 and 2 (mL/g-mole)

M_1, M_2 = molecular weights of components 1 and 2 (g/g-mole)

As with the liquid phase diffusion coefficient, the effect of approximating molar volume using a reference temperature rather than the boiling point was determined with the gas phase diffusion coefficient equation. Reference temperatures were 20 °C. The mean value of deviations between the gas phase diffusion coefficients using the approximated molar volume and coefficients using the published molar volumes was determined to be 3.3 % for 21 compounds, with a range of 0.7 % to 6.6 %. The mean deviation was deemed sufficiently small that the approximation of the molar volume could be used in the calculation of the gas phase diffusion

coefficient. The comparison of calculated gas phase diffusion coefficients also is provided in Appendix B.

3.3.2 Viscosities

3.3.2.1 Viscosity of Water

The viscosity of water is a parameter used in expressions for the liquid phase diffusion coefficient and liquid phase Schmidt number. The temperature-dependent relationship for the viscosity of water in APIDRAIN is (Bingham, 1922, from Perry et al., 1963):

$$\frac{1}{\mu_w} = 2.1482\left[(t-8.435)+\sqrt{8078.4+(t-8.435)^2}\right]-120 \qquad \textbf{(Equation 3-25)}$$

where: μ_w = viscosity of water (centipoise)

t = temperature (°C)

3.3.2.2 Viscosity of Air

The viscosity of air is used in the calculation of the gas phase Schmidt number. The relationship between air temperature and viscosity is expressed by the relationship (Arnold, 1933, from Perry and Chilton, 1973):

$$\mu_g = \frac{0.0027\,M^{0.5}T^{1.5}}{V_b^{2/3}(T+1.47\,T_b)} \qquad \textbf{(Equation 3-26)}$$

where: μ_g = gas phase viscosity (centipoise)

M = molecular weight of air (g/g-mole)

T = ambient temperature (°K)

T_b = boiling point of air (°K)

V_b = molar volume of air (mL/g-mole)

3.3.3 Phase Densities

3.3.3.1 Density of Water

The density of water, used in the liquid phase Schmidt number, displays an anomalous behavior, having the maximum density at approximately 4 °C. No mathematical expression of the temperature dependence of water was noted in the technical literature. An approximation of the relationship was prepared using a spreadsheet optimizing routine which minimized the sum of the squared differences between tabulated literature values of water density at different temperatures, with predicted values of water density.

The relationship derived was:

$$d_w = 1 - 2.134x10^{-5} T_w^{1.639} \qquad \textbf{(Equation 3-27)}$$

where: d_w = density of water (g/mL)
T_w = water temperature (°C)

This relationship does not account for the decrease in water density between 0 and 4 °C. The probability of dealing with process wastewaters in this temperature range, and the error that this relationship would instill in the density estimation, were considered negligible. The relationship is depicted in Figure 3.2.

3.3.3.2 Density of Air

The density of air is used in the estimation of the gas phase Schmidt number. The relationship used in APIDRAIN is (CRC, 1968):

$$d_a = \frac{0.001293P}{(1+0.00367T)76} \qquad \textbf{(Equation 3-28)}$$

where: d_a = density of air (g/mL)
P = ambient atmospheric pressure (cm of mercury)
T = ambient air temperature (°C)

Ambient atmospheric pressure is estimated in the model by the relationship (ASCE, 1992):

$$P_{el} = 14.7*(1 - 3.5*10^{-5}*h) \qquad \textbf{(Equation 3-29)}$$

where: P_{el} = atmospheric pressure (psia) at elevation h (ft) above mean sea level

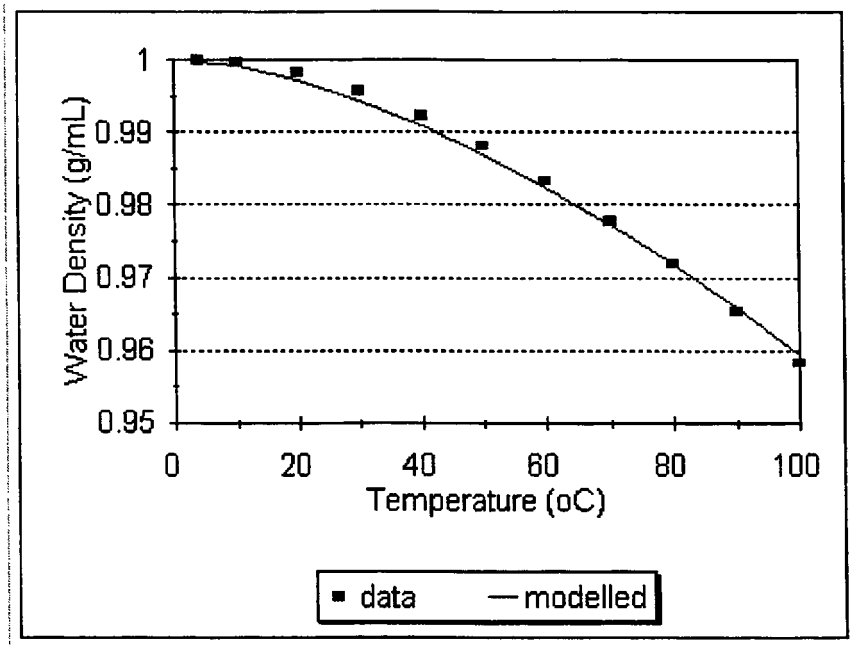

Figure 3.2 Modeled Density of Water by Non-Linear Least Squares Regression Technique

Section 4

MODEL "WORK-AROUNDS" FOR Excel™ 97

4.1 *Warning Display for Che_Namelist Formula Reference*

At start-up in Excel™ 97 (not in Excel™ Version 5), a warning dialog box may appear as shown below in Figure 4.1. This warning appears because of the macros used in the model. For the model to operate correctly, click "Yes" to the prompt in the dialog box any time it should appear at start-up of the model. Operation of the model is unaffected by this display.

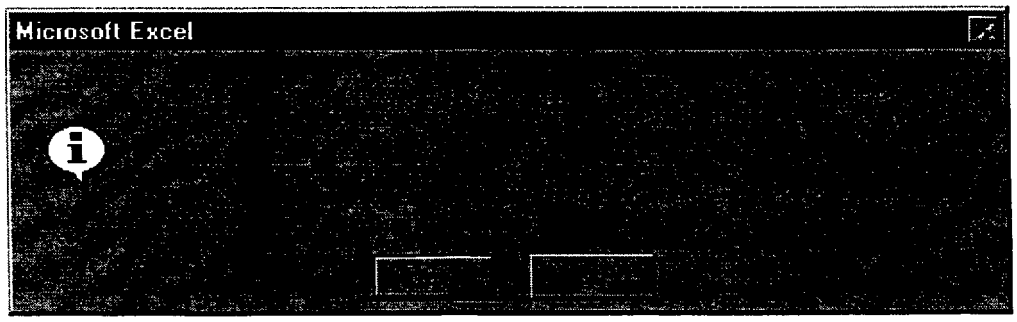

Figure 4.1 Dialog Box with Che_Namelist Formula Reference

4.2 *Initiation of Stripping Efficiency Model*

Use of the APIDRAIN model in Excel™ 97 may result in an improper display when the stripping efficiency procedure is used for the first time. The improper display occurs when the macro in this procedure defines cell references. A display as shown in Figure 4.2 results. Note that this improper display occurs only with Excel™ 97, and not with Excel™ Version 5. If this problem occurs, the model needs to be saved and then re-opened.

After creating and editing a selected drain in Excel™ 97 using the stripping efficiency procedure, the steps to eliminate the "#NAME" display are:

- From the menu, click on *File/Save Facility as;* a dialog box will appear on the screen prompting the user to provide a file name.
- After providing a file name (e.g., facility01.xls), click on the "save" button.

Previous page is blank.

- On the menu bar, click on *File/Open Facility.* A dialog box will appear on the screen listing the file name just saved earlier.
- Click on the file name and then the "Open" button. The facility summary worksheet will appear on the screen.
- On the menu bar, click on *Facility/Edit Selected Process Unit.* The process unit summary worksheet will again appear on the screen.
- Click on the menu item *Process Unit/Edit Selected Drain.*
- The drain worksheet will now appear on the screen as shown in Figure 4.3.

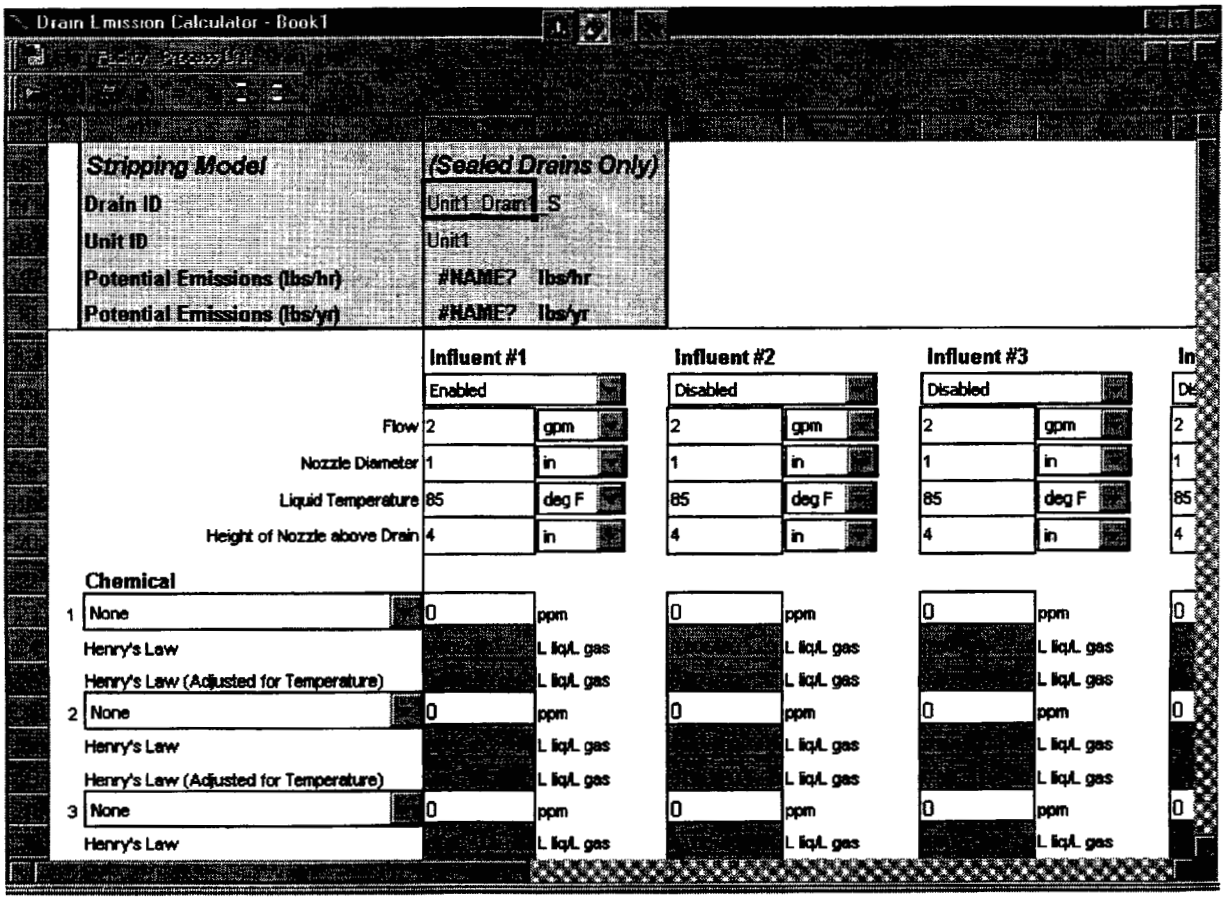

Figure 4.2 Stripping Efficiency Model Worksheet with "#NAME? Notation

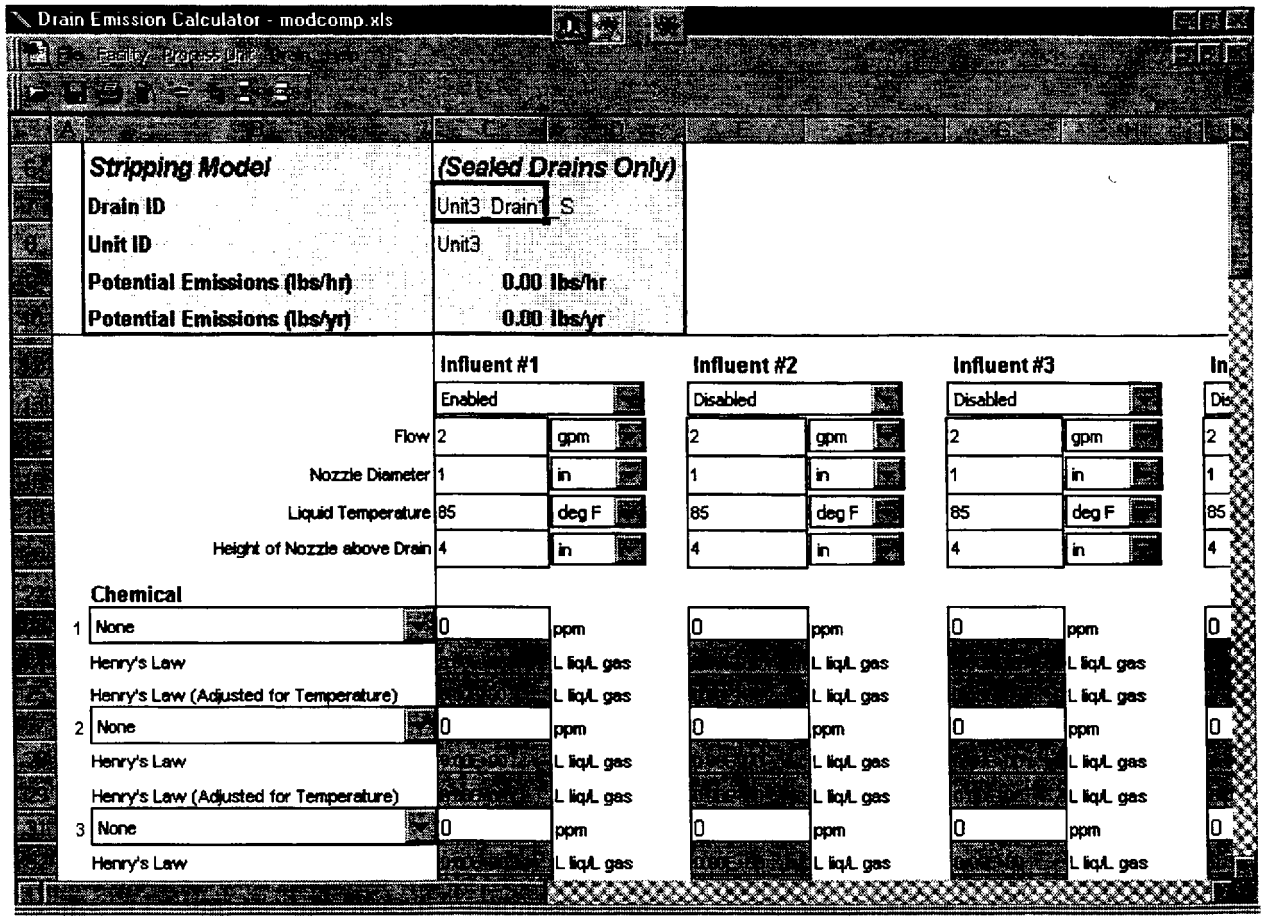

Figure 4.3 Stripping Efficiency Model Worksheet After Saving Procedure

Section 5

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Appendix A

COMPARISON OF METHODS FOR CALCULATING HENRY'S LAW COEFFICIENTS

Table A-1 Comparison of Henry's Law Coefficient Estimation Methods with Measured Data

COMPOUND	Antoine's Coefficients			Temp. (°C)	Measured Henry's Coefficient m^3_{liq}/m^3_{gas}	Error in Calculated Henry's Coefficient		Absolute Values of Errors w/o Zeros	
	A	B	C			Antoine	Gossett *et al.*	Antoine	Gossett *et al.*
Gossett (1987)									
Tetrachloroethylene	6.98	1386.92	217.53	9.6	0.00682	7.4%	34.9%	7.4%	34.9%
	6.98	1386.92	217.53	17.5	0.0117	0.5%	10.5%	0.5%	10.5%
	6.98	1386.92	217.53	24.8	0.0177	0.0%	0.0%		
	6.98	1386.92	217.53	34.6	0.0282	4.8%	-4.3%	4.8%	4.3%
Trichloroethylene	6.518	1018.6	192.7	9.6	0.00378	12.7%	31.7%	12.7%	31.7%
	6.518	1018.6	192.7	17.5	0.00632	4.2%	10.7%	4.2%	10.7%
	6.518	1018.6	192.7	24.8	0.00958	0.0%	0.0%		
	6.518	1018.6	192.7	34.6	0.0149	2.4%	1.5%	2.4%	1.5%
1,1,1-Trichloroethane	8.643	2136.6	302.8	9.6	0.00761	8.8%	17.5%	8.8%	17.5%
	8.643	2136.6	302.8	17.5	0.012	1.8%	4.7%	1.8%	4.7%
	8.643	2136.6	302.8	24.8	0.0172	0.0%	0.0%		
	8.643	2136.6	302.8	34.6	0.0249	6.8%	5.3%	6.8%	5.3%
Chloroethane	6.986	1030.01	238.61	10.3	0.00651	0.9%	-8.7%	0.9%	8.7%
	6.986	1030.01	238.61	17.5	0.00846	1.5%	-4.2%	1.5%	4.2%
	6.986	1030.01	238.61	24.8	0.0111	0.0%	0.0%		
	6.986	1030.01	238.61	34.6	0.0155	-1.1%	9.2%	1.1%	9.2%

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Table A1. Continued

Carbon tetrachloride	6.934	1242.43	230	10	0.0132	15.2%	21.8%	15.2%	21.8%
	6.934	1242.43	230	17.5	0.0211	3.5%	5.2%	3.5%	5.2%
	6.934	1242.43	230	24.8	0.0304	0.0%	0.0%		
	6.934	1242.43	230	34.6	0.046	0.2%	0.8%	0.2%	0.8%
Chloroform	6.493	929.44	196.03	9.6	0.0015	19.5%	27.2%	19.5%	27.2%
	6.493	929.44	196.03	17.5	0.00246	7.1%	8.9%	7.1%	8.9%
	6.493	929.44	196.03	24.8	0.00367	0.0%	0.0%		
	6.493	929.44	196.03	34.6	0.00563	-1.6%	-0.6%	1.6%	0.6%
Dichloromethane	7.409	1325.9	252.6	9.6	0.00115	0.6%	-1.0%	0.6%	1.0%
	7.409	1325.9	252.6	17.5	0.00131	24.2%	22.1%	24.2%	22.1%
	7.409	1325.9	252.6	24.8	0.00219	0.0%	0.0%		
	7.409	1325.9	252.6	34.6	0.00326	-2.2%	2.4%	2.2%	2.4%
Chloromethane	7.093	948.58	249.34	10.3	0.00391	44.6%	20.8%	44.6%	20.8%
	7.093	948.58	249.34	17.5	0.00584	21.4%	10.3%	21.4%	10.3%
	7.093	948.58	249.34	24.8	0.00882	0.0%	0.0%		
	7.093	948.58	249.34	34.6	0.0124	-6.4%	8.5%	6.4%	8.5%

Table A1. Continued

Ashworth *et al.* (1988)									
n-Hexane	6.876	1171.17	224.41	10	0.238	61.5%	69.2%	61.5%	69.2%
	6.876	1171.17	224.41	15	0.413	18.4%	20.9%	18.4%	20.9%
	6.876	1171.17	224.41	20	0.883	-30.3%	-29.9%	30.3%	29.9%
	6.876	1171.17	224.41	25	0.768	0.0%	0.0%		
	6.876	1171.17	224.41	30	1.56	-39.1%	-38.9%	39.1%	38.9%
Cyclohexane	6.841	1201.53	222.65	10	0.103	-16.4%	-9.9%	16.4%	9.9%
	6.841	1201.53	222.65	15	0.126	-12.2%	-8.7%	12.2%	8.7%
	6.841	1201.53	222.65	20	0.14	0.4%	1.9%	0.4%	1.9%
	6.841	1201.53	222.65	25	0.177	0.0%	0.0%		
	6.841	1201.53	222.65	30	0.223	-1.0%	-1.6%	1.0%	1.6%
Chlorobenzene	6.978	1431.05	217.55	10	0.00244	-39.7%	-22.7%	39.7%	22.7%
	6.978	1431.05	217.55	15	0.00281	-28.6%	-16.7%	28.6%	16.7%
	6.978	1431.05	217.55	20	0.00341	-20.7%	-14.9%	20.7%	14.9%
	6.978	1431.05	217.55	25	0.0036	0.0%	0.0%		
	6.978	1431.05	217.55	30	0.00473	0.1%	-5.6%	0.1%	5.6%
o-Xylene	6.998	1474.68	213.69	10	0.00285	-34.2%	-10.4%	34.2%	10.4%
	6.998	1474.68	213.69	15	0.00361	-27.6%	-12.3%	27.6%	12.3%
	6.998	1474.68	213.69	20	0.00474	-24.2%	-17.2%	24.2%	17.2%
	6.998	1474.68	213.69	25	0.00487	0.0%	0.0%		
	6.998	1474.68	213.69	30	0.00626	4.2%	-3.5%	4.2%	3.5%

Table A1. Continued

m-Xylene	7.009	1426.27	215.11	10	0.00411	-27.2%	-5.1%	27.2%	5.1%
	7.009	1426.27	215.11	15	0.00496	-17.2%	-2.5%	17.2%	2.5%
	7.009	1426.27	215.11	20	0.00598	-7.0%	0.3%	7.0%	0.3%
	7.009	1426.27	215.11	25	0.00744	0.0%	0.0%		
	7.009	1426.27	215.11	30	0.00887	10.9%	4.0%	10.9%	4.0%
Ethylbenzene	6.975	1424.26	213.21	10	0.00326	-4.2%	26.7%	4.2%	26.7%
	6.975	1424.26	213.21	15	0.00451	-4.4%	13.6%	4.4%	13.6%
	6.975	1424.26	213.21	20	0.00601	-2.4%	5.7%	2.4%	5.7%
	6.975	1424.26	213.21	25	0.00788	0.0%	0.0%		
	6.975	1424.26	213.21	30	0.0105	-0.4%	-6.9%	0.4%	6.9%
Toluene	6.954	1344.8	219.48	10	0.00381	-26.4%	-11.7%	26.4%	11.7%
	6.954	1344.8	219.48	15	0.00492	-24.0%	-15.2%	24.0%	15.2%
	6.954	1344.8	219.48	20	0.00555	-11.2%	-6.7%	11.2%	6.7%
	6.954	1344.8	219.48	25	0.00642	0.0%	0.0%		
	6.954	1344.8	219.48	30	0.00808	2.4%	-1.5%	2.4%	1.5%
Benzene	6.905	1211.03	220.79	10	0.0033	-23.5%	-16.1%	23.5%	16.1%
	6.905	1211.03	220.79	15	0.00388	-15.9%	-11.5%	15.9%	11.5%
	6.905	1211.03	220.79	20	0.00452	-7.7%	-5.8%	7.7%	5.8%
	6.905	1211.03	220.79	25	0.00528	0.0%	0.0%		
	6.905	1211.03	220.79	30	0.0072	-8.1%	-9.0%	8.1%	9.0%

Table A1. Continued

1,2-Dichloroethane	7.025	1272.3	222.9	10	0.00117	-43.7%	-36.8%	43.7%	36.8%
	7.025	1272.3	222.9	15	0.0013	-34.0%	-29.5%	34.0%	29.5%
	7.025	1272.3	222.9	20	0.00147	-24.8%	-22.7%	24.8%	22.7%
	7.025	1272.3	222.9	25	0.00141	0.0%	0.0%		
	7.025	1272.3	222.9	30	0.00174	2.4%	0.5%	2.4%	0.5%
1,1,1-Trichloroethane	8.643	2136.6	302.8	10	0.00965	-12.2%	-5.5%	12.2%	5.5%
	8.643	2136.6	302.8	15	0.0115	-5.6%	-1.6%	5.6%	1.6%
	8.643	2136.6	302.8	20	0.0146	-5.5%	-3.9%	5.5%	3.9%
	8.643	2136.6	302.8	25	0.0174	0.0%	0.0%		
	8.643	2136.6	302.8	30	0.0211	3.3%	2.3%	3.3%	2.3%
1,1,2-Trichloroethane	6.951	1314.41	209.2	10	0.00039	-3.6%	22.3%	3.6%	22.3%
	6.951	1314.41	209.2	15	0.00063	-18.8%	-6.1%	18.8%	6.1%
	6.951	1314.41	209.2	20	0.00074	-7.2%	-0.8%	7.2%	0.8%
	6.951	1314.41	209.2	25	0.00091	0.0%	0.0%		
	6.951	1314.41	209.2	30	0.00133	-10.4%	-15.1%	10.4%	15.1%
Tetrachloroethylene	6.98	1386.92	217.53	10	0.00846	-15.2%	6.0%	15.2%	6.0%
	6.98	1386.92	217.53	15	0.0111	-12.6%	0.2%	12.6%	0.2%
	6.98	1386.92	217.53	20	0.0141	-8.1%	-2.2%	8.1%	2.2%
	6.98	1386.92	217.53	25	0.0171	0.0%	0.0%		
	6.98	1386.92	217.53	30	0.0245	-8.9%	-13.4%	8.9%	13.4%

Table A1. Continued

Trichloroethylene	6.518	1018.6	192.7	10	0.00538	-14.6%	-0.6%	14.6%	0.6%
	6.518	1018.6	192.7	15	0.00667	-9.0%	-0.6%	9.0%	0.6%
	6.518	1018.6	192.7	20	0.00842	-6.0%	-2.3%	6.0%	2.3%
	6.518	1018.6	192.7	25	0.0102	0.0%	0.0%		
	6.518	1018.6	192.7	30	0.0128	1.5%	-1.2%	1.5%	1.2%
Chloroethane	6.986	1030.01	238.61	10	0.00759	-7.4%	-16.4%	7.4%	16.4%
	6.986	1030.01	238.61	15	0.00958	-11.4%	-17.9%	11.4%	17.9%
	6.986	1030.01	238.61	20	0.011	-7.6%	-11.3%	7.6%	11.3%
	6.986	1030.01	238.61	25	0.0121	0.0%	0.0%		
	6.986	1030.01	238.61	30	0.0143	0.0%	4.9%	0.0%	4.9%
Carbon tetrachloride	6.934	1242.43	230	10	0.0148	-1.1%	4.5%	1.1%	4.5%
	6.934	1242.43	230	15	0.0191	-2.3%	0.4%	2.3%	0.4%
	6.934	1242.43	230	20	0.0232	1.6%	2.5%	1.6%	2.5%
	6.934	1242.43	230	25	0.0295	0.0%	0.0%		
	6.934	1242.43	230	30	0.0378	-3.2%	-3.2%	3.2%	3.2%
Methylene chloride	7.409	1325.9	252.6	10	0.0014	12.8%	10.8%	12.8%	10.8%
	7.409	1325.9	252.6	15	0.00169	16.1%	13.9%	16.1%	13.9%
	7.409	1325.9	252.6	20	0.00244	-0.8%	-2.2%	0.8%	2.2%
	7.409	1325.9	252.6	25	0.00296	0.0%	0.0%		
	7.409	1325.9	252.6	30	0.00361	-0.4%	1.7%	0.4%	1.7%

Table A1. Continued

Chloroform	6.493	929.44	196.03	10	0.00172	21.0%	28.3%	21.0%	28.3%
	6.493	929.44	196.03	15	0.00233	14.2%	17.5%	14.2%	17.5%
	6.493	929.44	196.03	20	0.00332	1.3%	2.2%	1.3%	2.2%
	6.493	929.44	196.03	25	0.00421	0.0%	0.0%		
	6.493	929.44	196.03	30	0.00554	-5.9%	-5.8%	5.9%	5.8%
1,1,2,2-Tetrachloroethane	6.631	1228.1	179.9	10	0.00033	-74.5%	-60.3%	74.5%	60.3%
	6.631	1228.1	179.9	15	0.0002	-38.4%	-18.7%	38.4%	18.7%
	6.631	1228.1	179.9	20	0.00073	-75.8%	-72.4%	75.8%	72.4%
	6.631	1228.1	179.9	25	0.00025	0.0%	0.0%		
	6.631	1228.1	179.9	30	0.0007	-50.4%	-55.7%	50.4%	55.7%
1,2-Dichloropropane	6.98	1380.1	222.8	10	0.00122	28.1%	53.4%	28.1%	53.4%
	6.98	1380.1	222.8	15	0.00126	65.2%	84.2%	65.2%	84.2%
	6.98	1380.1	222.8	20	0.0019	44.3%	51.5%	44.3%	51.5%
	6.98	1380.1	222.8	25	0.00357	0.0%	0.0%		
	6.98	1380.1	222.8	30	0.00286	60.9%	54.8%	60.9%	54.8%
1,1,2-Trichlorotrifluoroethane	6.88	1099.9	227.5	10	0.154	9.9%	8.6%	9.9%	8.6%
	6.88	1099.9	227.5	15	0.215	-1.9%	-3.5%	1.9%	3.5%
	6.88	1099.9	227.5	20	0.245	6.3%	5.0%	6.3%	5.0%
	6.88	1099.9	227.5	25	0.319	0.0%	0.0%		
	6.88	1099.9	227.5	30	0.321	20.7%	23.3%	20.7%	23.3%

Table A1. Continued

Methyl ethyl ketone	6.9742	1209.6	216	10	0.00028	-78.4%	-75.7%	78.4%	75.7%
	6.9742	1209.6	216	15	0.00039	-79.8%	-78.3%	79.8%	78.3%
	6.9742	1209.6	216	20	0.00019	-46.4%	-44.8%	46.4%	44.8%
	6.9742	1209.6	216	25	0.00013	0.0%	0.0%		
	6.9742	1209.6	216	30	0.00011	49.5%	46.6%	49.5%	46.6%
Methyl isobutyl ketone	6.672	1168.4	191.9	10	0.00066	-76.5%	-69.0%	76.5%	69.0%
	6.672	1168.4	191.9	15	0.00037	-42.1%	-31.5%	42.1%	31.5%
	6.672	1168.4	191.9	20	0.00029	0.4%	8.4%	0.4%	8.4%
	6.672	1168.4	191.9	25	0.00039	0.0%	0.0%		
	6.672	1168.4	191.9	30	0.00068	-24.2%	-28.9%	24.2%	28.9%
Trichlorofluoromethane	6.884	1043.004	236.88	10	0.0536	7.9%	-1.2%	7.9%	1.2%
	6.884	1043.004	236.88	15	0.068	3.2%	-3.4%	3.2%	3.4%
	6.884	1043.004	236.88	20	0.0804	5.1%	1.3%	5.1%	1.3%
	6.884	1043.004	236.88	25	0.101	0.0%	0.0%		
	6.884	1043.004	236.88	30	0.122	-1.7%	2.7%	1.7%	2.7%
Average Absolute Error (%)								17.2%	16.4%

For 1,2-dichloropropane, the C coefficient in the AP-42 list appears to be off by an order of magnitude when compared to the coefficient value in EPA's "Air Emission Models for Waste and Wastewater". The c value for this compound from AP-42 gives an unreasonable correction at 30 °C while the c value from the Air Emission Models document appears in the expected range. Thus the latter c value was used in the spreadsheet.

Appendix B

ESTIMATION OF DIFFUSION COEFFICIENTS BY DIFFERENT CORRELATIONS

Table B-1 Comparison of Diffusion Coefficients by Gilliland and Wilke-Chang Correlations Using Molar Volume at Compound Boiling Point and at 20 °C

Compound	MW	Density	Temp	Mol. Vol. (cc/gmol)		Gas Diff. Coeff. (cm^2/s) for			Liquid Diff. Coeff. (cm^2/s) for		
	g/mol	g/cc	°C	at B.P.	at 20 °C	V at B.P.	V at 20 °C	% Error	V at B.P.	V at 20 °C	% Error
Benzene	78.11	0.879	20	96.5	88.86	0.0730	0.0754	3.3%	1.088	1.144	5.1%
Cyclohexane	84.16	0.779	20	117	108.04	0.0669	0.0691	3.3%	9.696	1.017	4.9%
Methanol	32.04	0.792	20	42.5	40.45	0.1172	0.1192	1.7%	1.780	1.834	3.0%
Acetone	58.08	0.792	20	77.5	73.33	0.0832	0.0850	2.1%	1.241	1.283	3.4%
n-Propanol	60.09	0.804	20	81.8	74.74	0.0810	0.0839	3.5%	1.202	1.269	5.6%
Methyl formate	60.05	0.974	20	62.8	61.65	0.0896	0.0902	0.7%	1.408	1.424	1.1%
Heptane	100.2	0.684	20	162	146.49	0.0572	0.0596	4.3%	7.976	8.473	6.2%
Acetonitrile	41.05	0.783	20	57.4	52.43	0.0994	0.1028	3.4%	1.486	1.570	5.6%
Fluorobenzene	96.11	1.0225	20	102	94.00	0.0695	0.0718	3.3%	1.053	1.106	5.0%
Bromobenzene	157.02	1.495	20	120	105.03	0.0621	0.0655	5.6%	9.550	1.034	8.3%
Chlorobenzene	112.56	1.107	20	115	101.68	0.0651	0.0684	5.1%	9.797	1.055	7.7%
Iodobenzene	204.01	1.8308	20	130	111.43	0.0590	0.0628	6.5%	9.102	9.984	9.7%
Ethyl propyl ether	88.15	0.7386	20	129	119.35	0.0638	0.0659	3.2%	9.144	9.581	4.8%
Acetic acid	60.05	1.049	20	64.1	57.24	0.0889	0.0927	4.3%	1.391	1.489	7.0%
Isobutyric acid	88.1	0.949	20	109	92.83	0.0684	0.0729	6.6%	1.011	1.114	10.1%
Ethyl acetate	88.1	0.901	20	106	97.78	0.0692	0.0715	3.3%	1.029	1.080	5.0%
Diethylamine	73.14	0.7056	20	109	103.66	0.0701	0.0716	2.0%	1.012	1.043	3.1%
Carbon tetrachloride	153.84	1.595	20	102	96.45	0.0664	0.0679	2.3%	1.053	1.089	3.4%
Ethyl mercaptan	62.13	0.839	20	75.5	74.05	0.0831	0.0837	0.7%	1.261	1.276	1.2%
Diethyl sulfide	90.18	0.837	20	118	107.74	0.0660	0.0685	3.8%	9.647	1.019	5.6%
Water	18.016	0.99823	20	18.7	18.05	0.1800	0.1820	1.1%	2.913	2.976	2.2%
Average Error								3.3%			5.1%

Molar volumes at normal boiling point from Reid, R.C. et al., The Properties of Gases and Liquids, McGraw-Hill (1987)

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Appendix C

CONVERSION FACTORS

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CONVERSION FACTORS

From	To	Multiply by
H_c (L_{liq}/L_{gas})	H_c ($atm.m^3/mol$) at 25 °C	1/(0.08205*(273+25))
$gpm/inch^2$	ft/s	0.321
°C	°F	°C*1.8 + 32

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American Petroleum Institute

STEP Strategies for Today's Environmental Partnership

American Petroleum Institute Environmental, Health, and Safety Mission and Guiding Principles

MISSION

The members of the American Petroleum Institute are dedicated to continuous efforts to improve the compatibility of our operations with the environment while economically developing energy resources and supplying high quality products and services to consumers. We recognize our responsibility to work with the public, the government, and others to develop and to use natural resources in an environmentally sound manner while protecting the health and safety of our employees and the public. To meet these responsibilities, API members pledge to manage our businesses according to the following principles using sound science to prioritize risks and to implement cost-effective management practices:

PRINCIPLES

- To recognize and to respond to community concerns about our raw materials, products and operations.
- To operate our plants and facilities, and to handle our raw materials and products in a manner that protects the environment, and the safety and health of our employees and the public.
- To make safety, health and environmental considerations a priority in our planning, and our development of new products and processes.
- To advise promptly, appropriate officials, employees, customers and the public of information on significant industry-related safety, health and environmental hazards, and to recommend protective measures.
- To counsel customers, transporters and others in the safe use, transportation and disposal of our raw materials, products and waste materials.
- To economically develop and produce natural resources and to conserve those resources by using energy efficiently.
- To extend knowledge by conducting or supporting research on the safety, health and environmental effects of our raw materials, products, processes and waste materials.
- To commit to reduce overall emission and waste generation.
- To work with others to resolve problems created by handling and disposal of hazardous substances from our operations.
- To participate with government and others in creating responsible laws, regulations and standards to safeguard the community, workplace and environment.
- To promote these principles and practices by sharing experiences and offering assistance to others who produce, handle, use, transport or dispose of similar raw materials, petroleum products and wastes.

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