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June 16, 1999

To: Consumers of API's *Amine Unit Air Emissions Model (AMINECalc) Version 1.0,* Software and User's Manual (Pub No. 4679)

From: The American Petroleum Institute: Health and Environmental Sciences Department

The telephone and fax numbers at DB Robinson Research Ltd. have recently changed.

For technical support, please contact DB Robinson Research Ltd., Edmonton, Canada by using the following:

Telephone: **(780) 463-8638**
Fax: **(780) 450-1668**
E-mail: **support@dbra.com**

Also, please note that there is a typographical error in the AMINECalc example print page for the Natural Gas Liquid (NGL) volumetric flow rate (gal/min). AMINECalc (version 1.0 prints the correct volumetric flow rate but the units are incorrectly printed as lb/h instead of gal/min (page B-17). The error does not effect the calculated results. The error will be corrected in the next version of AMINECalc.

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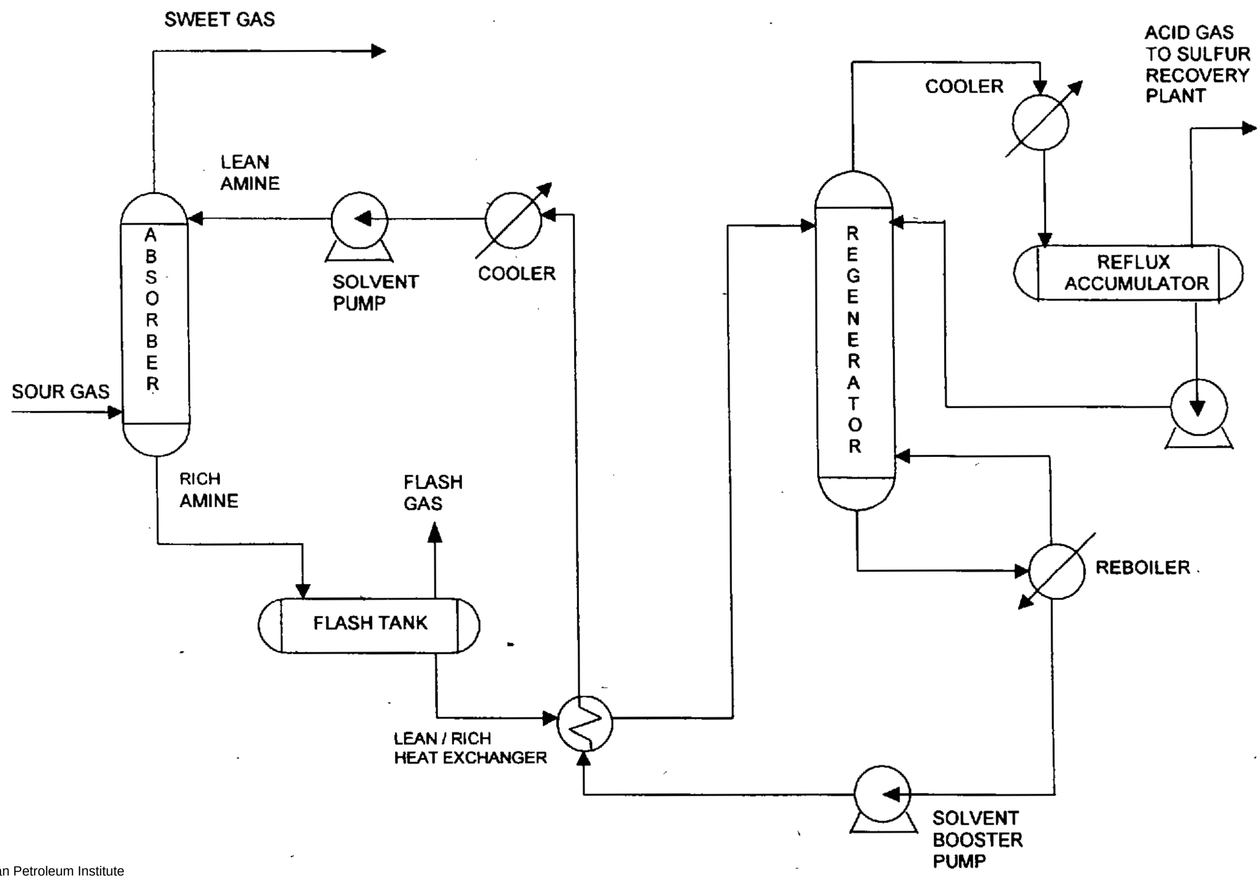
American Petroleum Institute

STEP Strategies for Today's Environmental Partnership

AMINE UNIT EMISSIONS MODEL

AMINECALC VERSION 1.0 USER'S MANUAL

HEALTH AND ENVIRONMENTAL SCIENCES DEPARTMENT
PUBLICATION NUMBER 4679
JANUARY 1999



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Record the AMINECalc Registration Number
from the enclosed registration form:
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Amine Unit Emissions Model

AMINECalc Version 1.0
User's Manual

Health and Environmental Sciences Department

API PUBLICATION NUMBER 4679

PREPARED UNDER CONTRACT BY:

DB ROBERTSON RESEARCH LTD.
EDMONTON, ALBERTA, CANADA

JANUARY 1999

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ACKNOWLEDGMENTS

THE FOLLOWING PEOPLE ARE RECOGNIZED FOR THEIR CONTRIBUTIONS OF TIME AND EXPERTISE DURING THIS STUDY AND IN THE PREPARATION OF THIS REPORT:

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CONTENTS

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CONTENTS (continued)

EXECUTIVE SUMMARY

This document describes a software simulation package called *Amine Unit Air Emissions Model* (AMINECalc Version 1.0). This package is designed to estimate hydrocarbon emissions from amine based sour gas and natural gas liquid (NGL) sweetening units. The output generated by the software package is suitable for regulatory reporting, which will be performed by the unit operators according to the schedule derived from the Clean Air Act Amendments (CAAA) of 1990.

The development of AMINECalc was funded by the American Petroleum Institute (API). The major objective of this project is to develop a comprehensive software simulator which, with its verifiable predictions, will gain acceptance of the U.S. Environmental Protection Agency (EPA). At the same time, the simulator, with its easy-to-use interface, will be accepted by amine unit operators.

The calculation algorithm of this package is based on commercial software developed originally by DB Robinson Research Ltd. Equipped with a rigorous non-equilibrium stage model and the Peng-Robinson equation of state, the commercial software was designed for providing accurate and reliable solutions to sour gas and liquefied petroleum gas processes. Traditionally, the emphasis of the commercial software was on acid gas (H_2S and CO_2) removal, and its predictions have been constantly checked against real plant data. In this study, the commercial software has been re-engineered and enhanced to accommodate three types of calculations (mass balance calculation, gas process simulation, and NGL process simulation) required by the AMINECalc project. Emphasis has been on hazardous air pollutants (HAPs) including benzene, toluene, ethylbenzene and xylenes (BTEX), and volatile organic compounds (VOCs) from amine unit emissions.

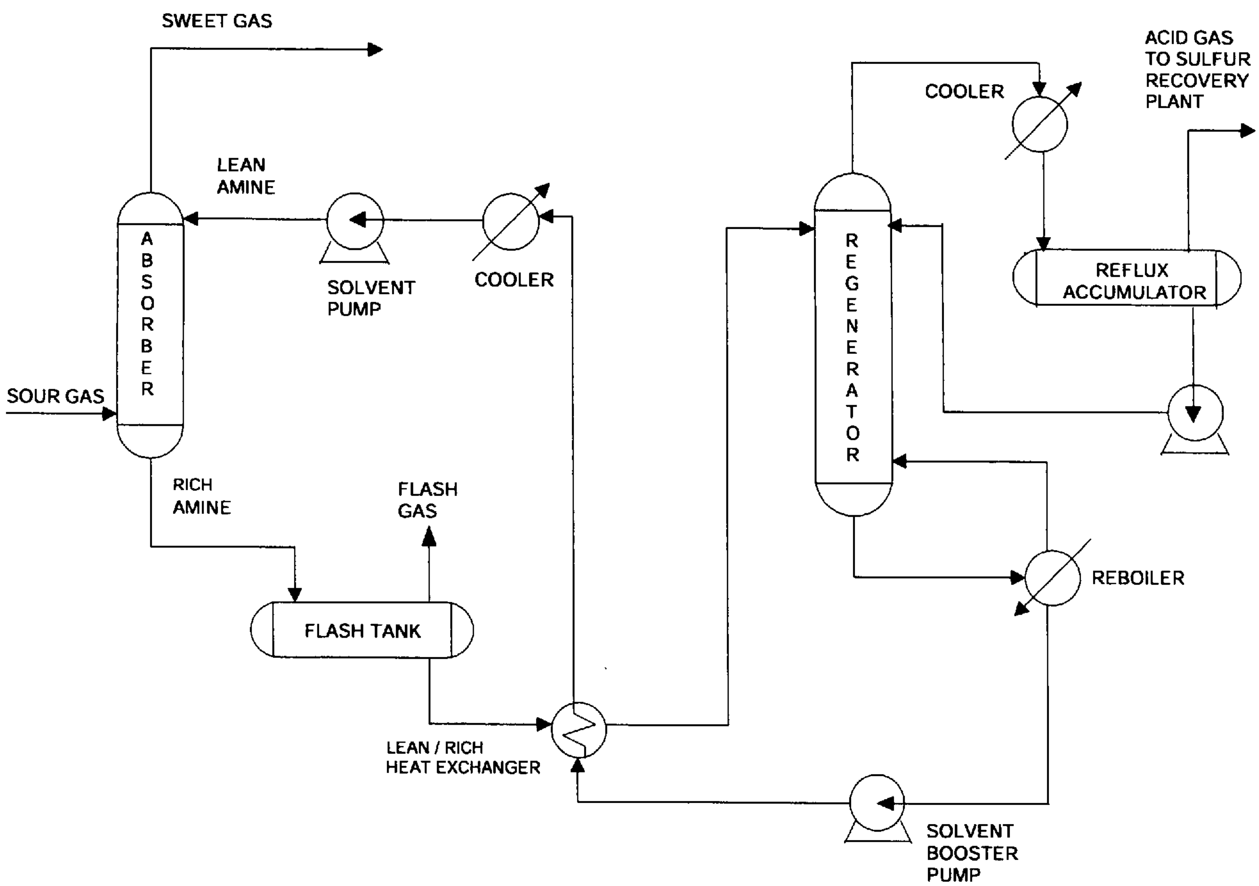
CHAPTER 1

INTRODUCTION

The removal of acid gases such as hydrogen sulfide (H_2S) and carbon dioxide (CO_2) from natural gas streams or natural gas liquid (NGL) streams is often required in gas plants and in oil refineries. Among many treating processes, the absorption technology using aqueous solutions of alkanolamines is popular for economic reasons.

The following figure depicts a simplified flow diagram of a typical amine sweetening unit.

Typical Flow Diagram of an Amine Sweetening Unit



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The system consists of two major operations: absorption and regeneration. A natural gas stream or a natural gas liquid stream containing acid gases (H_2S and/or CO_2) is introduced into an absorber column where the stream is counter-currently contacted with an amine solution. The acid gas contents are removed through chemical reactions with the amine. After the treatment, the natural gas or the natural gas liquid becomes suitable for consumer use or for further chemical processing. This process is often referred to as a gas sweetening process, and treated gas or liquid is called sweetened gas or liquid. On the other side, the amine solution, referred to as rich amine solution after selectively absorbing the acid gases from the stream requires regeneration before it can be used to sweeten sour gas again. The regeneration column serves the function of stripping absorbed acid gases from the rich amine solution. A flash tank is usually installed at the outlet of the absorber to permit the recovery of the dissolved and entrained hydrocarbons and to reduce the hydrocarbon contents of the acid gas product.

The flash gas from the flash tank and the stripped acid gas from the regenerator in amine units have the potential to emit hazardous air pollutants (HAPs), and therefore, the unit operators may be required to quantify and report the emissions. The regulatory report may include both Hazardous Air Pollutants (HAPs) and Volatile Organic Compounds (VOCs). As a consequence, the American Petroleum Institute (API) supported the development of a comprehensive software package for the estimation of emissions from amine sweetening units.

The objective of this current project is to develop a PC-based emission model for calculating HAPs and VOCs from the flash tank and solvent regenerator of a natural gas sweetening unit. The user of the model needs to determine if these gases are vented to the atmosphere and report the emissions to the appropriate regulatory agencies. This objective is achieved by modifying and enhancing an existing commercial software package.

To achieve a wide acceptance by those end users, special attention has been paid to the program interface design. No extensive computer literacy or simulation experience was assumed about the users. A user with a basic knowledge of Windows™ should find no difficulty in using AMINECalc. This document describes program operations and embedded calculation principles.

CHAPTER 2

INSTALLING AMINECalc

System Requirements

The minimum system requirements for running AMINECalc Version 1.0 are:

IBM PC 486 compatible or higher
8 MB RAM or more
Windows™ 95/98/NT

Approximately 2 megabytes (MB) of free hard disk space are required to hold the program and its supporting run-time libraries. For better interface viewing, it is recommended that the user set the monitor to a high color 16 bit (or higher) resolution.

Installing AMINECalc

To install AMINECalc:

1. Start Windows™ 95/98/NT and insert the AMINECalc diskette into drive A or B.
2. Click the Start button on the Windows™ Taskbar and select Run.
3. At the Run dialog box, type A:\SETUP32 or B:\SETUP32 and click OK.
4. Follow the instructions on the screen.

The default path for AMINECalc is *C:\Program Files\API\AMINECalc.* However, you may specify an alternative path. After the installation process is completed, a program group called AMINECalc will be created.

Congratulations! You have now successfully installed AMINECalc V1.0.

CHAPTER 3

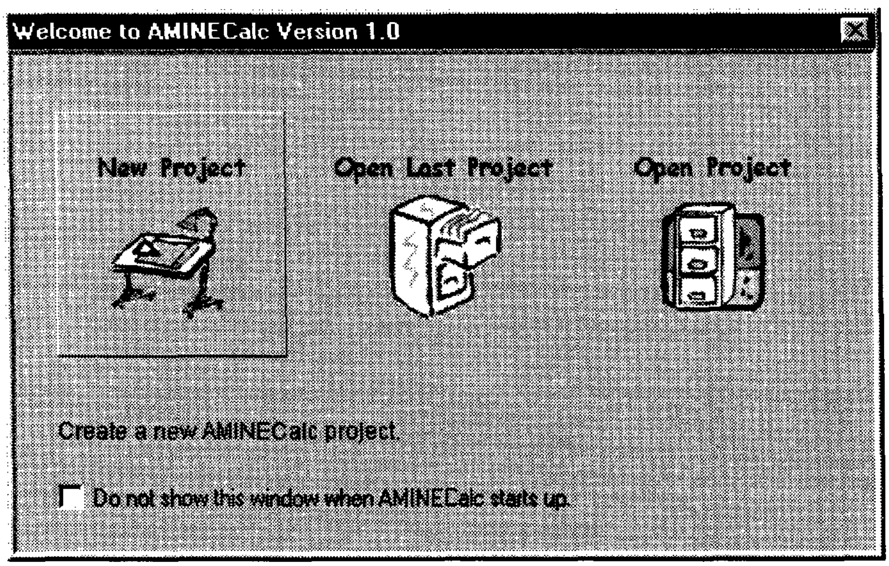
GETTING STARTED

This chapter will show you how to start AMINECalc and set up a new project. You will also be introduced to the AMINECalc desktop and learn how to use some important function keys.

Starting AMINECalc

After installing the application, you are ready to run AMINECalc. To start the program, double-click on the file *AMINECalc.exe* under *C:\Program Files\API\AMINECalc* from the Windows™ Explorer. Alternatively, you may also create an AMINECalc shortcut icon on the Windows desktop and start the program by double-clicking the icon.

After starting the program, an opening screen followed by the API disclaimer screen will be displayed. Click the *Continue* button after reading the disclaimer message. A welcome screen will be activated. You can create a new project, open the last project, open an existing project or close the welcome window.



Select *New Project.*

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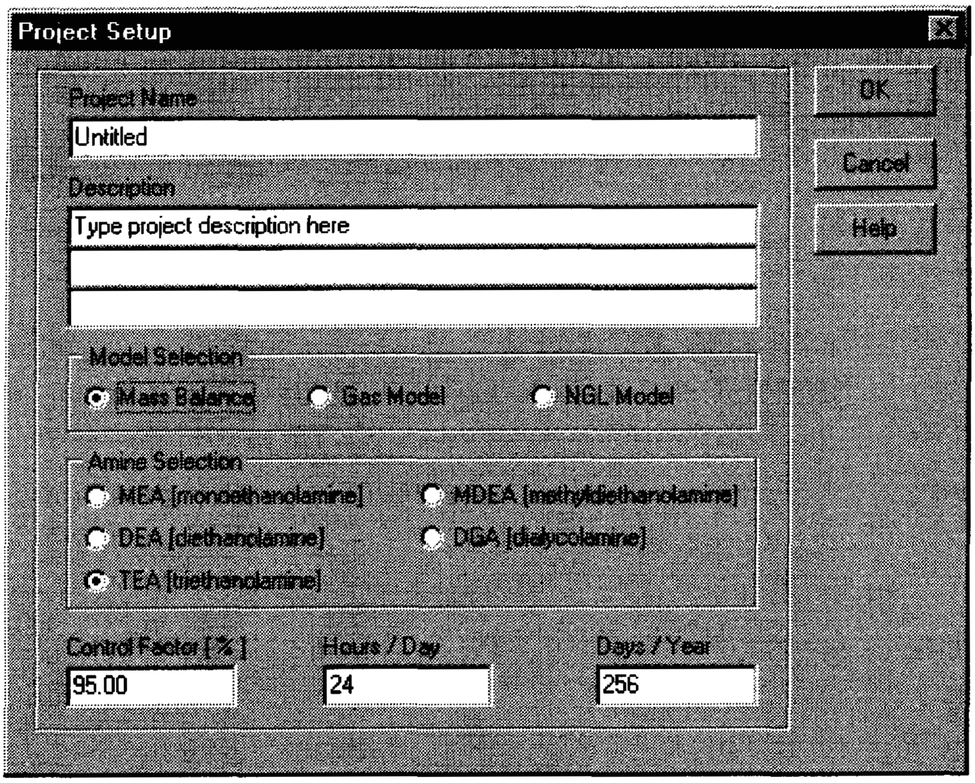
Project Setup

Upon opening a new project, a Project Setup dialog box will appear.

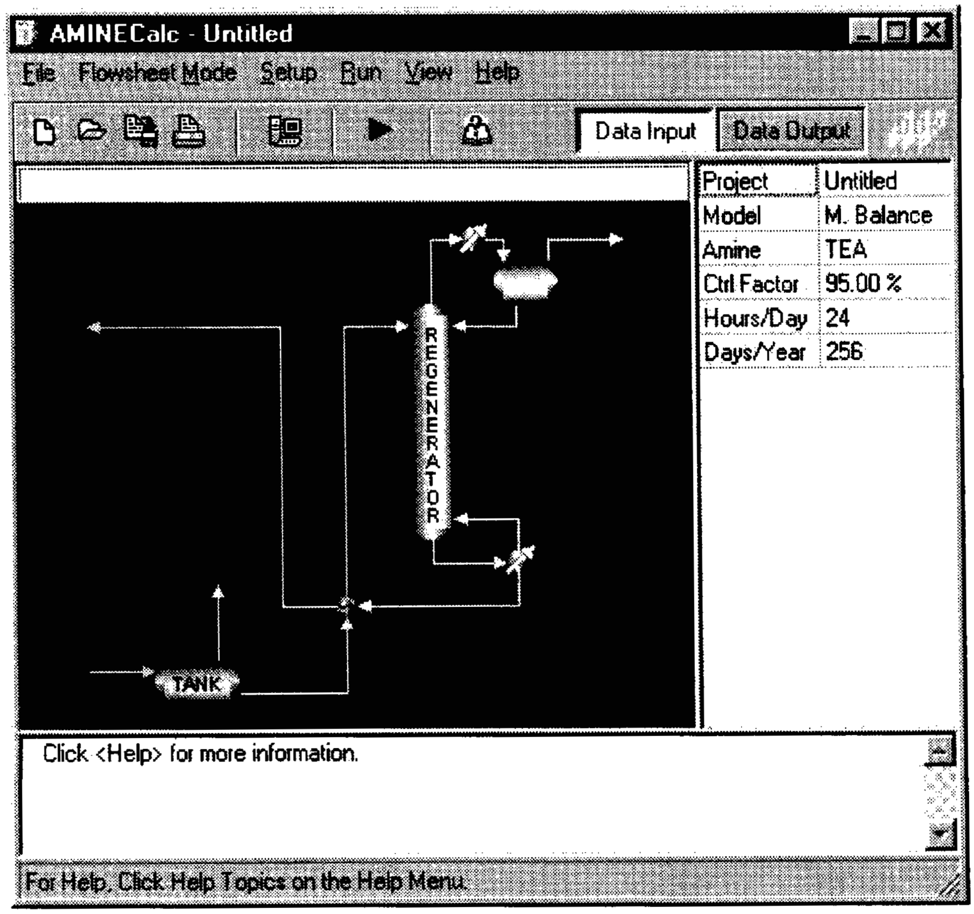


Once the setup is completed, click OK. The AMINECalc desktop will appear.

The rest of this chapter will help users to become familiarized with the basic functions and features of the program. If you are comfortable with Windows™ working environment, proceed to Chapter 4 now.

AMINECalc Desktop

The AMINECalc Desktop can be separated into several working areas.



Menu Bar

There are six drop-down menus in the menu bar located at the top of the AMINECalc desktop:

File – to create, open, reopen, save, print or close your AMINECalc projects

Flowsheet Mode – to change the flowsheet mode

Setup – to setup a project or to edit setup of an existing project

Run – to run a simulation based on the data you entered

View – to manage your working screen

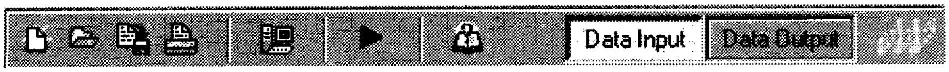
Help – to access on-line help on various topics

➡ **To select a command from a menu**

Click on the menu and select the command.

Toolbar

The toolbar consists of buttons for frequently-used commands in AMINECalc:



New Project – to create a new project

Open Project – to open an existing project

Save Project – to save the current project

Print Report – to view and print current project simulation results

Project Setup – to edit the project setup

Run – to execute a simulation

Help – to access on-line help

Data Input – to turn on the flowsheet input mode

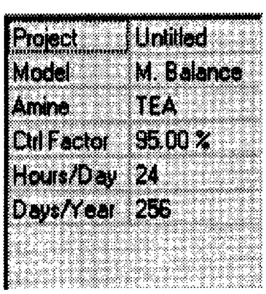
Data Output – to turn on the flowsheet output mode

Note The Toolbar can be turned on/off by clicking on Toolbar from the View menu.

➡ **To select a command from the toolbar**

Click on the button for the desired command.

Project Setup Viewing Box



Project	Untitled
Model	M. Balance
Amine	TEA
Ctrl Factor	95.00 %
Hours/Day	24
Days/Year	256

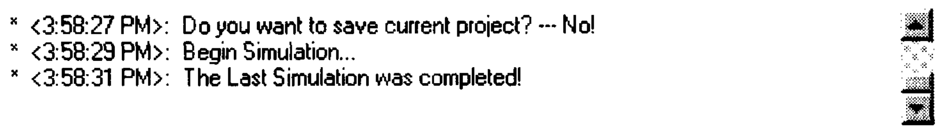
The Project Setup viewing box located to the right of the flowsheet allows users to view and to edit the setup for the current project. The Project Setup viewing box can be turned on/off by clicking on Project Setup from the View menu.

➡ **To edit Project Setup**

Click on the Project Setup button on the toolbar or double-click on the Project Setup viewing area.

Message Box

Message Box displays a list of commands previously-executed on projects on screen.



Note The Message Box can be turned on/off by clicking on Message Box from the View menu.

Status Bar

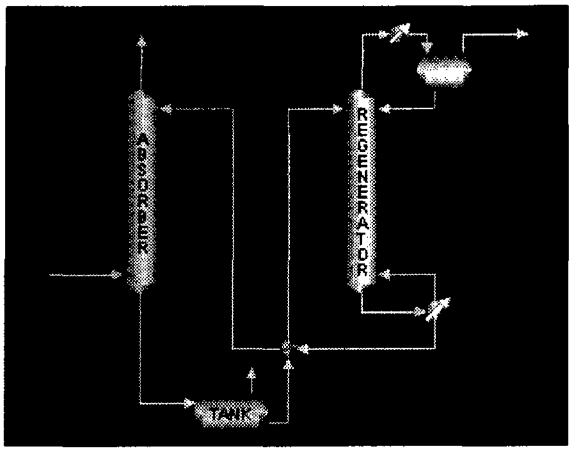
The Status Bar provides information on the current status of the project and the current flowsheet mode.

Note The Status Bar can be turned on/off by clicking on Status Bar from the View menu.

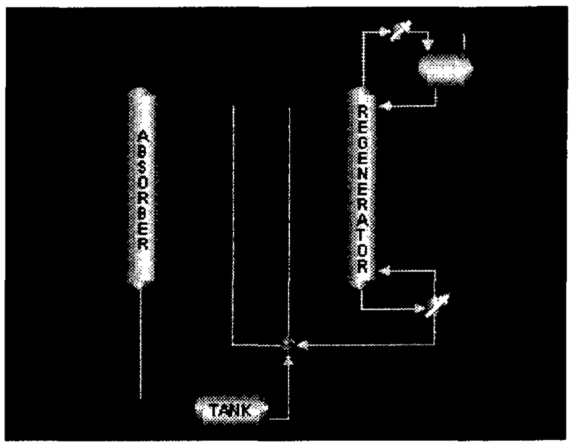
Process Flowsheet

The Flowsheet window displays the process flow diagram for the project. There are two flowsheet modes: Data Input and Data Output.

Data Input Mode
Input Mode allows you to provide input information for the project. When the flowsheet is in Input Mode, only devices and process lines that are colored green require input. These items colored green are also referred to as hotspots.



Data Output Mode
This mode allows you to view simulation output or to print simulation reports. Users can only view the simulation output for process lines that are colored red.



➡ **To change the flowsheet mode from the Flowsheet Mode menu**

Click on the Flowsheet Mode menu and select mode.

➡ **To change the flowsheet mode from the toolbar**

Click on the desired flowsheet mode.

Unit Systems

Two unit systems are used in AMINECalc: Engineering and SI units. You can specify the unit system separately for each input and output dialog boxes.

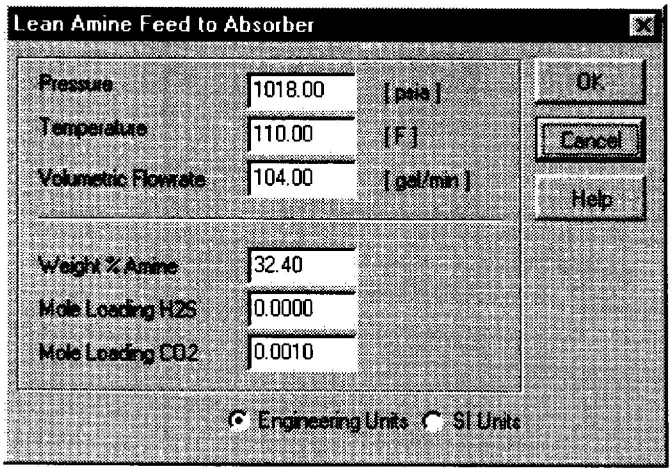
➧ **To specify a unit system for an input/output dialog box**

Click on the desired unit button in the input/output dialog box.

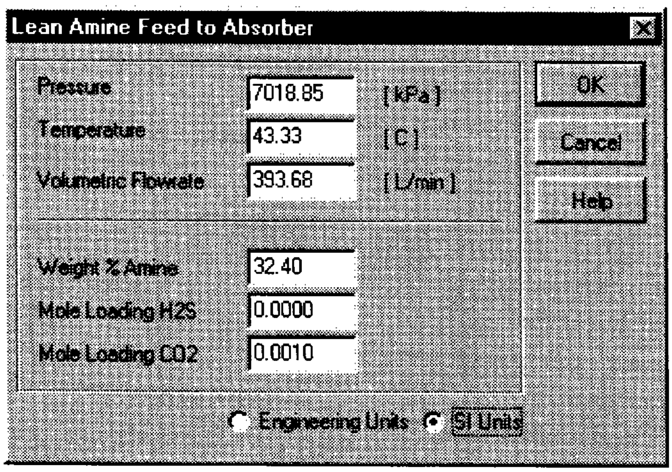
➧ **To view unit conversions**

In the active dialog box, click on one unit button and then the other.

Engineering Units



International System (SI) Units



CHAPTER 4

RUNNING AMINECalc

In this chapter, you will be shown how to input data and execute simulations for each model in AMINECalc.

Calculation Models

There are three calculation options (models) in AMINECalc:

1. Mass Balance Calculation
2. Gas Process Simulation
3. NGL Process Simulation.

Mass Balance Calculation

Mass Balance Calculation is a descriptive calculation that uses available plant stream data and calculates the flow rate and compositions of the flash vent gas and the contents of the stripped acid gas from the regenerator.

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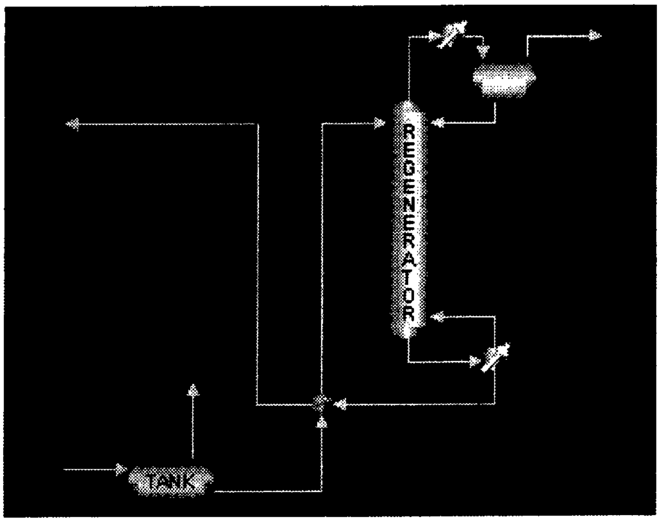
Process Flowsheet



Input Data

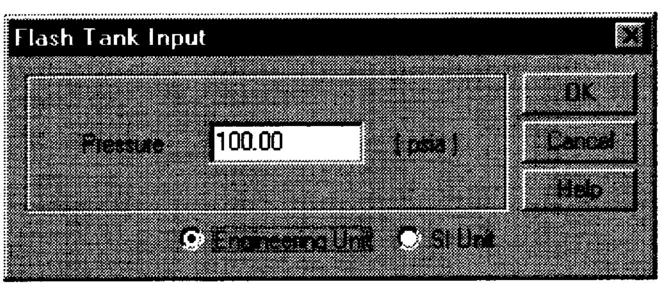
Input data required for the Mass Balance Calculation are the Flash Tank Pressure, the stream data of Lean Amine to Flash Tank, and the stream data of Lean Amine from Regenerator.

➡ To input data

Click on the green equipment and streams on the input-mode flowsheet.

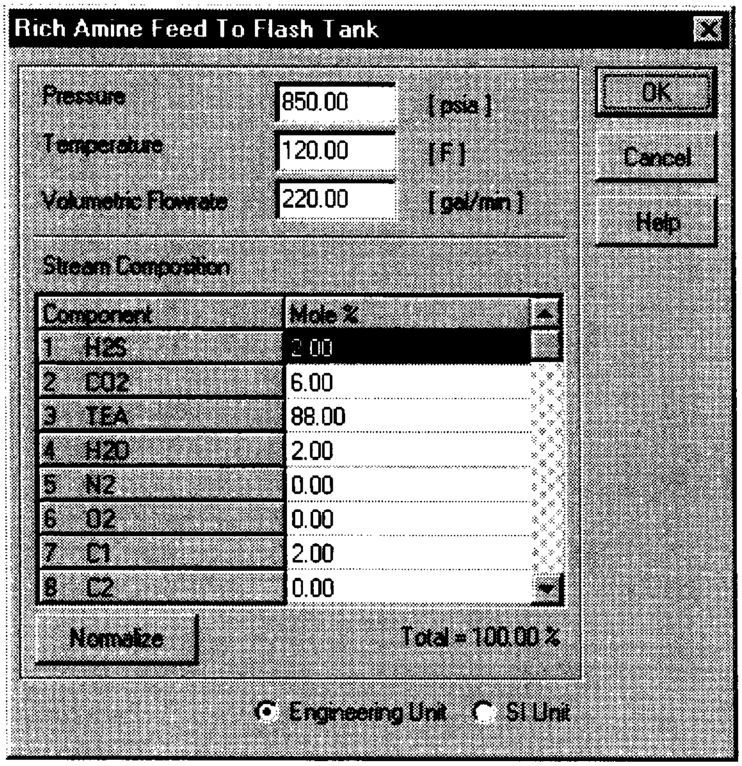
Note The values present in the input dialog boxes are default values. The purpose of these default values is to provide you with some hints on the magnitude or the range of the input data. These default values also serve as reasonable guesses when complete input information is not available.

Flash Tank Pressure



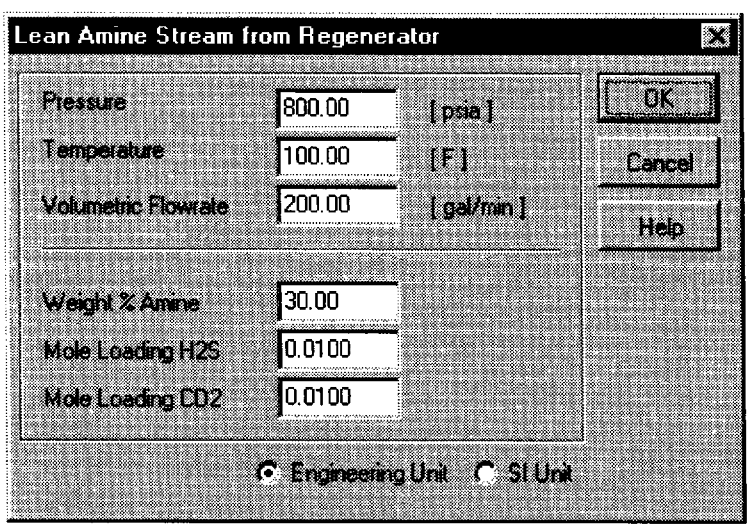
Enter the flash tank pressure. Click OK to exit the dialog box.

Rich Amine to Flash Tank



Enter Temperature, Pressure, Flow Rate, and the detailed stream composition for the stream. Click the Normalize button to normalize compositions. Click OK to exit the dialog box.

Lean Amine from Regenerator



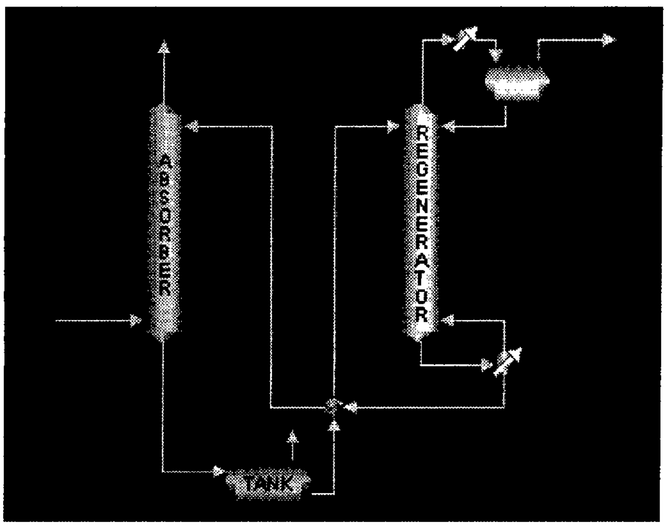
Enter Temperature, Pressure, Feed Rate, Weight % Amine, and the Mole Loading of the acid gas (or mole acid gas/mole amine) for the stream.

After the data input is completed, click OK to exit the dialog box.

Gas Process Simulation

Gas Process Simulation is a rigorous process model that predicts emissions from sour gas amine units.

Process Flowsheet



Input Data

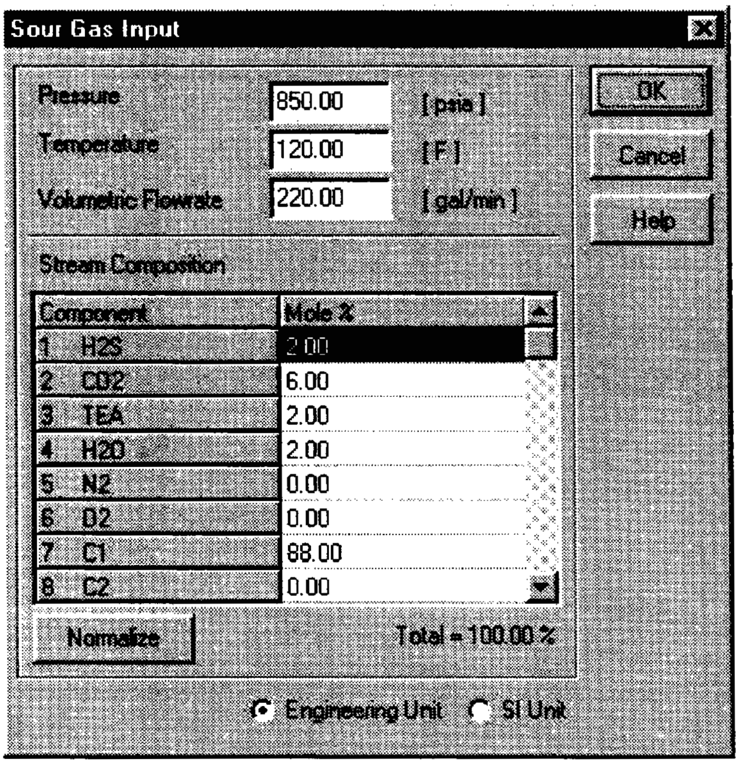
Input data required for the Gas Process Simulation are the Flash Tank Pressure, the Gas Feed, the number of actual trays of the Absorber, and the Lean Amine leaving the Regenerator.

Note The Values present in the input dialog boxes are default values. The purpose of these default values is to provide you with some hints on the magnitude or the range of the input data. These default values also serve as reasonable guesses when complete input information is not available.

● To input data

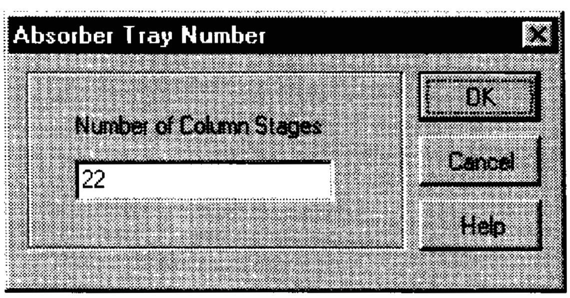
Click on the green equipment and streams on the input-mode flowsheet.

Sour Gas Feed



Enter Temperature, Pressure, Feed Rate, and stream composition for the Sour Gas Feed. Click the Normalize button to normalize compositions. Click OK to exit the dialog box.

Absorber



Enter the actual number of trays (stages) of the absorber.

Click OK to exit the dialog box.

Note Maximum number of column stages is 22.

Flash Tank Pressure

Refer to Flash Tank Pressure under Mass Balance Calculation (page 16).

Lean Amine from Regenerator

Refer to Lean Amine from Regenerator under Mass Balance Calculation (page 17).

Natural Gas Liquid (NGL) Process Simulation

The NGL Process Simulation is a rigorous process model that predicts emissions from amine units that treat natural gas liquid.

Process Flowsheet

The Process Flowsheet for the NGL Process Simulation is similar to that of the Gas Process Simulation. Refer to the process flowsheet for Gas Process Simulation.

Input Data

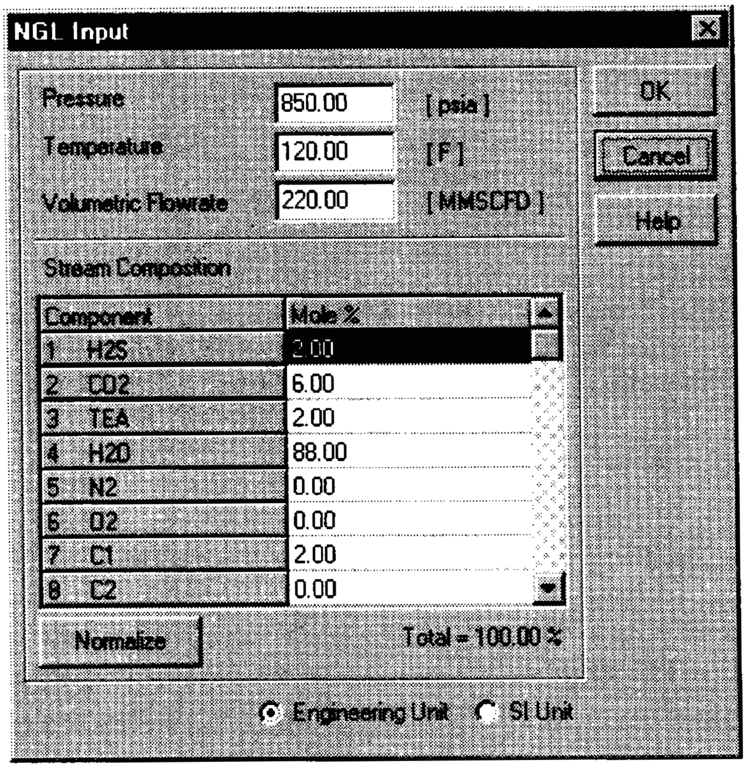
The input data required for the NGL Process Simulation are the Flash Tank Pressure, the NGL Feed, the number of actual trays of the Absorber and the Lean Amine leaving the Regenerator.

Note The values present in input dialog boxes are default values. The purpose of these default values is to provide you with some hints on the magnitude or the range of the input data. These default values also serve as reasonable guesses when complete input information is not available.

➡ **To input data**

Click on the green equipment and streams on the flowsheet. An input dialog box will appear.

Natural Gas Liquid Feed



Enter Temperature, Pressure, Feed Rate, and stream composition for the NGL Feed.

Click the Normalize button to normalize compositions. Click OK to exit the dialog box.

Absorber

Refer to Absorber under Gas Process Simulation (page 19).

Flash Tank Pressure

Refer to Flash Tank Pressure under Mass Balance Calculation (page 16).

Lean Amine from Regenerator

Refer to Lean Amine from Regenerator under Mass Balance Calculation (page 17).

Executing Simulations

The process of executing a simulation applies to all of the models in AMINECalc.

Note Before executing a simulation in AMINECalc, it is advisable to shut down all other programs that are currently open on the system.

➧ **To execute a simulation**

Click the Run button located on the toolbar. A message informing the user that the calculation is in progress will be displayed.

After the simulation is completed, the flow diagram will be switched to Data Output mode:

Note If at any time the user would like to return to the input mode, click on the Input Mode button on the toolbar.

CHAPTER 5

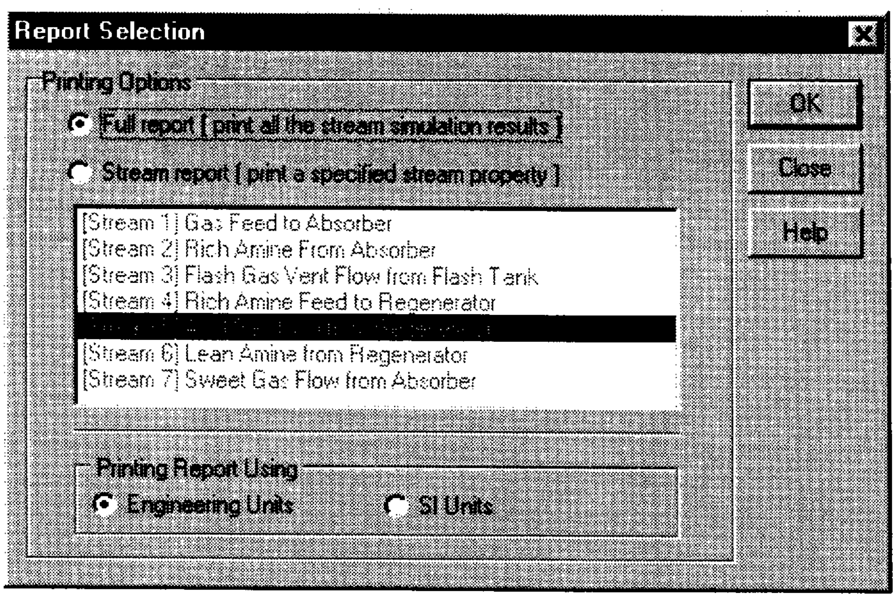
VIEWING AND PRINTING RESULTS

After the project is executed successfully, the process flowsheet will be switched automatically to Data Output mode.

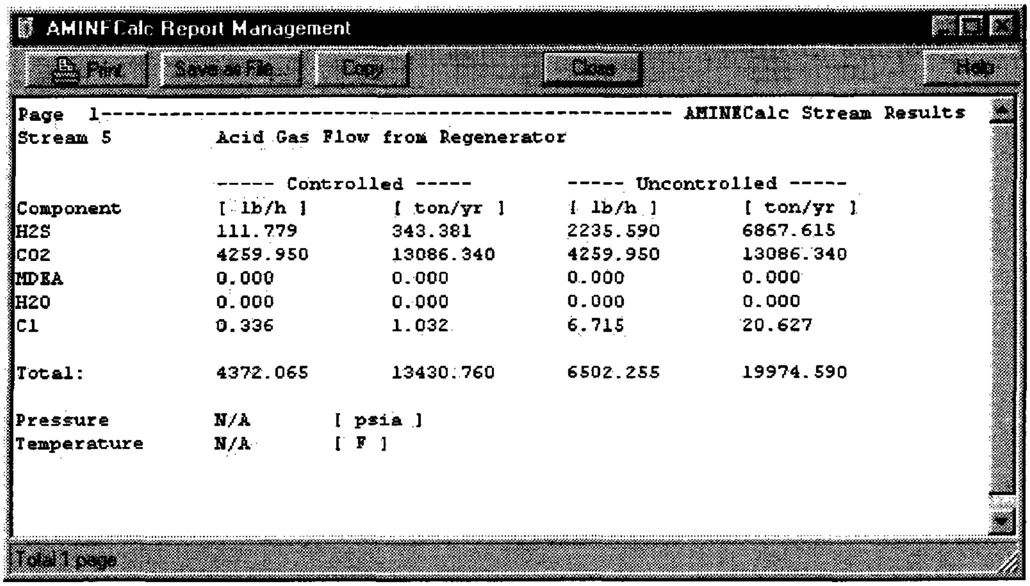
Note To view and print results, the process flowsheet is required to be in Data Output mode.

Viewing and Printing Full Reports

In AMINECalc, the same function key is used to preview and print simulation results. Click on the *Printing Report* button on the toolbar. The Report Selection window will appear.



Choose *Full report*, or *Stream report*. Click OK to preview the report. The Report Management window will appear. The function of the Report Management window is similar to that of a print preview window.



Page 1--- AMINECalc Stream Results

Stream 5 Acid Gas Flow from Regenerator

	----- Controlled -----		----- Uncontrolled -----	
Component	[lb/h]	[ton/yr]	[lb/h]	[ton/yr]
H2S	111.779	343.381	2235.590	6867.615
CO2	4259.950	13086.340	4259.950	13086.340
MDEA	0.000	0.000	0.000	0.000
H2O	0.000	0.000	0.000	0.000
C1	0.336	1.032	6.715	20.627
Total:	4372.065	13430.760	6502.255	19974.590

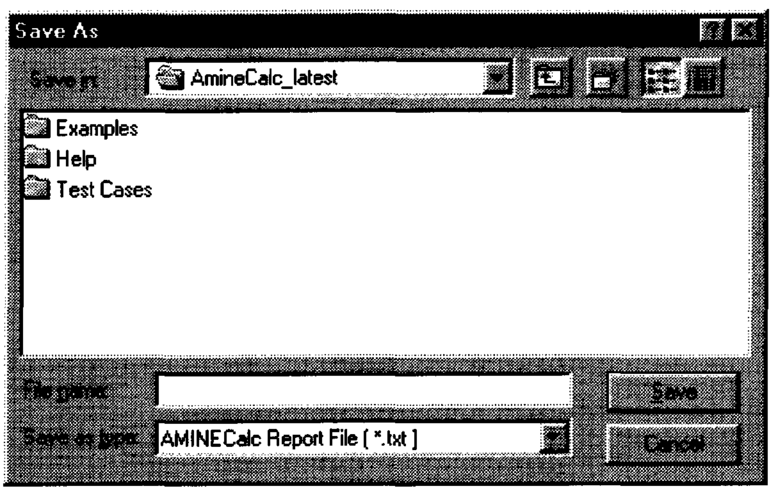
Pressure	N/A	[psia]
Temperature	N/A	[F]

Click *Print* to start printing report.

Saving and Copying Reports

AMINECalc also allows you to save results as output files or copy results to another Windows™ application. These functions can be accessed from the Report Management window.

➡ To save outputs



Click *Save as File...* in the Report Management window. A Save As window will appear.

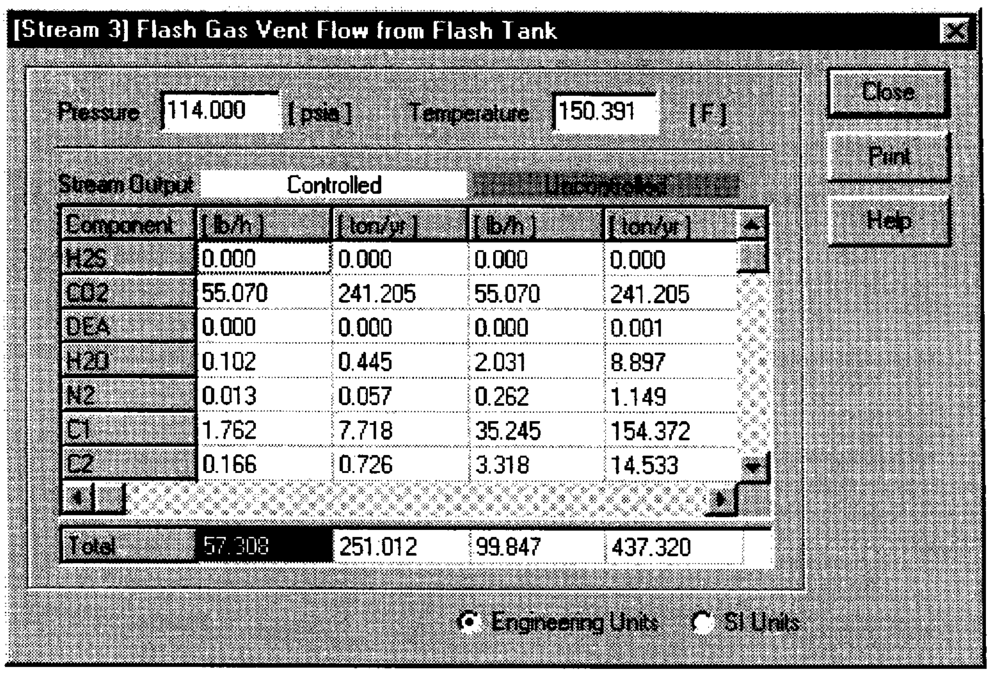
Choose a path to save the output file. Click *Save* to save or *Cancel* to cancel the activity.

➡ **To copy outputs**

1. While in the Report Management window, use the mouse to select the output area to copy.
2. Click *Copy.*
3. Proceed to a Windows™ application and click paste.

Viewing and Printing a Stream Output

Click on the desired red process stream on the flowsheet. The Stream Output window will appear.



Use the scroll bars to the view complete stream output when necessary. Click *Print* to activate the Report Management window. In the Report Management window, click *Print* again to start printing the report or *Close* to exit the window.

APPENDIX A

TECHNICAL BACKGROUND OF AMINECalc

Thermodynamic Models

The framework of the thermodynamics of sour gas or NGL treating is based on two types of equilibria: vapor-liquid or liquid-liquid phase equilibria (VLE or LLE) and chemical equilibria in liquid phase.

Phase Equilibria

For any system that is at vapor-liquid equilibrium at a specified temperature and pressure, the fugacities of both phases must be equal for all components in the mixture, that is:

$$f_i^V = f_i^L \tag{A-1}$$

In the case of the gaseous components dissolved in the aqueous solution, the equilibrium condition can be written in the form of Henry's Law:

$$y_i \Phi_i^V P = H_i m_i \tag{A-2}$$

where H_i is the Henry's Law constant, m_i is the concentration of molecular species i in liquid, y_i is the mole fraction of the gaseous component i, Φ_i^V is the vapor fugacity coefficient for component i, and P is the system pressure .

The experimental measurement of the value of the Henry's Law constant is comparatively straight forward in the case of physical solvents. All that is needed is a determined equilibrium curve of partial pressure versus composition. In the ideal case, H is simply the slope of such a curve near the origin.

In the case of chemical solvents, the situation is considerably more complex because the value of H cannot be extracted from VLE data. If H^0 represents the value of the Henry's Law constant in a non-reactive solution, the value of H in the reactive solution will be appreciably different from H^0.

The fugacity coefficients can be calculated by an equation of state, such as the Peng-Robinson equation of state developed by Peng and Robinson in 1976[1]:

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$$P=\frac{RT}{v-b}-\frac{a(T)}{v(v+b)+b(v-b)} \quad \text{(A-3)}$$

where a and b are the equation parameters, R is the universal gas constant, and P, v and T are the system pressure, volume and temperature, respectively.

Chemical Equilibria

In this study, the important chemical dissociation reactions in the H_2S-CO_2-R_1R_2NH (primary or secondary amine)/-$R_1R_2R_3N$ (tertiary amine)-H_2O system are as follows:

$R_1R_2NH + H_2O \rightarrow R_1R_2NH_2^+ + OH^-$

$R_1R_2R_3N + H_2O \rightarrow R_1R_2R_3NH^+ + OH^-$

$R_1R_2NH + CO_2 \rightarrow R_1R_2NCOO^- + H^+$

$H_2O \rightarrow H^+ + OH^-$

$H_2S \rightarrow H^+ + HS^-$

$CO_2 + H_2O \rightarrow H^+ + HCO_3^-$

$HS^- \rightarrow H^+ + S^=$

$HCO_3^- \rightarrow H^+ + CO_3^=$

The equilibrium constants, K_j, can be expressed by the reacting species

$$K_j = \prod_i (x_i\gamma_i)^{\beta_{ij}} \quad \text{(A-4)}$$

where x_i and γ_i are the mole fraction and activity coefficient of species i, respectively, and β_{ij}, the stoichiometric coefficient for component i in reaction j.

The determination of the equilibrium compositions of all molecular and ionic species in both the vapor and liquid phases involves the simultaneous solution of a set of nonlinear equations which describe the phase and chemical equilibrium, electroneutrality and mass balance of the electrolytes in the aqueous solution are given as follows:

Chemical Equilibrium:

$K_1 = [H^+][R_1R_2NH]/[R_1R_2NH_2^+]$ (A-5)

$K_2 = [H^+][R_1R_2R_3N]/[R_1R_2R_3NH^+]$ (A-6)

$K_3 = [HCO_3^-][R_1R_2NH]/[R_1R_2NCOO^-][H_2O]$ (A-7)

$K_4 = [H^+][OH^-]/[H_2O]$ (A-8)

$K_5 = [H^+][HS^-]/[H_2S]$ (A-9)

$K_6 = [H^+][HCO_3^-]/[CO_2][H_2O]$ (A-10)

$K_7 = [H^+][S^=]/[HS^-]$ (A-11)

$K_8 = [H^+][CO_3^=]/[HCO_3^-]$ (A-12)

Electroneutrality:

$[H^+]+[R_1R_2NH_2^+]+[R_1R_2R_3NH^+]$

$= [OH^-]+[R_1R_2NCOO^-]+[HCO^{3-}]+[HS^-]+2[CO^{3=}]+2[S^=]$ (A-13)

Mass Balance:

$C_{1,2\text{-amine}} = [R_1R_2NH] + [R_1R_2NH_2^+] + [R_1R_2NCOO^-]$ (A-14)

$C_{3\text{-amine}} = [R_1R_2R_3N] + [R_1R_2R_3NH^+]$ (A-15)

$C_{CO2} = (C_{1,2\text{-amine}} + C_{3\text{-amine}})\alpha_{CO2}$

$= [CO_2] + [R_1R_2NCOO^-] + [HCO_3^-] + [CO_3^=]$ (A-16)

$C_{H2S} = (C_{1,2\text{-amine}} + C_{3\text{-amine}})\alpha_{H2S}$

$= [H_2S] + [HS^-] + [S^=]$ (A-17)

In the above equations, C is the concentration of a molecular species in the liquid, and α is the acid gas loading in the liquid.

Mass Transfer with Chemical Reaction

The absorption of acid gases into an amine solution is a gas-liquid mass transfer process accompanied by complex chemical reactions. The rate of absorption is strongly influenced or enhanced by the rate of chemical reactions taking place in the liquid phase.

The occurrence of the chemical reactions has two distinct effects on the overall behavior of the system. The first effect is to maintain a high driving force for mass transfer in the liquid phase. When component A is absorbed into the liquid phase, it is consumed by the chemical reactions and therefore its concentration in the bulk of the liquid is kept low. This implies that the driving force for absorption remains higher than it would be if no chemical reactions were taking place.

The second effect is subtler. At a given level of driving force, the actual rate of mass transfer may be significantly larger when chemical reactions are taking place than it would be in the absence of chemical reactions. The rate of enhanced mass transfer may be very large (up to two orders of magnitude or even more).

In the absence of chemical reactions, the mass transfer rate in the liquid phase is given by:

$$N^o = k_L^o(a_i - a_o) \tag{A-18}$$

The actual rate in the presence of chemical reactions may be larger than the rate that would be observed under the same driving force in the absence of chemical reactions:

$$N = k_L(a_i - a_o) \tag{A-19}$$

In the above equations, N is the mass transfer rate, and k_L and $k_L{}^0$ are the mass transfer coefficients in the presence or absence of chemical reactions respectively, whereas a_i and a_0 are the concentrations of component a at the vapor-liquid interface (a_i) and in the bulk of the liquid (a_0), respectively. The enhancement factor, I, is defined as the ratio of the actual mass-transfer rate and the rate in the absence of chemical reaction.

$$I=\frac{N}{N^0}=\frac{k_L(a_i-a_0)}{k_L^0(a_i-a_0)}=\frac{k_L}{k_L^0} \qquad \text{(A-20)}$$

A group of differential equations which describe the mass transfer with chemical reactions needs to be solved to obtain the enhancement factors. Besides the mass transfer coefficients, the experimental values of the chemical reaction coefficients and the molecular diffusion coefficients are also needed to solve those equations[2].

Non-Equilibrium Stage Model

A rigorous non-equilibrium stage model is employed to calculate stage efficiencies of individual components for column simulation. For a vapor-liquid absorber, a modified form of the Murphree vapor stage efficiency η_{ij} is used to characterize the condition of each component (i) on any stage (j) within the column.

$$\eta_{ij}=\frac{(V_j+SV_j)y_{i,j}-V_{j+1}y_{i,j+1}}{(V_j+SV_j)K_{i,j}x_{i,j}-V_{j+1}y_{i,j+1}} \qquad \text{(A-21)}$$

where V_j and SV_j are the molar vapor flow rate on stage j and molar flow rate of side vapor on stage j, respectively. $x_{i,j}$ and $y_{i,j}$ are the mole fraction of component i on stage j in the liquid and vapor, respectively.

For a sieve-tray liquid-liquid contactor, the stage efficiency η may be expressed after some simplification [3]:

$$\eta = \frac{4.4K_f + 2K_r}{1 + 0.4K_f + K_r} \tag{A-22}$$

where K_f and K_r are the overall mass-transfer coefficients during drop formation and drop rise, respectively.

Combining this definition with the material and energy balances for each stage in a column, a system of non-linear algebraic equations is generated. Using the reliable convergence technique initially proposed by Ishii and Otto [4], the program obtains a converged set of stage compositions, phase rates and temperatures.

Calculation Options of AMINECalc

There are three calculation options (models) in AMINECalc:

Option 1: Mass Balance Calculation

The mass balance calculation option requires the input of flow rates and chemical species concentrations of the rich amine stream that come from an absorber column, and the flow rates of the lean amine stream from the regenerator. As shown in the figure in the following page, a rich amine stream with relatively high pressure goes to a flash tank with relatively low pressure. The program executes a flash calculation and calculates the flash tank vent gas flow rate and composition. The calculated information of the flash tank liquid stream and the input data of the lean amine stream are used in a mass balance calculation to give an estimate of the stripped acid gas contents from the top of the regeneration column. The details of the input requirements are summarized in the table on page A-11.

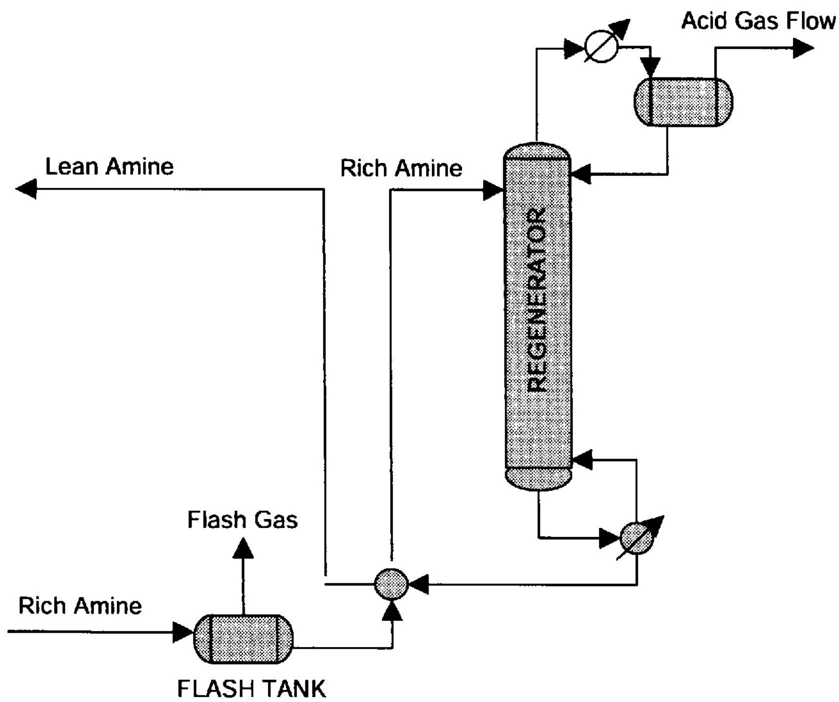
Option 2: Gas Process Simulation

The gas process simulation requires the input of sour gas feed data and lean amine circulation rate to the absorber as well as the number of the trays of the absorber column. See the flow diagram on page 10 for the sour gas treating process. The program will rigorously simulate the operation of the absorber column and calculate the hydrocarbon contents in rich amine stream. The calculated information of the rich amine stream will then be used to predict the flash tank vent gas and the stripped acid gas vent flow from the solvent regeneration section in the same way as described in Option 1. The details of the input requirements are summarized in the table on page A-11.

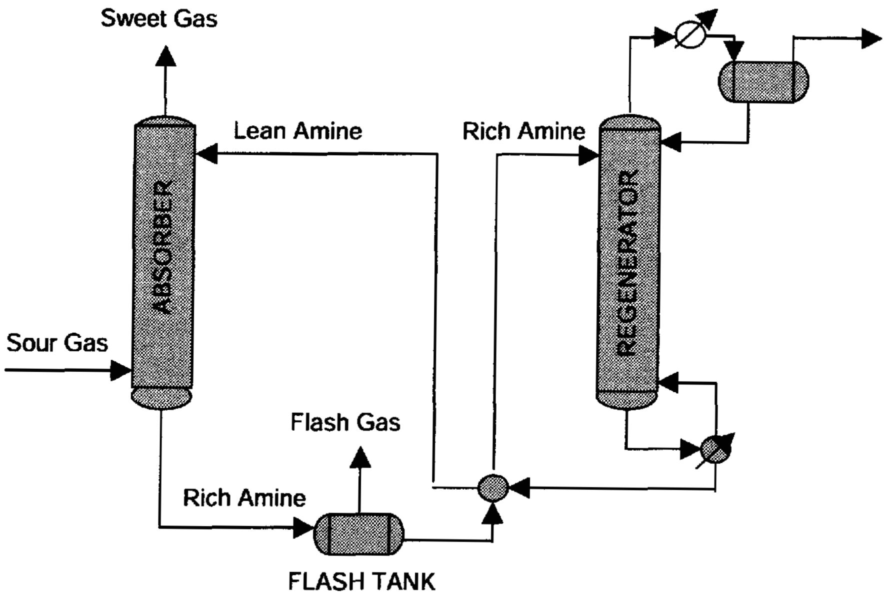
Option 3: NGL Process Simulation

The NGL process simulation shares the same flow diagram with Option 2, and requires the same input information. The difference between Option 3 and Option 2 is that the feed to the absorber column in Option 3 is in the liquid state, and the column is actually a liquid-liquid contactor. Instead of a vapor-liquid absorption process simulation, Option 3 offers a liquid-liquid extraction process simulation. The contents of the sweetened NGL from the top of the column along with the flash tank vent flow and the stripped acid gas vent flow are predicted.

Flow Diagram for Mass Balance Calculation



Flow Diagram for Sour Gas/NGL Process Simulation



Input Requirements for Each Calculation Option

Input Variables	Option 1	Option 2	Option 3
Sour Gas Feed			
Flow rate (MMSCF/D)		X	
Compositions (mole%)		X	
Temperature/Pressure (^{0}F/psia)		X	
NGL Feed			
Flow rate (gpm)			X
Compositions (mole%)			X
Temperature/Pressure (^{0}F/psia)			X
Lean Amine			
Temperature/Pressure (^{0}F/psia)	X	X	X
Flow rate (gpm)	X	X	X
Amine concentration (wt%)	X	X	X
Acid gas loadings (mole/mole)	X	X	X
Rich Amine			
Temperature/Pressure (^{0}F/psia)	X		
Flow rate (gpm)	X		
Compositions (mole%)	X		
Absorber			
Tray numbers		X	X
Flash Tank			
Pressure (psia)	X	X	X

Chemical Components

The AMINECalc program contains data for the alkanolamines that are commonly used by the industry, and hydrocarbons, gases and sulfur species encountered in sour gas/NGL treating. A list of the chemical species follows.

Alkanolamine Types:

Monoethanolamine	(MEA)
Diethanolamine	(DEA)
Triethanolamine	(TEA)
Methyldiethanolamine	(MDEA)
Diglycolamine	(DGA)

Hydrocarbons:

Methane	Octanes
Ethane	Nonanes
Propane	C_{10+}
i-Butane	Benzene
n-Butane	Toluene
i-Pentane	Ethylbenzene
n-Pentane	Xylenes
Hexanes	n-Hexane
Heptanes	2,2,4-Trimethylpentane

Non-Hydrocarbon Gases:

H_2S	N_2
CO_2	O_2

Sulfur Compounds:

Methyl mercaptan	(MeSH)
Ethyl mercaptan	(EtSH)

Program Limitations

The program contains a correlation of data that restrict its use to certain conditions of pressure, temperature and composition. These limitations are given below.

Amine Concentration

Equilibrium solubility data have been correlated over the following concentration ranges:

Amine	Concentration Range (wt%)
MEA	0 to 30
DEA	0 to 50
TEA	0 to 50
MDEA	0 to 50
DGA	50 to 70

Acid Gas Loading

The data have not been correlated above H_2S or CO_2 loadings of 1.0 mole acid gas / mole amine.

Temperature

The equilibrium solubility data have not been correlated beyond the range of temperatures from 25 °C to 125 °C (77 to 260 °F).

Stage Model

At present, the non-equilibrium stage model will accept up to 22 real stages in the absorber column.

Program Validation

The program predictions were verified against six sets of field data.

APPENDIX B

STANDARD EXAMPLES

MASS BALANCE CALCULATION

GAS PROCESS SIMULATION

NGL PROCESS SIMULATION

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MASS BALANCE CALCULATION

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AMINECalc Input Data

Project Name:	Untitled Type project description here	
Model:	Mass Balance	
Amine:	MDEA	
Lean Amine Pressure:	800.000	[psia]
Lean Amine Temperature:	100.000	[F]
Lean Amine Flowrate:	200.000	[gal/min]
Lean Amine Weight:	30.000	[%]
H2S Loading:	0.010	[mol/mol]
CO2 Loading:	0.010	[mol/mol]
Emission Control Efficiency	95.000	
Operating Hours/Day:	24	[hours/day]
Operating Days/Year:	256	[days/year]
Rich Amine Pressure:	800.000	[psia]
Rich Amine Temperature:	110.000	[F]
Rich Amine Flowrate:	200.000	[lb/h]
Flash Tank Pressure:	100.000	[psia]
H2S	1.00000	[%]
CO2	0.55000	[%]
MDEA	6.00000	[%]
H2O	92.45000	[%]
N2	0.00000	[%]
O2	0.00000	[%]
C1	0.10000	[%]
C2	0.00000	[%]
C3	0.00000	[%]
i-C4	0.00000	[%]
n-C4	0.00000	[%]
i-C5	0.00000	[%]
n-C5	0.00000	[%]
Hexanes	0.00000	[%]
Heptanes	0.00000	[%]
Octanes	0.00000	[%]
Nonanes	0.00000	[%]
C10+	0.00000	[%]
MeSH	0.00000	[%]
EtSH	0.00000	[%]
Benzene	0.00000	[%]
Toluene	0.00000	[%]
Ethylbenzene	0.00000	[%]
Xylenes	0.00000	[%]
n-C6	0.00000	[%]
224Trimeth	0.00000	[%]

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Stream 2 Rich Amine From Absorber

Component	Mol Fraction	[lb/h]	[ton/yr]
H2S	0.009990	1460.750	4487.348
CO2	0.005495	1037.627	3187.536
MDEA	0.059940	30651.060	94158.450
H2O	0.923576	71407.000	219358.600
C1	0.000999	68.772	211.264
Total:	1.000000	104625.200	321403.200

Pressure	800.000	[psia]
Temperature	110.000	[F]

Stream 3 Flash Gas Vent Flow from Flash Tank

	----- Controlled -----		----- Uncontrolled -----	
Component	[lb/h]	[ton/yr]	[lb/h]	[ton/yr]
H2S	0.028	0.085	0.556	1.707
CO2	0.371	1.139	0.371	1.139
MDEA	0.000	0.000	0.000	0.001
H2O	0.041	0.126	0.818	2.512
C1	2.986	9.174	59.728	183.482
Total:	3.426	10.524	61.473	188.841

Pressure	100.000	[psia]
Temperature	110.000	[F]

Stream 4 Rich Amine Feed to Regenerator

Component	Mol Fraction	[lb/h]	[ton/yr]
H2S	0.009995	1460.194	4485.640
CO2	0.005497	1037.256	3186.398
MDEA	0.059993	30651.060	94158.450
H2O	0.924383	71406.180	219356.100
C1	0.000131	9.044	27.783
Total:	1.000000	104563.700	321214.300

Pressure	100.000	[psia]
Temperature	110.000	[F]

Stream 5 Acid Gas Flow from Regenerator

Component	----- Controlled ----- [lb/h]	[ton/yr]	----- Uncontrolled ----- [lb/h]	[ton/yr]
H2S	68.591	210.709	1371.822	4214.167
CO2	923.122	2835.783	923.122	2835.783
MDEA	0.000	0.000	0.000	0.000
H2O	0.000	0.000	0.000	0.000
C1	0.452	1.389	9.044	27.783
Total:	992.165	3047.880	2303.989	7077.733

Pressure	N/A	[psia]
Temperature	N/A	[F]

Stream 6 Lean Amine from Regenerator

Component	Mol Fraction	[lb/h]	[ton/yr]
H2S	0.000608	88.372	271.474
CO2	0.000608	114.134	350.614
MDEA	0.060781	30905.200	94939.160
H2O	0.938003	72112.130	221524.700
C1	0.000000	0.000	0.000
Total:	1.000000	103219.800	317086.000

Pressure	800.000	[psia]
Temperature	100.000	[F]

GAS PROCESS SIMULATION

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AMINECalc Input Data

Project Name:	Untitled	
	Type project description here	
Model:	Gas Model	
Amine:	MDEA	
Lean Amine Pressure:	800.000	[psia]
Lean Amine Temperature:	100.000	[F]
Lean Amine Flowrate:	200.000	[gal/min]
Lean Amine Weight:	30.000	[%]
H2S Loading:	0.010	[mol/mol]
CO2 Loading:	0.010	[mol/mol]
Emission Control Efficiency	95.000	
Operating Hours/Day:	24	[hours/day]
Operating Days/Year:	256	[days/year]
Gas Feed Pressure:	805.000	[psia]
Gas Feed Temperature:	100.000	[F]
Gas Feed Flowrate:	30.000	[MMSCFD]
Number of Trays in Column:	20	
Flash Tank Pressure:	100.000	[psia]
H2S	2.00000	[%]
CO2	6.00000	[%]
MDEA	0.00000	[%]
H2O	0.00000	[%]
N2	0.00000	[%]
O2	0.00000	[%]
C1	92.00000	[%]
C2	0.00000	[%]
C3	0.00000	[%]
i-C4	0.00000	[%]
n-C4	0.00000	[%]
i-C5	0.00000	[%]
n-C5	0.00000	[%]
Hexanes	0.00000	[%]
Heptanes	0.00000	[%]
Octanes	0.00000	[%]
Nonanes	0.00000	[%]
C10+	0.00000	[%]
MeSH	0.00000	[%]
EtSH	0.00000	[%]
Benzene	0.00000	[%]
Toluene	0.00000	[%]
Ethylbenzene	0.00000	[%]
Xylenes	0.00000	[%]
n-C6	0.00000	[%]
224Trimeth	0.00000	[%]

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Stream 1 Gas Feed to Absorber

Component	Mol Fraction	[lb/h]	[ton/yr]
H2S	0.020000	2244.855	6896.077
CO2	0.060000	8697.857	26719.360
MDEA	0.000000	0.000	0.000
H2O	0.000000	0.000	0.000
C1	0.920000	48616.430	149347.100
Total:	1.000000	59559.140	182962.600

Pressure	805.000	[psia]
Temperature	100.000	[F]

Stream 2 Rich Amine From Absorber

Component	Mol Fraction	[lb/h]	[ton/yr]
H2S	0.015453	2332.352	7164.863
CO2	0.022542	4394.047	13498.280
MDEA	0.058552	30905.160	94939.040
H2O	0.902585	72030.240	221273.100
C1	0.000867	61.635	189.339
Total:	1.000000	109723.400	337064.700

Pressure	805.000	[psia]
Temperature	136.463	[F]

Stream 3 Flash Gas Vent Flow from Flash Tank

	----- Controlled -----		----- Uncontrolled -----	
Component	[lb/h]	[ton/yr]	[lb/h]	[ton/yr]
H2S	0.419	1.289	8.389	25.769
CO2	19.958	61.308	19.958	61.308
MDEA	0.000	0.000	0.001	0.003
H2O	0.094	0.288	1.876	5.764
C1	2.746	8.436	54.923	168.719
Total:	23.217	71.321	85.146	261.565

Pressure	100.000	[psia]
Temperature	136.463	[F]

Stream 4 Rich Amine Feed to Regenerator

Component	Mol Fraction	[lb/h]	[ton/yr]
H2S	0.015413	2323.961	7139.088
CO2	0.022461	4374.084	13436.960
MDEA	0.058608	30905.160	94939.030
H2O	0.903424	72028.360	221267.400
C1	0.000095	6.715	20.627
Total:	1.000000	109638.300	336803.100

Pressure	100.000	[psia]
Temperature	136.463	[F]

Stream 5 Acid Gas Flow from Regenerator

	----- Controlled -----		----- Uncontrolled -----	
Component	[lb/h]	[ton/yr]	[lb/h]	[ton/yr]
H2S	111.779	343.381	2235.590	6867.615
CO2	4259.950	13086.340	4259.950	13086.340
MDEA	0.000	0.000	0.000	0.000
H2O	0.000	0.000	0.000	0.000
C1	0.336	1.032	6.715	20.627
Total:	4372.065	13430.760	6502.255	19974.590

Pressure	N/A	[psia]
Temperature	N/A	[F]

Stream 6 Lean Amine from Regenerator

Component	Mol Fraction	[lb/h]	[ton/yr]
H2S	0.000608	88.372	271.474
CO2	0.000608	114.134	350.614
MDEA	0.060781	30905.200	94939.160
H2O	0.938003	72112.130	221524.700
C1	0.000000	0.000	0.000
Total:	1.000000	103219.800	317086.000

Pressure	800.000	[psia]
Temperature	100.000	[F]

Stream 7 Sweet Gas Flow from Absorber

Component	Mol Fraction	[lb/h]	[ton/yr]
H2S	0.000008	0.873	2.683
CO2	0.032059	4418.250	13572.630
MDEA	0.000000	0.019	0.058
H2O	0.001451	81.843	251.419
C1	0.966482	48554.730	149157.600
Total:	1.000000	53055.720	162984.400

Pressure	800.000	[psia]
Temperature	101.559	[F]

NGL PROCESS SIMULATION

AMINECalc Input Data

Project Name:	Untitled Type project description here	
Model:	NGL Model	
Amine:	DEA	
Lean Amine Pressure:	815.000	[psia]
Lean Amine Temperature:	80.000	[F]
Lean Amine Flowrate:	16.000	[gal/min]
Lean Amine Weight:	7.000	[%]
H2S Loading:	0.010	[mol/mol]
CO2 Loading:	0.300	[mol/mol]
Emission Control Efficiency	95.000	
Operating Hours/Day:	24	[hours/day]
Operating Days/Year:	365	[days/year]
NGL Feed Pressure:	815.000	[psia]
NGL Feed Temperature:	85.000	[F]
NGL Feed Flowrate:	120.000	[lb/h]
Number of Trays in Column:	10	
Flash Tank Pressure:	80.000	[psia]
H2S	0.00150	[%]
CO2	0.64898	[%]
DEA	0.00000	[%]
H2O	0.00000	[%]
N2	0.00400	[%]
O2	0.00000	[%]
C1	0.35399	[%]
C2	37.68903	[%]
C3	40.76484	[%]
i-C4	3.88278	[%]
n-C4	11.11446	[%]
i-C5	2.12293	[%]
n-C5	2.30993	[%]
Hexanes	0.00000	[%]
Heptanes	0.00000	[%]
Octanes	0.00000	[%]
Nonanes	0.00000	[%]
C10+	0.00000	[%]
MeSH	0.00000	[%]
EtSH	0.00000	[%]
Benzene	0.00100	[%]
Toluene	0.00050	[%]
Ethylbenzene	0.00010	[%]
Xylenes	0.00000	[%]
n-C6	1.10597	[%]
224Trimeth	0.00000	[%]

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Stream 1	NGL Feed to Absorber		
Component	Mol Fraction	[lb/h]	[ton/yr]
H2S	0.000015	0.386	1.692
CO2	0.006490	215.826	945.303
DEA	0.000000	0.000	0.000
H2O	0.000000	0.000	0.000
N2	0.000040	0.847	3.708
C1	0.003540	42.914	187.960
C2	0.376890	8563.866	37509.100
C3	0.407648	13583.640	59495.350
i-C4	0.038828	1705.375	7469.414
n-C4	0.111145	4881.636	21381.200
i-C5	0.021229	1157.443	5069.514
n-C5	0.023099	1259.397	5516.066
Benzene	0.000010	0.590	2.585
Toluene	0.000005	0.348	1.524
Ethylbenzene	0.000001	0.080	0.352
n-C6	0.011060	720.214	3154.482
Total:	1.000000	32132.560	140738.200
Pressure	815.000	[psia]	
Temperature	85.000	[F]	

Stream 2	Rich Amine From Absorber		
Component	Mol Fraction	[lb/h]	[ton/yr]
H2S	0.000130	1.939	8.492
CO2	0.011058	213.808	936.465
DEA	0.012600	582.011	2549.163
H2O	0.975183	7719.446	33810.600
N2	0.000000	0.000	0.001
C1	0.000004	0.031	0.138
C2	0.000611	8.076	35.371
C3	0.000402	7.789	34.114
i-C4	0.000002	0.045	0.196
n-C4	0.000005	0.128	0.562
i-C5	0.000001	0.043	0.191
n-C5	0.000001	0.047	0.207
Benzene	0.000001	0.051	0.225
Toluene	0.000000	0.000	0.000
Ethylbenzene	0.000000	0.005	0.022
n-C6	0.000001	0.032	0.138
Total:	1.000000	8533.452	37375.890
Pressure	815.000	[psia]	
Temperature	84.510	[F]	

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Stream 3 Flash NGL Vent Flow from Flash Tank

	Controlled		Uncontrolled	
Component	[lb/h]	[ton/yr]	[lb/h]	[ton/yr]
H2S	0.001	0.004	0.021	0.093
CO2	1.730	7.575	1.730	7.575
DEA	0.000	0.000	0.000	0.000
H2O	0.003	0.013	0.058	0.254
N2	0.000	0.000	0.000	0.001
C1	0.001	0.007	0.028	0.122
C2	0.348	1.526	6.967	30.517
C3	0.345	1.512	6.906	30.249
i-C4	0.002	0.010	0.045	0.195
n-C4	0.006	0.028	0.128	0.559
i-C5	0.002	0.010	0.043	0.190
n-C5	0.002	0.010	0.047	0.206
Benzene	0.000	0.001	0.005	0.022
Toluene	0.000	0.000	0.000	0.000
Ethylbenzene	0.000	0.000	0.000	0.002
n-C6	0.001	0.007	0.030	0.131
Total:	2.441	10.702	16.008	70.115

Pressure	80.000	[psia]
Temperature	84.510	[F]

Stream 4 Rich Amine Feed to Regenerator

Component	Mol Fraction	[lb/h]	[ton/yr]
H2S	0.000128	1.918	8.399
CO2	0.010980	212.078	928.886
DEA	0.012613	582.011	2549.163
H2O	0.976148	7719.388	33810.350
N2	0.000000	0.000	0.000
C1	0.000000	0.003	0.015
C2	0.000084	1.109	4.857
C3	0.000046	0.883	3.866
i-C4	0.000000	0.000	0.001
n-C4	0.000000	0.001	0.002
i-C5	0.000000	0.000	0.001
n-C5	0.000000	0.000	0.001
Benzene	0.000001	0.046	0.203
Toluene	0.000000	0.000	0.000
Ethylbenzene	0.000000	0.004	0.020
n-C6	0.000000	0.002	0.008
Total:	1.000000	8517.443	37305.770

Pressure	80.000	[psia]
Temperature	84.510	[F]

Stream 5 Acid Gas Flow from Regenerator

Component	----- Controlled ----- [lb/h]	[ton/yr]	----- Uncontrolled ----- [lb/h]	[ton/yr]
H2S	0.002	0.007	0.032	0.138
CO2	138.992	608.773	138.992	608.773
DEA	0.000	0.000	0.000	0.000
H2O	0.000	0.000	0.000	0.000
N2	0.000	0.000	0.000	0.000
C1	0.000	0.001	0.003	0.015
C2	0.055	0.243	1.109	4.857
C3	0.044	0.193	0.883	3.866
i-C4	0.000	0.000	0.000	0.001
n-C4	0.000	0.000	0.001	0.002
i-C5	0.000	0.000	0.000	0.001
n-C5	0.000	0.000	0.000	0.001
Benzene	0.002	0.010	0.046	0.203
Toluene	0.000	0.000	0.000	0.000
Ethylbenzene	0.000	0.001	0.004	0.020
n-C6	0.000	0.000	0.002	0.008
Total:	139.095	609.227	141.072	617.885

Pressure	N/A	[psia]
Temperature	N/A	[F]

Stream 6 Lean Amine from Regenerator

Component	Mol Fraction	[lb/h]	[ton/yr]
H2S	0.000127	1.886	8.262
CO2	0.003805	73.086	320.112
DEA	0.012685	582.011	2549.163
H2O	0.983383	7732.428	33867.460
N2	0.000000	0.000	0.000
C1	0.000000	0.000	0.000
C2	0.000000	0.000	0.000
C3	0.000000	0.000	0.000
i-C4	0.000000	0.000	0.000
n-C4	0.000000	0.000	0.000
i-C5	0.000000	0.000	0.000
n-C5	0.000000	0.000	0.000
Benzene	0.000000	0.000	0.000
Toluene	0.000000	0.000	0.000
Ethylbenzene	0.000000	0.000	0.000
n-C6	0.000000	0.000	0.000
Total:	1.000000	8389.411	36745.000

Pressure	815.000	[psia]
Temperature	80.000	[F]

Stream 7 Sweet NGL Flow from Absorber

Component	Mol Fraction	[lb/h]	[ton/yr]
H2S	0.000013	0.334	1.462
CO2	0.002267	75.112	328.987
DEA	0.000000	0.000	0.000
H2O	0.000957	12.980	56.851
N2	0.000040	0.846	3.707
C1	0.003551	42.883	187.822
C2	0.378001	8555.789	37473.720
C3	0.409001	13575.850	59461.230
i-C4	0.038978	1705.330	7469.216
n-C4	0.111574	4881.507	21380.640
i-C5	0.021311	1157.399	5069.322
n-C5	0.023188	1259.350	5515.858
Benzene	0.000009	0.539	2.360
Toluene	0.000005	0.348	1.524
Ethylbenzene	0.000001	0.075	0.330
n-C6	0.011102	720.182	3154.343
Total:	1.000000	31988.530	140107.400

Pressure	815.000	[psia]
Temperature	85.859	[F]

APPENDIX C

REFERENCES

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REFERENCES

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