

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:

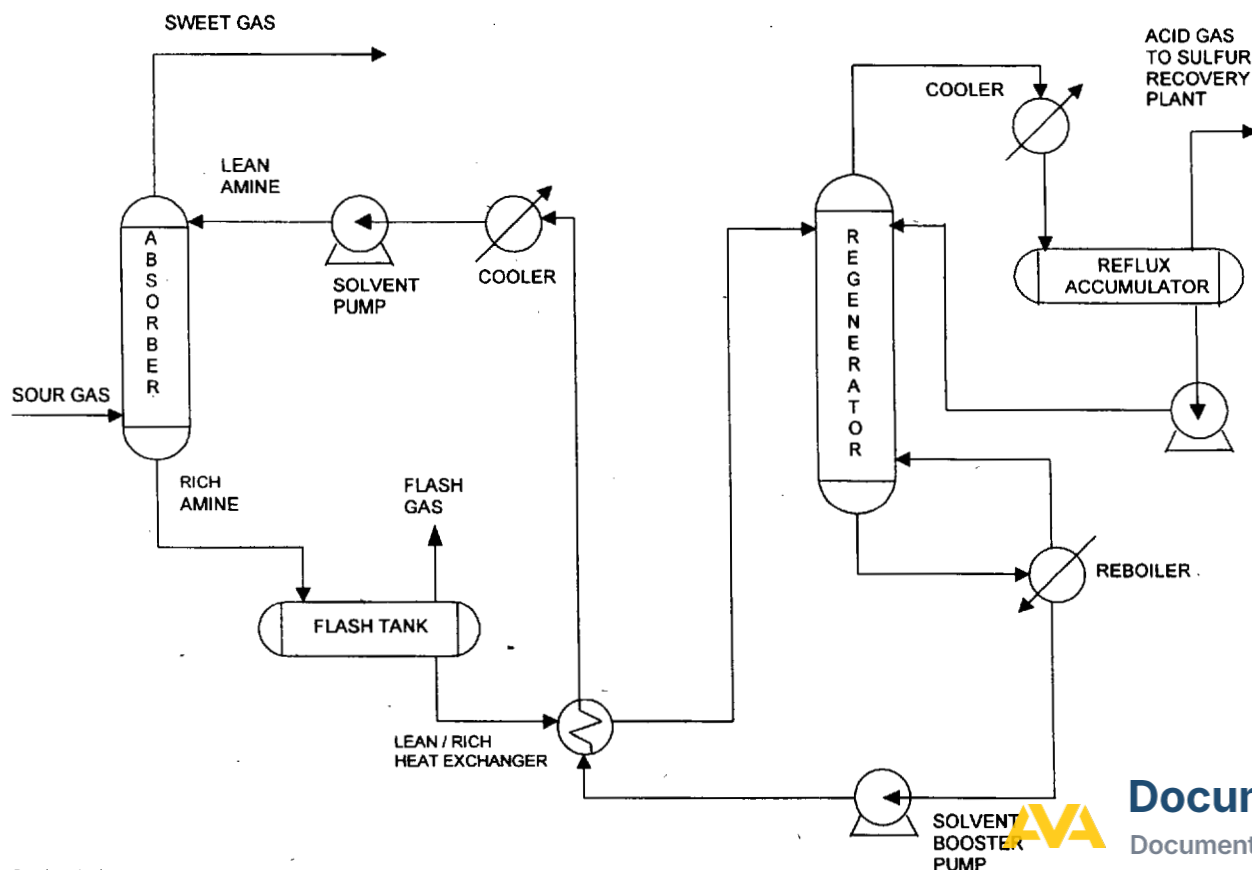
Telephone: (780) 463-8638
Fax: (780) 450-1668
E-mail: support@dbra.com

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.

AMINE UNIT EMISSIONS MODEL

AMINECALC VERSION 1.0 USER'S MANUAL

HEALTH AND ENVIRONMENTAL SCIENCES DEPARTMENT
PUBLICATION NUMBER 4679
JANUARY 1999



For Technical Support:

(403) 463-8638

DB ROBINSON AND ASSOCIATES, LTD.

9419-20 AVENUE

EDMONTON, ALBERTA T6N 1E5

CANADA

FAX: (403) 450-1668

Record the AMINECalc Registration Number
from the enclosed registration form:

I46790 - _ _ _

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

FOREWORD

API PUBLICATIONS NECESSARILY ADDRESS PROBLEMS OF A GENERAL NATURE. WITH RESPECT TO PARTICULAR CIRCUMSTANCES, LOCAL, STATE, AND FEDERAL LAWS AND REGULATIONS SHOULD BE REVIEWED.

API IS NOT UNDERTAKING TO MEET THE DUTIES OF EMPLOYERS, MANUFACTURERS, OR SUPPLIERS TO WARN AND PROPERLY TRAIN AND EQUIP THEIR EMPLOYEES, AND OTHERS EXPOSED, CONCERNING HEALTH AND SAFETY RISKS AND PRECAUTIONS, NOR UNDERTAKING THEIR OBLIGATIONS UNDER LOCAL, STATE, OR FEDERAL LAWS.

NOTHING CONTAINED IN ANY API PUBLICATION IS TO BE CONSTRUED AS GRANTING ANY RIGHT, BY IMPLICATION OR OTHERWISE, FOR THE MANUFACTURE, SALE, OR USE OF ANY METHOD, APPARATUS, OR PRODUCT COVERED BY LETTERS PATENT. NEITHER SHOULD ANYTHING CONTAINED IN THE PUBLICATION BE CONSTRUED AS INSURING ANYONE AGAINST LIABILITY FOR INFRINGEMENT OF LETTERS PATENT.

All rights reserved. No part of this work may be reproduced, stored in a retrieval system, or transmitted by any means, electronic, mechanical, photocopying, recording, or otherwise, without prior written permission from the publisher. Contact the publisher, API Publishing Services, 1220 L Street, N.W., Washington, D.C. 20005.

Copyright © 1999 American Petroleum Institute

ACKNOWLEDGMENTS

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

API STAFF CONTACT

Paul Martino, Health and Environmental Sciences Department

MEMBERS OF THE PROJECT GROUP

Tom Backhouse, Phillips Petroleum

Vance Burton, Mobil E & P

William Fishback, Mobil E & P

Wayne Hamilton, Shell

Robert Lott, GRI

Jim McCarthy, GRI

Vernon Schievelbein, Texaco

Andy Shah, Conoco

Dan Van Der Zanden, Chevron

Charles Wallace, Shell

Gary Webster, Canadian Assn. of Petroleum Producers

Jenny Yang, Marathon

CONTENTS

EXECUTIVE SUMMARY	1
CHAPTER 1 INTRODUCTION.....	3
Typical Flow Diagram of an Amine Sweetening Unit.....	3
CHAPTER 2 INSTALLING AMINECalc	5
System Requirements	5
Installing AMINECalc	5
CHAPTER 3 GETTING STARTED	7
Starting AMINECalc	7
Project Setup	8
AMINECalc Desktop	9
Menu Bar	9
Toolbar.....	10
Project Setup Viewing Box	10
Message Box.....	11
Status Bar	11
Process Flowsheet.....	12
Data Input Mode.....	12
Data Output Mode	12
Unit Systems	13
Engineering Units.....	13
International System (SI) Units.....	13
CHAPTER 4 RUNNING AMINECalc.....	15
Calculation Models	15
Mass Balance Calculation	15
Process Flowsheet.....	16
Input Data	16
Flash Tank Pressure	16
Rich Amine to Flash Tank	17
Lean Amine from Regenerator.....	17
Gas Process Simulation.....	18
Process Flowsheet.....	18
Input Data	18
Sour Gas Feed	19
Absorber	19
Flash Tank Pressure	20
Lean Amine from Regenerator.....	20

CONTENTS (continued)**CHAPTER 4 RUNNING AMINECalc (continued)**

Natural Gas Liquid (NGL) Process Simulation	20
Process Flowsheet.....	20
Input Data	20
NGL Feed.....	21
Absorber	21
Flash Tank Pressure	21
Lean Amine from Regenerator.....	21
Executing Simulations.....	22

CHAPTER 5 VIEWING AND PRINTING RESULTS 23

Viewing and Printing Full Reports	23
Saving and Copying Reports.....	24
Viewing and Printing a Stream Output	25

APPENDIX A TECHNICAL BACKGROUND OF AMINECalc..... A-1

Thermodynamic Models	A-3
Phase Equilibria	A-3
Chemical Equilibria	A-4
Mass Transfer with Chemical Reaction	A-6
Non-Equilibrium Stage Model.....	A-7
Calculation Options of AMINECalc.....	A-8
Option 1: Mass Balance Calculation.....	A-8
Option 2: Gas Process Simulation.....	A-8
Option 3: NGL Process Simulation.....	A-9
Flow Diagram for Mass Balance Calculation	A-9
Flow Diagram for Sour Gas/NGL Process Simulation	A-10
Input Requirements for Each Calculation Option.....	A-11
Chemical Components	A-12
Program Limitations.....	A-13
Program Validation	A-13

APPENDIX B STANDARD EXAMPLES B-1

Mass Balance Calculation.....	B-3
Gas Process Simulation.....	B-9
NGL Process Simulation.....	B-15

APPENDIX C: REFERENCES C-1

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.

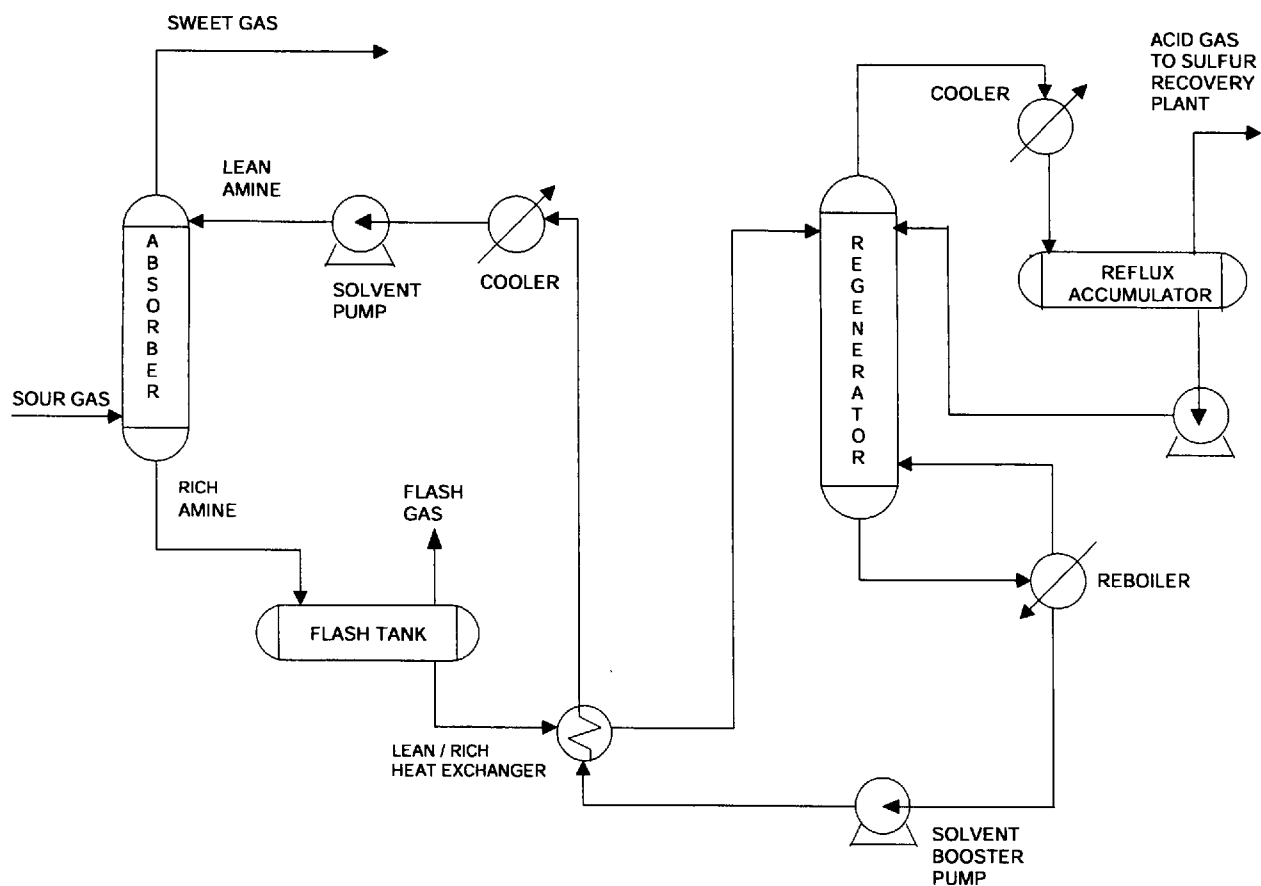
CHAPTER 1

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



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

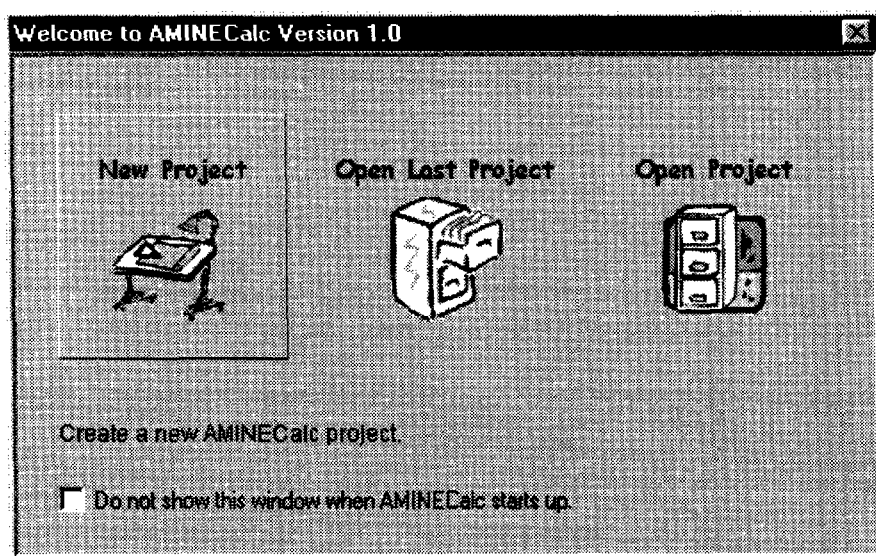
GETTING STARTED

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*.

Project Setup

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

Project Setup

Project Name
Untitled

Description
Type project description here

Model Selection
☒ Mass Balance ☐ Gas Model ☐ NGL Model

Amine Selection
☐ MEA [monoethanolamine] ☐ MDEA [methyldiethanolamine]
☐ DEA [diethanolamine] ☐ DGA [diglycolamine]
☒ TEA [triethanolamine]

Control Factor [%] Hours / Day Days / Year
 95.00 24 256

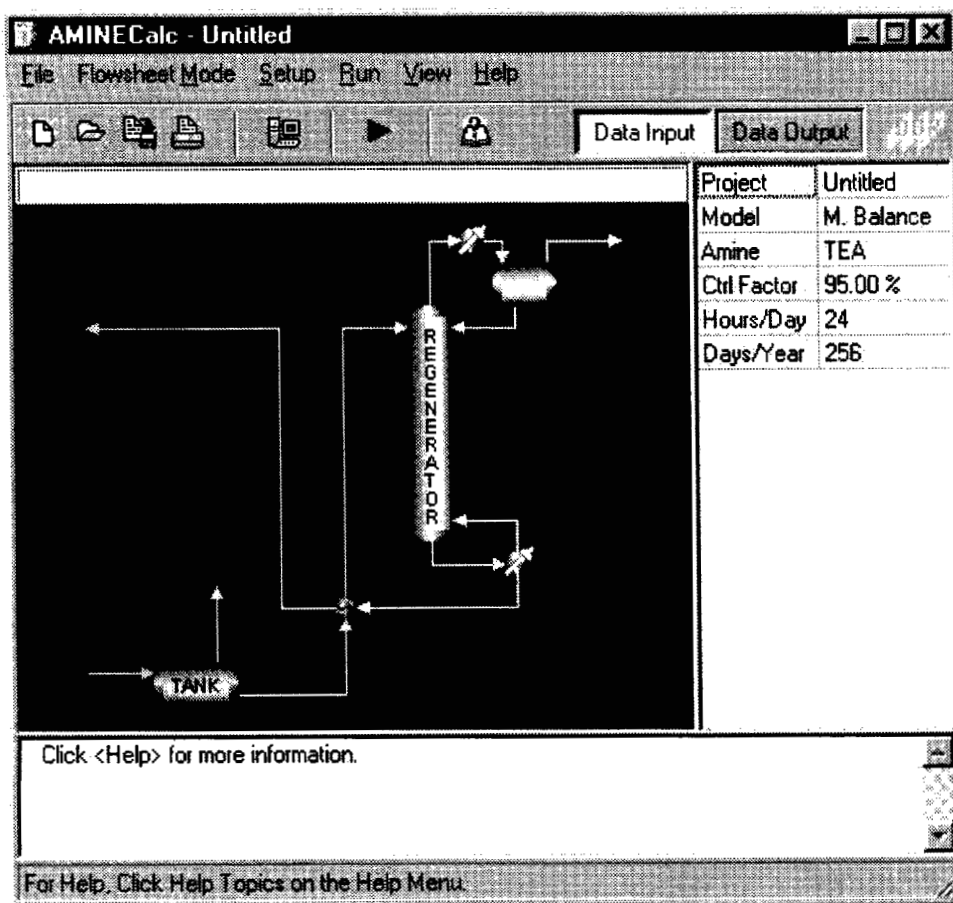
OK Cancel Help

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.

- * <3:58:27 PM>: Do you want to save current project? --- No!
- * <3:58:29 PM>: Begin Simulation...
- * <3:58:31 PM>: The Last Simulation was completed!



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.



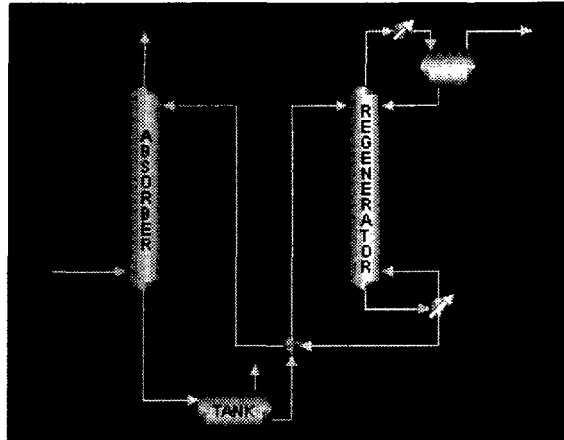
Note The Status Bar can be turned on/off by clicking on Status Bar from the View menu.

Process Flowsheet

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

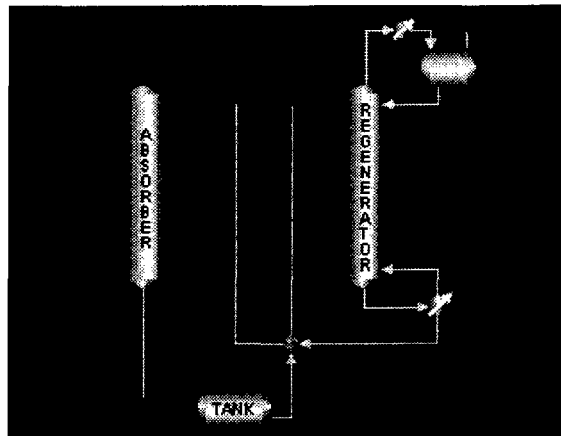
Data Input Mode

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

The screenshot shows the 'Lean Amine Feed to Absorber' dialog box with the following values and units:

Pressure	1018.00	[psia]
Temperature	110.00	[F]
Volumetric Flowrate	104.00	[gal/min]
Weight % Amine	32.40	
Mole Loading H ₂ S	0.0000	
Mole Loading CO ₂	0.0010	

At the bottom, the 'Engineering Units' radio button is selected, and the 'SI Units' radio button is unselected. Buttons for 'OK', 'Cancel', and 'Help' are on the right.

International System (SI) Units

The screenshot shows the 'Lean Amine Feed to Absorber' dialog box with the following values and units:

Pressure	7018.85	[kPa]
Temperature	43.33	[C]
Volumetric Flowrate	393.68	[L/min]
Weight % Amine	32.40	
Mole Loading H ₂ S	0.0000	
Mole Loading CO ₂	0.0010	

At the bottom, the 'SI Units' radio button is selected, and the 'Engineering Units' radio button is unselected. Buttons for 'OK', 'Cancel', and 'Help' are on the right.