CHEMCAD

User Guide

CHEMCAD User Guide

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Chemstations™

Chapter 1

Introduction to CHEMCAD

Welcome to CHEMCAD, a powerful and effective software tool for chemical process simulation. Whether you're a new or experienced CHEMCAD user, you'll appreciate the program's user-friendly, feature-rich interface. Creating flowsheets and running simulations is fast and easy with CHEMCAD, and the program is highly customizable to fit your needs and the way you work.

This User Guide will help you get up and running with CHEMCAD, from installation and licensing to details on using dynamics and data interfaces.

Overview of CHEMCAD and Its Uses

Today's chemical processing industry (CPI) faces numerous challenges: unpredictable fuel and feedstock costs, reduced engineering staff, shorter product life cycles, increased global competition, and increased regulation. These challenges require that CPI companies seek out and use the best tools to increase productivity and improve engineering decisions.

CHEMCAD is a powerful and flexible chemical process simulation environment, built around three key values of innovation, integration, and open architecture. These values create important advantages for CHEMCAD users:

- The latest chemical engineering techniques at your fingertips
- All functionality united in a single software environment
- Seamless connection to the chemical engineering computing environment, with links to tools such as MS Excel and Word and interfaces such as COM, DCOM, OPC, CAPE-OPEN, and XML

CHEMCAD combines a state-of-the-art graphical user interface (GUI), an extensive chemical component database, a large library of thermodynamic data, and a library of the most common unit operations to give users the ability to provide significant and measurable returns on their investment. In addition, the program is customizable to allow custom chemicals, thermodynamics, unit operations, calculations, and reporting—all ingredients for a powerful user experience.

CHEMCAD is capable of modeling continuous, batch, and semi-batch processes, and it can simulate both steady-state and dynamic systems. This program is used extensively around the world for the design, operation, and maintenance of chemical processes in a wide variety of industries, including oil and gas exploration, production, and refining; gas processing; commodity and specialty chemicals; pharmaceuticals; biofuels; and process equipment manufacturing.

Within all these industries, chemical engineers work every day with CHEMCAD to address a variety of challenges:

- Initial design of new processes
- Optimization or de-bottlenecking of existing processes
- Performance monitoring of processes
- Design and rating of process equipment such as vessels, columns, heat exchangers, piping, valves, and instrumentation
- Evaluation of safety relief devices
- Heat exchanger sizing
- Pressure and flow balancing of complex piping networks
- Reconciliation of plant data
- Economic comparisons of process alternatives
- Advanced process control (APC), including model predictive control (MPC), real-time optimization (RTO), and operator training systems (OTS)
- Scale-up of processes from lab-scale to pilot-scale, and from pilot-scale to full-scale
- Binary interaction parameter (BIP) regression from process or lab data
- Batch reaction rate regression from process or lab data

No matter how complex your process, CHEMCAD is capable of delivering the results you need to stay competitive in an increasingly fast and fluid global market. Easy to learn and highly customizable, CHEMCAD can put future-proof solutions within easy reach of your engineering staff.

CHEMCAD Products and Features

The CHEMCAD suite consists of several modules that serve specific purposes. Depending on your particular needs, you may have purchased some or all of these modules. The following are brief descriptions of the various CHEMCAD modules and their most common uses.

CC-STEADY STATE

The main CHEMCAD product, known as CC-STEADY STATE, enables you to design new processes, rate existing processes, and optimize processes in steady state.

CC-DYNAMICS

The module known as CC-DYNAMICS makes it possible to design new and rate existing processes using a dynamic simulation. This module is fully integrated with CHEMCAD to make switching between steady state and dynamics easy and intuitive. Using CC-DYNAMICS, you can easily simulate everything from simple vessel accumulation to complex control systems on columns. This module also provides tools for simulation of continuous stirred-tank reactors (CSTRs), including complex reaction rate and pressure calculation.

CC-BATCH

The CC-BATCH product enables you to design, rate, or optimize a batch distillation column. CC-BATCH includes a scheduling interface to allow an "operation step" approach to simulation of batch columns.

CC-THERM

The CC-THERM product lets you design a single heat exchanger, or vet a vendor's heat exchanger design. It is also ideal for customers who want to rate existing exchangers in new service, or to perform calculations on hypothetical situations. CC-THERM can simulate shell-and-tube, air-cooled, plate-and-frame, and double-pipe exchangers. Full integration with CHEMCAD makes it possible to calculate exit conditions from exchanger geometry for high-fidelity simulations.

CC-SAFETY NET

The CC-SAFETY NET product provides the capability to design or rate piping networks and safety relief devices and systems, in both steady-state and dynamic systems. The steady-state features of CC-SAFETY NET are included with CC-STEADY STATE. This product enables users to make simultaneous flow- and pressure-balanced simulations—even in reverse-flow situations—for single- or multi-phase flow.

CC-FLASH

The CC-FLASH module provides physical property and phase equilibrium data, as well as property prediction and regression. CC-FLASH is a subset of CC-STEADY STATE, and is meant for customers who do not need full flowsheet simulation tools.

CHEMCAD Features by Module

The following matrix lists the features associated with each component of the CHEMCAD suite. For a more detailed explanation, or to inquire about a particular component or feature, please contact Chemstations or your CHEMCAD distributor (see complete contact information at www.chemstations.com).

	CC-STEADY STATE	CC-DYNAMICS	CC-BATCH	CC-THERM	CC-SAFETY NET	CC-FLASH
VB/COM/OPC/Data Map	✓	✓				
Sensitivity/optimization	✓	✓			✓	
Sizing (line/valve/orifice/vessel)	✓	✓			✓	
Run steady state	✓		✓	✓	✓	✓
Run dynamics		✓			✓	
Run recycles	✓	✓			✓	
Costing	✓	✓			✓	
Reconciliation	✓	✓				
Sizing columns	✓	✓	✓			
Sizing heat exchangers				✓		
Economics	✓	✓				
Reports (incl. Excel)	✓	✓	✓	✓	✓	✓
DIERS	✓	✓			✓	
CO_2 solid	✓	✓			✓	✓
Hydrates	✓	✓			✓	✓
Depress	✓	✓			✓	✓
TOC/COD	✓	✓			✓	✓
Pure regression	✓	✓	✓	✓	✓	✓
BIP regression	✓	✓	✓	✓	✓	✓
Electrolyte regression	✓	✓	✓	✓	✓	✓
Rate regression	✓	✓				
Units calculator	✓	✓	✓	✓	✓	✓
Execute parser	✓	✓				
Environmental report	✓	✓	✓	✓	✓	✓
Simple calculator	✓	✓	✓	✓	✓	✓
Spec sheet	✓	✓	✓	✓	✓	

UnitOps by Module

The availability of certain unit operations, or UnitOps, in CHEMCAD simulations is a function of which modules you have licensed. The following matrix lists all available UnitOps and the CHEMCAD modules associated with them.

	CC-STEADY STATE	CC-DYNAMICS	CC-BATCH	CC-THERM	CC-SAFETY NET	CC-FLASH
Baghouse filter	✓	✓				
Batch column			✓			
Calculator	✓	✓				
Centrifuge	✓	✓				
Component separator	✓	✓				
Compressor	✓	✓			✓	
Control valve	✓	✓			✓	
Controller	✓	✓			✓	
Crusher/grinder	✓	✓				
Crystallizer	✓	✓				
Cyclone	✓	✓				
Divider	✓	✓			✓	✓
Electrostatic precipitator	✓	✓				
Equilibrium reactor	✓	✓				
Excel unit	✓	✓				
Expander	✓	✓			✓	
Fired heater	✓	✓				
Flash	✓	✓			✓	✓
Gibbs reactor	✓	✓				
Heat exchanger	✓	✓		✓	✓	
Hydrocyclone	✓	✓				
Kinetic reactor	✓	✓				
Liquid/liquid extractor	✓	✓				
LNGH exchanger	✓	✓				
Loop	✓	✓				
Membrane	✓	✓				
Mixer	✓	✓			✓	✓

	CC-STEADY STATE	CC-DYNAMICS	CC-BATCH	CC-THERM	CC-SAFETY NET	CC-FLASH
Node	✓	✓			✓	
PID controller	✓	✓			✓	
Pipe simulator	✓	✓			✓	
Polymer reactor						
Pump	✓	✓			✓	
Ramp controller	✓	✓			✓	
Relief device	✓	✓				
Run subflowsheet META unit	✓	✓				
SCDS distillation column	✓	✓				
Screen	✓	✓				
Sedimentator	✓	✓				
Shortcut column	✓	✓				
Solids dryer	✓	✓				
Solids washer	✓	✓				
Stoichiometric reactor	✓	✓				
Stream reference	✓	✓				
Tank			✓			
Time delay		✓			✓	
Time switch		✓	✓			
Tower distillation column	✓	✓				
Tower plus distillation column	✓	✓				
User-added module	✓	✓				
Vacuum filter	✓	✓				
Valve	✓	✓			✓	
Venturi scrubber	✓	✓				
Vessel	✓	✓				
Vessel reactor		✓			✓	

Chapter 2

Getting Started with CHEMCAD

To start using CHEMCAD, you'll need to obtain the software, install it on your computer, and set up a valid software license. This chapter provides step-by-step instructions for these tasks.

Before you begin, please ensure that your PC meets the recommended system requirements, as listed below. It's also a good idea to find out whether your copy of CHEMCAD will rely on a network license; if it will, make sure to ask your network administrator for all the information that you'll need when installation is complete and it's time to set up licensing.

CHEMCAD System Requirements

Processor: 1 GHz or faster, 32- or 64-bit

Operating system: Windows 7 or later (all 32- and 64-bit versions)

RAM: 1 GB for 32-bit, or 2 GB for 64-bit

Video card: DirectX 9 graphics device with WDDM 1.0 or higher driver

Display resolution: 1920 x 1080 or higher

Hard disk space: 16 GB (32-bit) or 20 GB (64-bit) for installation, 1 GB free space recommended

Productivity software: Some features require

If you'll be using a hardware dongle to license CHEMCAD, make sure the dongle is inserted into a USB port before you attempt to run the program.

To obtain the CHEMCAD installation file, you'll need a live Internet connection and a web browser. You can either download the file directly onto the system where you plan to install CHEMCAD, or download the file and place it onto a portable drive for installation

on a different computer. In either case, the download process requires that you log into Chemstations' User Support Center.

Creating a User Support Center Account

The first time you visit Chemstations' User Support Center, you'll need to set up a user account. Follow the steps below to do this.

1. On the Chemstations website home page (**www.chemstations.com**), click the **User Login** button in the upper right area of the screen.
2. On the login screen, click the **Forgot your password?** button.

*Figure 2-01: Clicking the **Forgot your password?** button on the login screen*

3. On the next screen, enter a valid e-mail address, and click the **Send** button. Be sure to use your company address, as the login system will match your address against our customer database.
4. If your address is found, you will receive an e-mail from CHEMCAD Technical Support, offering a link to reset your password. Follow the instructions in the e-mail and at the password reset screen to complete your registration.

Note: In the event you do not receive a password reset e-mail within 24 hours, your address may not have been found in our database. Please contact Chemstations Technical Support (**support@chemstations.com**) for assistance.

Downloading the Software

Once your user login is established, you can download the latest version of CHEMCAD from the Chemstations website (**www.chemstations.com**).

On the home page, click the **User Login** button. The next screen will invite you to sign in. When you have done this, click the **Downloads** link at the top of the screen.

The resulting Downloads list will include the .exe version of the latest CHEMCAD installation file. When you have downloaded this file to your local system, you can begin installation.

Installing the software

Locate the installation file, called **CHEMCAD_*version number*_Setup.exe**, and double-click it to start the installation. The first InstallShield Wizard screen appears.

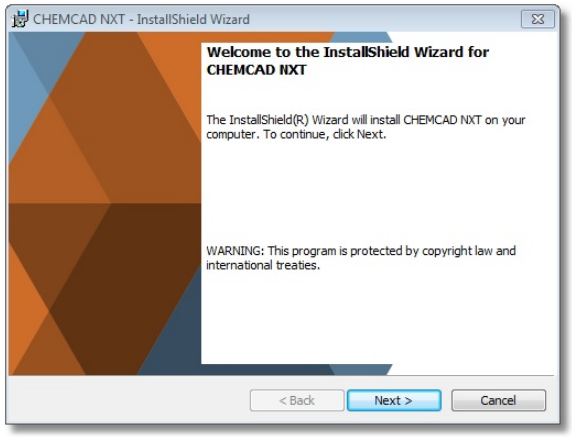


Figure 2-02: The CHEMCAD NXT - InstallShield Wizard screen

Click **Next** to begin the installation process. The License Agreement screen appears, listing the terms of the CHEMCAD standard license. Once you've read and understood the license terms, you'll need to click the *I accept the terms in the license agreement* button before you can click **Next** to proceed. Note that you have the option to print a copy of the license agreement from this screen.

Figure 2-03: The License Agreement screen

The Destination Folder screen appears next, displaying the name of the folder into which the CHEMCAD files will be installed by default. Normally, this destination is **C:\Program Files\Chemstations\CHEMCAD** (or some variation, based on your version of Windows), and it is recommended that you use this location unless you have a specific need to install the program elsewhere. Click the **Change** button if you want to change the file destination, or click **Next** to accept the suggested destination and proceed.

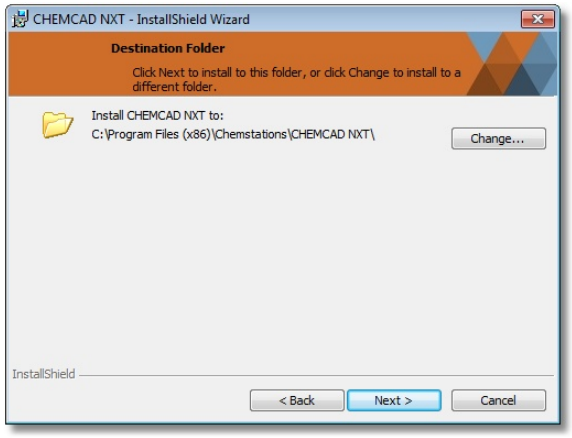


Figure 2-04: The Destination Folder screen

The Setup Type screen now appears, offering a choice between complete and custom installation. Each type of installation is described on the screen. Either accept the default setting of **Complete** or click **Custom** to select specific components to install, then click **Next** to proceed.

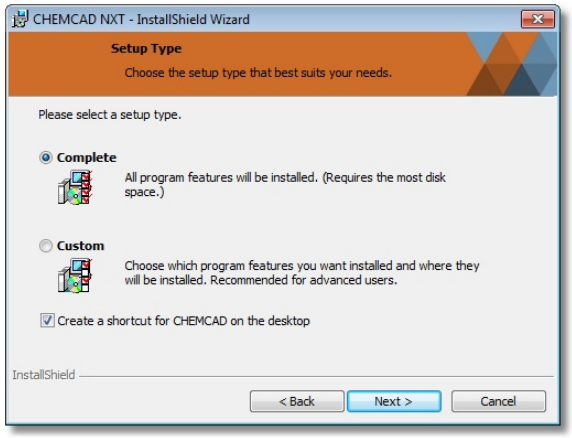


Figure 2-05: The Setup Type screen

This brings you to the Ready to Install the Program screen. Note that on this screen, and in fact on any screen in the installation process, you can click **Back** to return to a previous screen and verify or change your installation options. If you are satisfied with your settings as they are, click **Install** to start the installation.

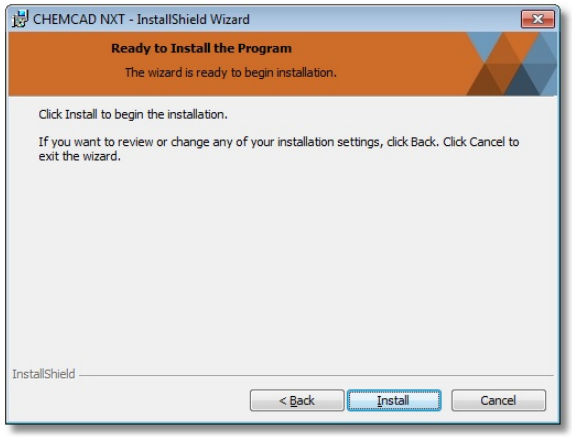


Figure 2-06: The Ready to Install the Program screen

The Installing CHEMCAD Suite screen appears, showing the progress of your installation with a green status bar.

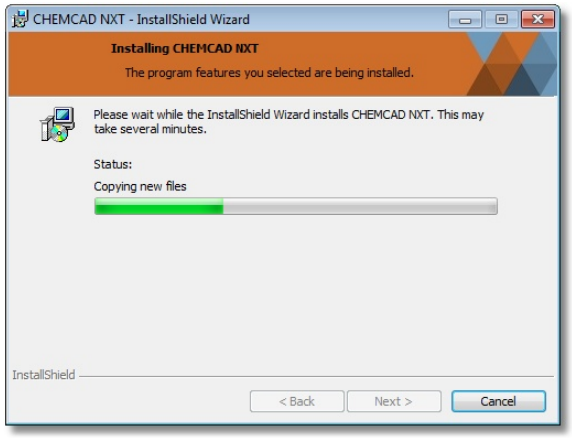


Figure 2-07: Status bar showing the progress of CHEMCAD installation

During installation, you may notice a second, smaller installation window that pops up. This shows the progress of various software components that are being found and installed so that CHEMCAD installation may proceed. To ensure successful completion of the install procedure, be sure to leave this window open; it will close automatically when all components are in place.

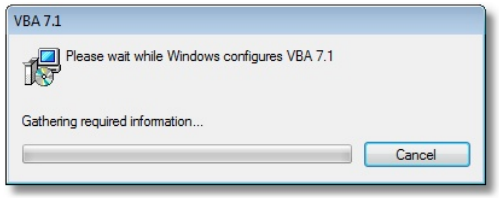


Figure 2-08: Software component installation message

When installation is complete, you'll see one final screen, which states that the InstallShield Wizard has completed installation of the CHEMCAD Suite. Click **Finish** to close the installer window.

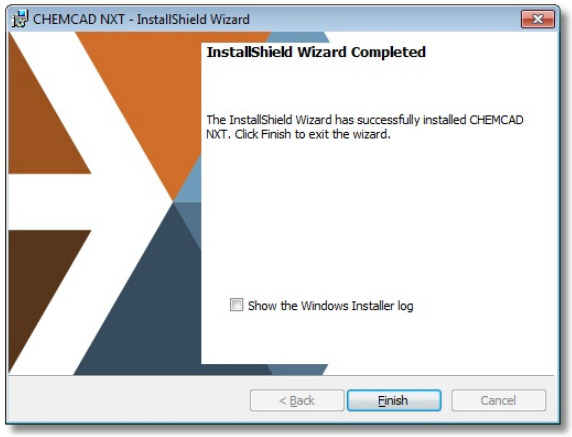


Figure 2-09: The InstallShield Wizard Completed screen

Licensing CHEMCAD

Before you can use CHEMCAD, you'll need to set up a licensing scheme of some type. Depending on your particular licensing agreement, you will use one of several types of licenses to run CHEMCAD.

Types of CHEMCAD Licenses

The various types of CHEMCAD licenses are designed to fit different users' software, hardware, and networking needs. Most licenses require the use of a hardware device, commonly known as a *dongle*, to run the program.

The dongle simply plugs into a USB port on the computer, and must be plugged in any time the program runs. If you work on a network with other CHEMCAD users, your license may rely on a dongle plugged into a network server elsewhere in your organization, rather than one plugged directly into your computer.

You or your organization may use one of the following types of dongles:

- SuperPro single-user dongle
- SuperProNet dongle for network use

In some instances, software licensing is provided without the use of a hardware device:

- RMS License Manager software, which runs over a local- or wide-access network
- System Authorization, a method that authorizes a single-user machine for a limited time (used for software evaluation)

License Settings

To run CHEMCAD for the first time, make sure that your dongle (if applicable) is plugged in properly, and then start the program. From the Windows Start menu, select **All Programs** > **Chemstations** > **CHEMCAD NXT**.

Note: A Standard License screen appears ***only the first time*** that you run CHEMCAD after installation. After you have reviewed the license agreement, click **Yes** to continue.

The program opens, displaying a CHEMCAD splash screen. After a short time, this screen is replaced by the CHEMCAD License Monitor dialog box, which displays information about the license(s) that your computer is using to run CHEMCAD.

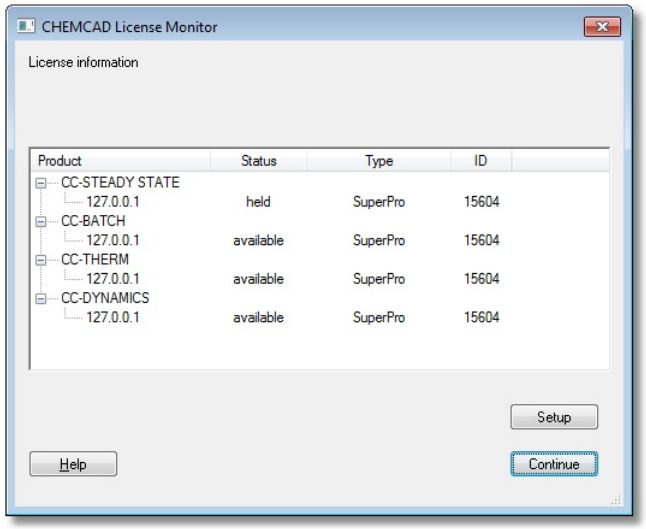


Figure 2-10: The CHEMCAD License Monitor, displaying licenses from a local hardware dongle

Note: In some cases, this dialog may initially display with the title *Searching for Licenses*, indicating that CHEMCAD has not yet detected a valid license. If your computer is experiencing slow communication with the license server system, CHEMCAD may simply need more time to detect the license(s). As soon as any valid license is found, the *CHEMCAD License Monitor* title will appear and licensing will proceed.

Normally, this dialog box remains in view for only a few seconds, listing all product licenses that CHEMCAD has obtained. During that time, you can click anywhere in the dialog box to keep it open. If you do not click in the dialog box, it disappears from view, but you can bring it back up at any time by clicking the **File** tab and then selecting **Licensing**.

While the CHEMCAD License Monitor dialog box is open, you can view the various CHEMCAD licenses detected for your system and see what method (and where applicable, which server) is being used to obtain those licenses. If your organization uses RMS License Manager or a SuperProNet hardware key, you can also see which other users currently hold various product licenses.

For network licenses, you can right-click a server name under a particular product and select a licensing preference (**on demand**, **always**, or **never**) as shown below.

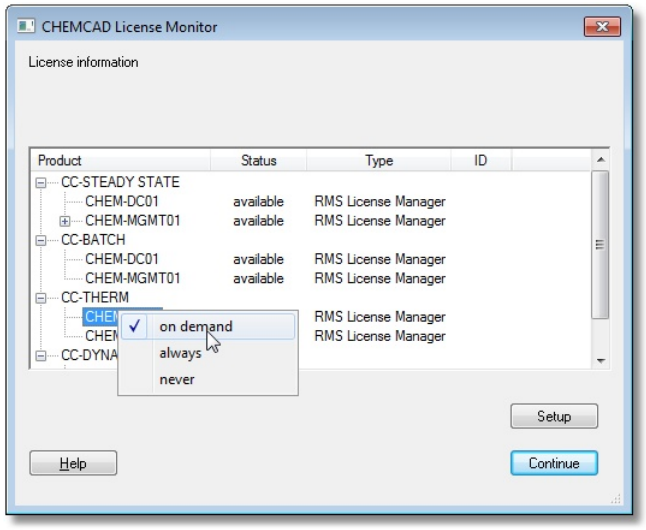


Figure 2-11: Selecting a network licensing preference

You can use the **always** or **never** setting to turn licensing for a product absolutely on or off, respectively. The **on demand** setting secures a license *only* when you begin to use a specific CHEMCAD feature controlled by a certain product. This setting is ideal in most situations, as it leaves unused licenses available for other users.

To close the CHEMCAD License Monitor screen, click the **Continue** button, or click the **X** in the top right corner of the screen.

Updating a License

CHEMCAD dongles require re-programming on a regular basis—either once a year or more often, depending on your licensing agreement. This is a security measure to reduce the likelihood that your dongle will be stolen and misused.

The dongle that you use is programmed to work only through the licensed time period, and when that time has elapsed, the dongle must be updated before you can continue using CHEMCAD.

Updating a dongle is a relatively simple procedure. Before your license expiration, you or your software administrator should receive an e-mail from Chemstations, with what's known as a *configuration file* included as an attachment. You should save this file to your Windows desktop as soon as you receive it.

Note: If you've updated the same dongle in the past, the new configuration file should have the exact same file name as the previous one. If, while saving the file to your desktop, you see a Windows message about an existing file with the same name, you should overwrite the old file (which in any case cannot be used again), replacing it with the new one.

It's important to ensure that your configuration file matches your dongle. The configuration file should be a .DNG file whose name includes a four- or five-digit code; this code must match the number stamped onto your dongle. If the numbers

don't match, contact your software administrator or Chemstations support to resolve the issue.

The update e-mail also specifies the date on which you'll need to update your dongle. Before that date arrives, follow this procedure to perform the update:

1. Start the CHEMCAD program and click the **File** tab. On the command list at left, click **Licensing**. This brings up the CHEMCAD License Monitor dialog box, which displays the status of all applicable CHEMCAD product licenses, along with your dongle type and number.

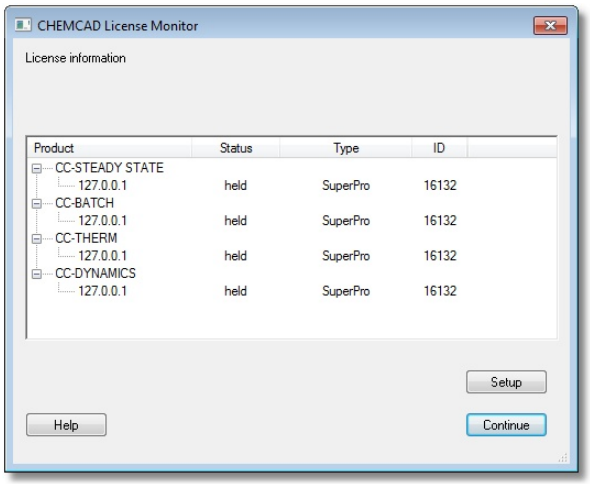


Figure 2-12: The CHEMCAD License Monitor dialog box

2. Click **Setup** to bring up the License Setup dialog box, then click **Update dongle** as shown below.

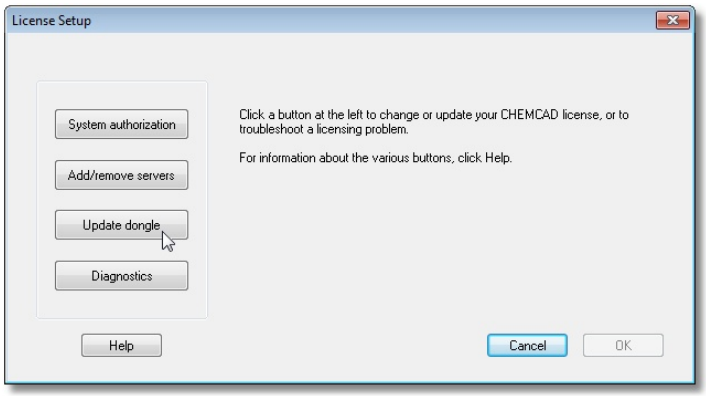


*Figure 2-13: Clicking **Update dongle** within the License Setup dialog box*

3. The dialog box now lists all licensing dongles and displays a field for entering the full path and file name for the dongle update file. Click **Browse** to navigate to the update file.

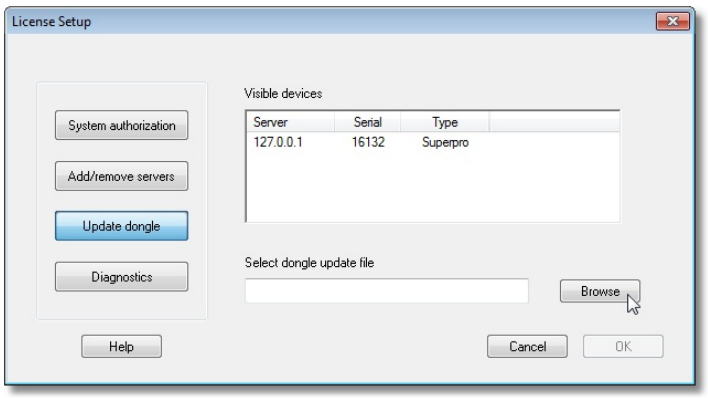


Figure 2-14: Browsing for the dongle update file

4. In the Open dialog box, navigate to the location where you saved the .DNG configuration file. Normally, this is the Windows desktop; if you saved your configuration file there, click **Desktop** to tell CHEMCAD where to look for the file, then select the .DNG file and click **Open**.

5. The License Setup dialog box now displays the directory path and file name for the selected .DNG file. Click **OK** to update the dongle.

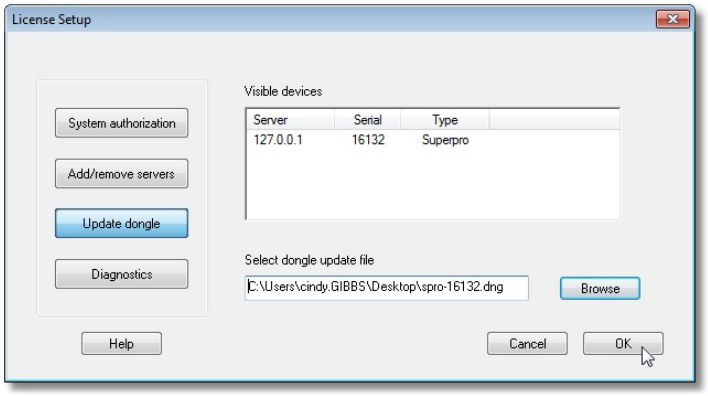


Figure 2-15: Updating the dongle with the selected update file

6. CHEMCAD re-programs the dongle, and then displays a pop-up window stating that the update is complete.

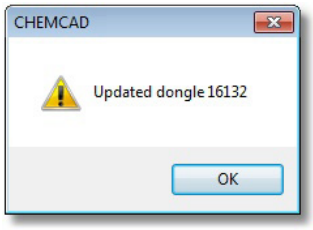


Figure 2-16: Successful re-programming of a CHEMCAD dongle

7. Click **OK** to close the pop-up window. If the CHEMCAD License Monitor screen appears, click **Continue** to close it.

You should now be able to proceed normally in CHEMCAD.

Getting Help with CHEMCAD

If you find that you have questions that are not addressed in this User Guide, you can turn to several resources for CHEMCAD help.

Online Help

At any time while running CHEMCAD in an active window, you can press the **[F1]** key to bring up the CHEMCAD Help screen that's most appropriate to the task you are currently performing or the dialog box currently displayed.

In some situations, pressing **[F1]** will bring up the main CHEMCAD Help window instead of a particular help screen. From there, you can click the **Contents**, **Index**, or **Search** tab in the upper left corner of the CHEMCAD Help window, and use these tools to find the information you need.

You can also go directly to the main CHEMCAD Help window by clicking **Help** in the top right corner of the program screen. Regardless of how you open CHEMCAD Help, it always opens in a separate window that does not interfere with the operation of the CHEMCAD program.

The Chemstations Website

To find the most recent updates of the CHEMCAD software, manuals, and various training tools, go to **www.chemstations.com**. There you'll find the following items available for download:

- The latest release of CHEMCAD
- A list of updates implemented in the most recent release
- CHEMCAD documentation and demos

Contacting Chemstations Technical Support

If you are unable to solve a problem or find the answer to a question using this User Guide or the other tools listed here, you can contact Chemstations' technical support staff for assistance.

Our technical support engineers are available via e-mail, or by phone Monday through Friday, 7:00 AM through 6:00 PM Central Standard Time.

Phone:	**713.978.7700**
Toll-free (U.S. and Canada):	**800.243.6223**
FAX:	**713.978.7727**
E-mail:	**support@chemstations.com**

Outside of the United States, please see **www.chemstations.com** for regional contact information.


Chemstations™

Chapter 3

The CHEMCAD Interface

This chapter takes you on a tour of the CHEMCAD screen, including the tabbed command ribbon, the main areas of the screen, and the flowsheet drawing tools. It also shows you some ways that you can customize the screen and various features so that they best suit your own way of working.

The CHEMCAD Window

When you launch the CHEMCAD program for the first time, you'll see a screen with a tabbed ribbon at the top, a large open area in the middle, and various *panes*, or specialized areas, at the edges of the screen.

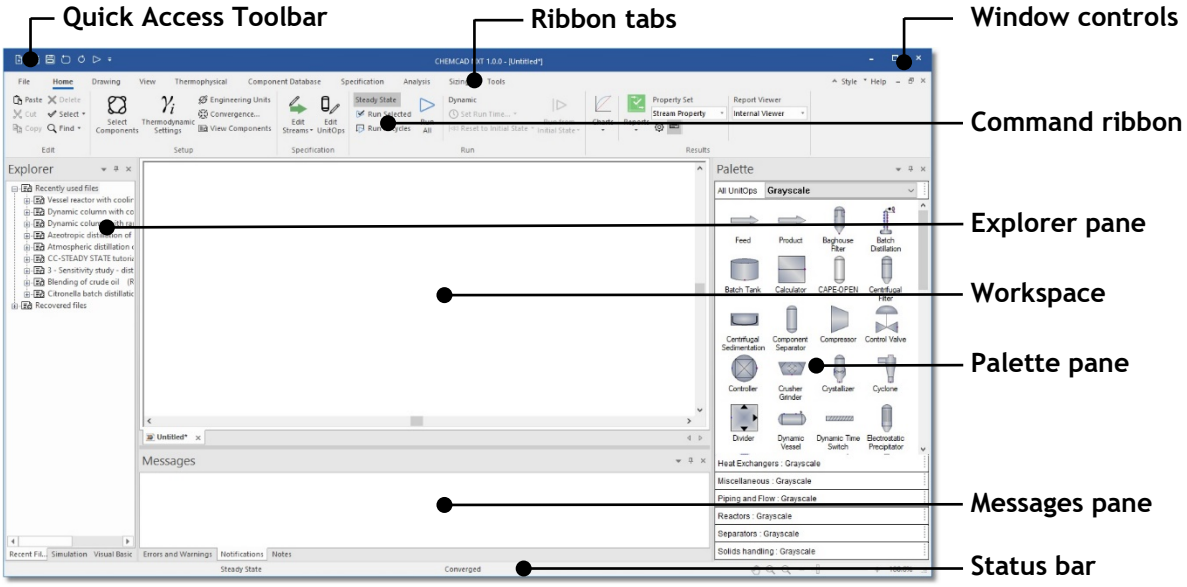


Figure 3-01: The full CHEMCAD program window

The Command Ribbon

The commands for using CHEMCAD are arranged into a tabbed *ribbon*, which is located at the top of the program window. Each tab brings up a different set of commands, with items grouped according to topic.

When you launch the program, the **Home** tab is selected, showing the most commonly used CHEMCAD commands. To access any other groups of commands (known as command *categories*), simply click the corresponding tab.

Some of the tab names are commonly found in Windows programs—namely **File**, **Home**, **View**, **Tools**—while other tabs items such as **Thermophysical, Component Database,** and **Sizing** are more specific to chemical process simulation. Once you click any tab, the ribbon will display a series of related commands.

To discover the use of any item on the command ribbon, simply point your mouse cursor at the button and watch for the tooltip to appear, as shown below.

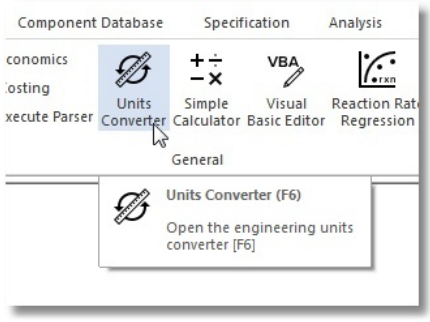


Figure 3-02: Viewing a button's tooltip

Note that the **File** tab behaves differently than the other tabs. Clicking this tab brings up a list of commands that are applied at the file or program level, including opening, closing, or saving a simulation; printing a flowsheet or simulation notes; and setting up licensing and various program preferences. It's a good idea to take a few minutes to familiarize yourself with these commands as you begin to work with the program.

The Quick Access Toolbar

Above the command ribbon, in the top left corner of the CHEMCAD screen, you'll find the Quick Access Toolbar. This toolbar provides one-click access to important and commonly used commands—**New**, **Open**, **Save**, **Undo**, **Redo**, and **Run All**—regardless of which command ribbon is currently selected.

Like most other areas of the CHEMCAD interface, the Quick Access Toolbar can be customized to fit your needs. Click the down arrow at the right end of the toolbar to access the customization options, which include turning off any of the default commands or displaying the Quick Access Toolbar below the command ribbon.

Figure 3-03: The default commands on the Quick Access Toolbar

The Workspace

The area in the middle of the screen is known as the *workspace*. This is the main focus of the CHEMCAD window, the place where you'll build and edit flowsheets, view charts and reports, and run and tweak process simulations.

When you first launch CHEMCAD, the workspace is empty. When you start to build a flowsheet or open an existing simulation, the flowsheet displays in the workspace.

The workspace uses *tabs* to enable you to switch between an open simulation and any related features, such as Excel Data Maps, reports, and charts. At the bottom of the workspace area, you'll see one or more tabs whenever a simulation is open.

Each workspace tab includes a button marked with an **x**; to close any tab, simply click that tab's **x** button.

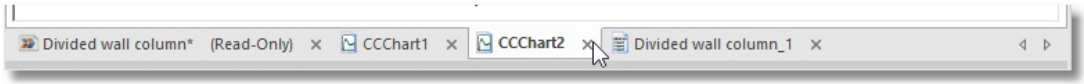


Figure 3-04: The bottom of the workspace area, showing several tabs and their x buttons

Note that any time you've closed a simulation and haven't yet opened another file, the workspace displays as an empty space.

The Explorer Pane

Along the left edge of the CHEMCAD window, you'll see an area with a title bar at the top that reads *Explorer*. At the bottom of the Explorer pane are three tabs called **Recent Files**, **Simulation**, and **Visual Basic**. To view the contents of a tab, simply click the tab name.

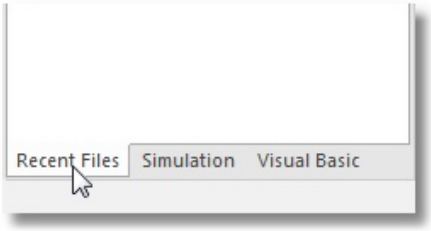


Figure 3-05: Explorer pane tabs

The Explorer pane tabs are presented in a *tree format*, with items organized into a multi-level hierarchy. The default view shows only top-level items, but you can expand each item to view second-level items, third-level items, and so forth.

At the left of each top-level item is a small triangle that points to the right. To expand an item, click the triangle. Two things happen simultaneously when you click: the tree expands to show that item's contents, and the triangle shifts to point downward. You can hide (or *collapse*) the lower-level items again by clicking the triangle again. Figure 3-06 shows an example of an Explorer item in collapsed and expanded view.

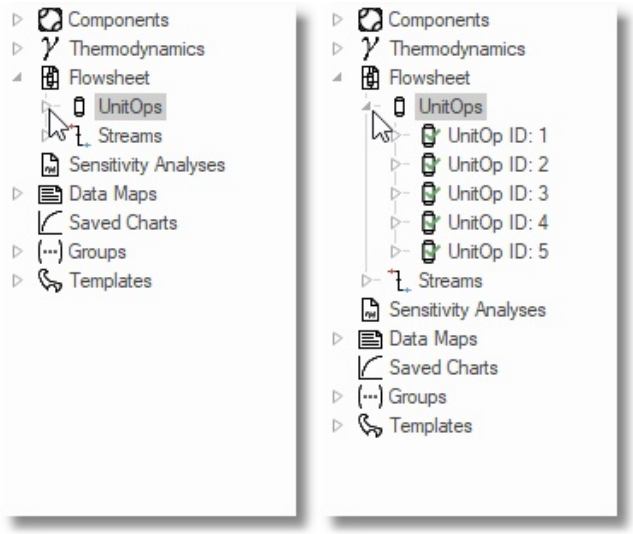


Figure 3-06: Clicking to expand an item (left); the resulting view (right)

Expanding and collapsing items in the Explorer tabs is one way that you can make the best use of your screen space when working in CHEMCAD.

The Recent Files Tab

The Recent Files tab is selected by default when you first launch CHEMCAD. This tab lists all the simulation files that you have opened lately, starting with the most recent. When you first install CHEMCAD, the list is empty, but with every simulation that you open—new files or existing ones such as built-in examples—the list will grow, providing convenient access to files that you use frequently.

To open a simulation from the Recent Files list, simply double-click the file name in the list.

The Simulation Tab

The Simulation tab displays by default any time a simulation is open. It provides a series of shortcuts to common commands and settings, including:

- **Components:** Includes one-click access to component, electrolyte, and solids selection
- **Thermodynamics:** Provides quick access to thermodynamic settings and transport properties
- **Flowsheet:** Allows quick editing of UnitOp and stream data
- **Sensitivity Analyses: Provides a convenient way to create, edit, and run sensitivity analyses**
- **Data Maps:** Enables you to create or set execution rules for a Data Map without using the menu
- **Saved Charts: Provides quick access to previously saved charts for this simulation**

- **Groups:** Provides an easy way to categorize UnitOps, streams, and components
- **Templates:** Stores and organizes stream and UnitOp specifications that you can "clone" for re-use

Expand any of these items to see and use specific features, which are described in further detail in the appropriate chapters of this user guide.

The Visual Basic Tab

If you use Visual Basic to customize CHEMCAD, this tab provides quick and easy access to your Visual Basic code. You can expand the **Reactions**, **Properties**, or **UnitOps** item to view available subroutines for that category. Clicking the name of a subroutine opens a Visual Basic editor in a separate window.

The Palette Pane

Along the right side of the CHEMCAD window is a pane titled *Palette*, which is a repository for the various unit operation icons needed to create flowsheets. This pane is highly customizable, so you can arrange the icons to best suit the way you work.

By default, the Palette pane displays the **All UnitOps** palette. As the name suggests, this palette shows all available UnitOps, listed in alphabetical order.

Below this palette, you'll see other palette titles such as **Heat Exchangers** and **Piping and Flow**. Each of these palettes includes a subset of the available UnitOp types, focusing on one general type of equipment.

To change what you see in the Palette pane, you can do any or all of the following:

- Select a different palette
- Change the color scheme of a palette
- Change the order of UnitOp symbols on a palette
- Remove unwanted UnitOp symbols from a palette
- Reset all palettes to default configuration

Selecting a Palette

To select a palette, simply click its title bar. The selected palette expands in place, as shown in Figure 3-07.

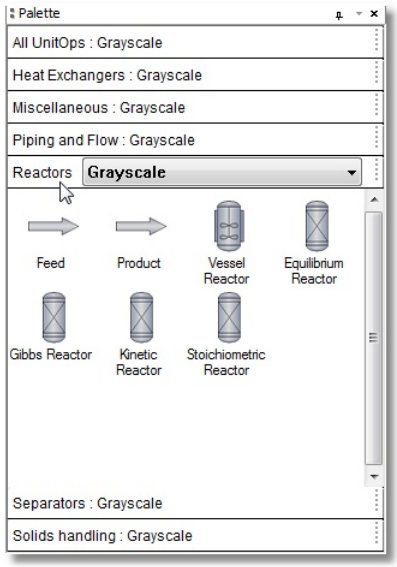


Figure 3-07: The expanded Reactors palette

Changing the Color Scheme of a Palette

CHEMCAD offers three built-in color schemes for UnitOp symbols: **Grayscale**, **System Color**, and **Wireframe**. Both the System Color and Grayscale color schemes use color shading to give symbols a three-dimensional appearance. The Wireframe color scheme uses no shading, for a more PFD-ready appearance.

Examples of each color scheme are shown in Figure 3-08.

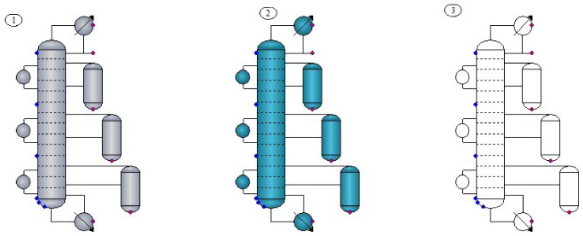


Figure 3-08: A Tower Plus icon in (left to right) Grayscale, System Color, and Wireframe color schemes

You can apply a color scheme to any UnitOp palette, to determine the appearance of any new UnitOps you add from that palette to a flowsheet.

Before you apply a color scheme to a palette, first ensure that the desired palette is open. Then click the current color scheme name, which is displayed next to the palette name; this will cause a selection list to drop down. Simply click a color scheme name to switch to that scheme.

Once you have applied a color scheme to a palette, the icons you drag from that palette onto the flowsheet will look just like the examples on the palette. Changing the color scheme of a palette does not affect any icons previously added to the flowsheet from that palette.

Changing the Order of UnitOp Icons in a Palette

If you prefer to see UnitOp symbols in a different order than they appear on a palette, you can rearrange them.

Note: Before you attempt to rearrange symbols on a palette, make sure that the **Lock Palette** feature is turned off. Normally, this setting protects you from unintentionally moving symbols around when you are placing items onto a flowsheet.

To turn the feature on or off, right-click any palette's title bar and look for the **Lock Palette** menu item. A check mark indicates that the feature is turned on; simply click to clear the check mark and unlock all palettes. It's a good idea to return palettes to a locked state when you are not actively editing them.

To move a UnitOp symbol to a new location on the palette, click and drag the symbol. Release the mouse button when the symbol is situated where you want it. Other symbols on the palette will shift their positions to make room for the newly placed item.

Removing UnitOp Symbols from a Palette

If you have identified some equipment types that you never use, you can remove those UnitOp symbols from your palette. This can save time spent searching through the list of UnitOps for the item you want.

To remove a symbol, first make sure that the **Lock Palette** feature is turned off. Then hold down **[CTRL]** and right-click the UnitOp symbol you want to remove. Select **Delete** from the resulting menu, then confirm the deletion by clicking **Yes**. The symbol will disappear from the open palette.

Resetting All Built-in Palettes to Default Configuration

If at any time you want to return all of the built-in UnitOp palettes to their default settings—with their original contents and the Grayscale color scheme—you can do so with a single command. Simply right-click any palette heading and select **Reset All Palettes**.

The Messages Pane

The Messages pane is located at the bottom edge of the CHEMCAD workspace. At the bottom of this pane are three tabs: **Errors and Warnings**, **Notifications**, and **Notes**.

The Errors and Warnings Tab

This tab displays a running list of error and warning messages that have been generated while the current simulation file has been open. The oldest messages display at the top of the list. When there are too many cumulative messages to display in the pane, the most recent messages display and the older messages scroll

off the top edge of the pane. If needed, you can use the vertical scroll bar on the right side of the pane to scroll up and review earlier messages.

To clear all messages from this tab, right-click anywhere within the tab and click **Refresh Errors and Warnings**.

The Notifications Tab

This tab displays diagnostic messages from each UnitOp every time a simulation is run. This information is helpful in troubleshooting a simulation that is not working properly.

The text on the Notifications tab is not saved with the simulation. The text refreshes with each run and clears when you close the simulation.

The Notes Tab

This tab provides a handy place to store additional information, in text form, about the simulation. You can use it to list any details about the simulation, such as its origin and any assumptions that are being made.

Any notes that you add or change are saved as part of the simulation. To delete text from a note, simply click and drag to select the text and then press **[DELETE]** on your keyboard.

Other CHEMCAD Window Commands

The upper right corner of the CHEMCAD window has the usual **Minimize**, **Restore**/**Maximize**, and **Close** buttons for the main program window. Beneath those commands is an identical set of commands that control the open simulation window.

To the left of the window commands are three other items:

- **Minimize the Ribbon:** To minimize the command ribbon, click the caret symbol (just to the left of **Style**). When the ribbon is minimized, only the ribbon tabs are visible, and you must click a tab to see the corresponding commands. Alternatively, you can press **[CTRL]** + **[F1]** to toggle the full ribbon on or off.
- **Modify Visual Style:** To change the color scheme of the CHEMCAD interface, click the **Style** drop-down and make a selection.
- **Help (F1):** Click **Help** to open the CHEMCAD Help and Reference file.

Customizing the CHEMCAD Screen

When you first install CHEMCAD, the screen is laid out with the command ribbon at the top, the Explorer pane on the left, the Palette pane on the right, and the Messages pane below the workspace.

If having all of these items visible leaves you less workspace than you would prefer, or if the location of one or more panes is less than optimal for the way that you work, you can hide or move panes to customize your CHEMCAD screen.

Viewing and Hiding Screen Elements

You can view or hide the various panes and other screen elements to make optimal use of your screen space.

To toggle a pane on or off, click the **View** tab and then choose **Explorer**, **Palette**, or **Messages in the Show group. Items that are currently displayed have a background color that differs from the ribbon's background.** The **Status Bar** item controls the visibility of the status bar at the bottom of the CHEMCAD window.

Resizing and Moving Items

In addition to determining which screen elements to display, you can customize your CHEMCAD window to determine exactly where each of these items will appear.

Resizing a Pane

The simplest way to alter the appearance of a pane is to resize it. You can make the Explorer and Palette panes wider or narrower, or make the Messages pane shorter or taller, by moving the inside edge, or *wall*, of the pane toward or away from the edge of the main window.

To resize a pane, start by positioning your mouse cursor at the inside wall of the pane—that is, the right edge of the Explorer pane, the left edge of the Palette pane, or the top edge of the Messages pane. When the cursor is in the correct position for resizing, the normal pointer will be replaced with a two-headed arrow as shown in Figure 3-09.

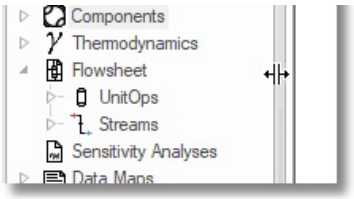


Figure 3-09: The two-headed arrow cursor used for resizing panes

When you see the two-headed arrow, click and drag in the direction you want to move the pane wall. A thick gray line shows a preview of the new pane size; when you release the mouse button, the resized pane appears.

Moving a Pane

In addition to resizing, you can also move any of the panes in the CHEMCAD window, either to a different edge of the screen or to the middle of the screen.

Initially, all the panes are *docked*, meaning that they are "snapped into" an edge of the screen. When you *undock* a pane, you can put it in the location of your choice, away from the screen edge.

To undock a pane, click and drag the pane's *title bar*, that is, the bar at the top of the pane that shows the pane name. Release the mouse button when the pane is in the desired location.

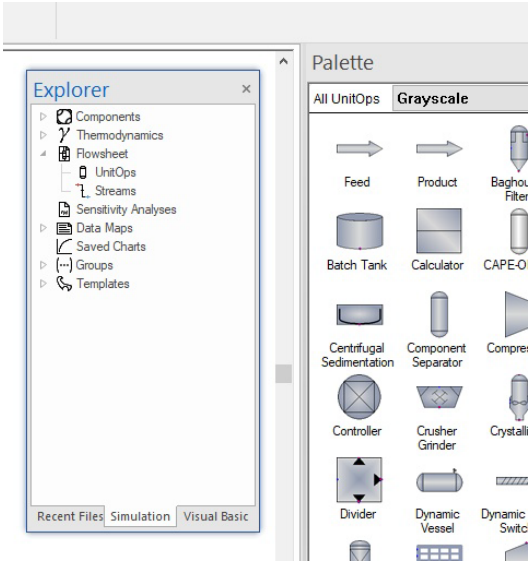


Figure 3-10: The Explorer pane, undocked and moved onto the workspace

You can also dock a pane to a different edge of the screen. To do this, click the pane's title bar and begin to drag it away from its current location. A selection box appears near the center of the workspace, showing all available docking locations. When your mouse cursor points at any of these docking icons, the corresponding area of the screen will be highlighted, as shown in Figure 3-xx. Release the mouse button to dock the pane to that location.

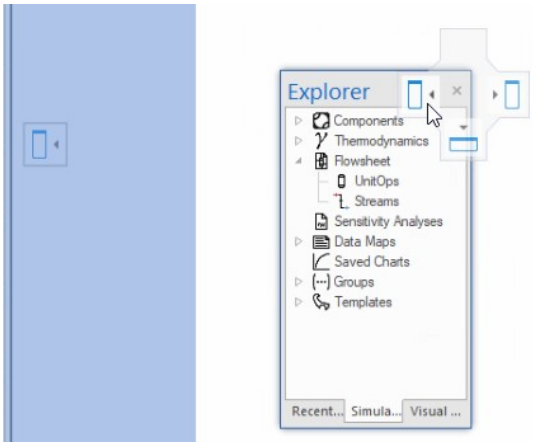


Figure 3-11: Selecting a location for an undocked pane

Pinning and Unpinning Panes

In addition to moving and resizing the various panes, there's another way that you can customize your CHEMCAD screen: *pinning* and *unpinning* the Explorer and Palette panes.

These two panes can take up a fair amount of horizontal screen space, and making them very narrow isn't an ideal way to work. Pinning and unpinning provide a way to view full-width Explorer and Palette panes when you need these tools, while also freeing up space when you aren't using them.

Whenever either of these panes is docked at an edge of the screen, it is in one of two states:

- Pinned, meaning that the pane is always visible
- Unpinned, meaning that the pane is mostly hidden from view, and appears only on demand

By default, all CHEMCAD panes are initially pinned in place. You can choose to unpin a pane if you prefer to have some extra space on the screen. To unpin a pane, find the tiny pushpin icon in the pane's title bar, next to the **x** icon that enables you to close the pane. If the pane is stationary, you'll see that the pin is upright with its point down.

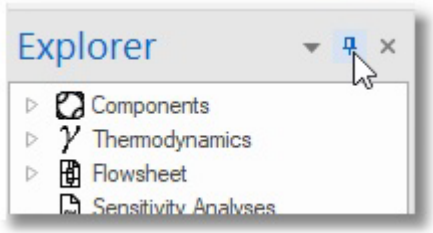


Figure 3-12: The icon indicating a pinned, or stationary, pane

If you click the pin icon, the pane suddenly disappears from view—but it isn't gone. Instead, a small tab bearing the name of the palette appears at the edge of the screen where the pane is docked. To see the pane reappear, you only have to roll your mouse over that tab. When the pane appears, you'll notice that the pushpin icon is now horizontal. Use the tools on the Explorer or Palette normally; then, when you no longer need the pane, just move the mouse pointer elsewhere. The pane will automatically hide itself until the next time you roll the mouse over the tab.

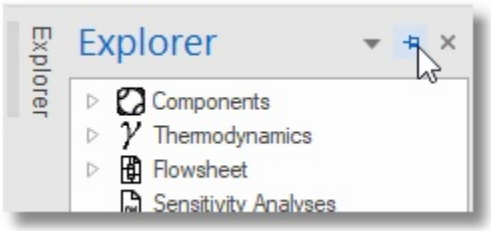


Figure 3-13: An unpinned pane in use; note the horizontal pin icon and the Explorer tab at left

To re-pin an unpinned pane, point to the tab to make the pane appear and then click the pin icon. The pin turns so that it is once again upright, and the pane is once again a permanent fixture on the CHEMCAD screen.

Flowsheet Drawing Tools

Most of the commands used for drawing flowsheets are accessed via the **Drawing** tab. The drawing commands are grouped by function, for easy access.

The Workspace Group

The Workspace group includes features that help with alignment of flowsheet objects, behavior of stream lines, and text objects on the flowsheet.

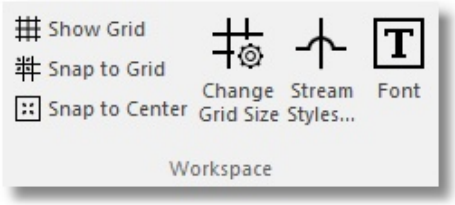


Figure 3-14: The Drawing tab's Workspace group

You can turn on a visible workspace grid to use as a guide while creating your flowsheet. Click **Show Grid** to toggle this feature on or off.

The option called **Snap to Grid** can help with alignment of objects on the flowsheet. When this option is turned on, items that you move on the workspace will align themselves with the nearest vertical and horizontal grid lines.

The **Snap to Center** feature helps you to neatly line up flowsheet elements relative to one another. When this option is turned on, items that you move around on the workspace will show when they are centrally aligned with nearby objects, as indicated by a blue dotted line.

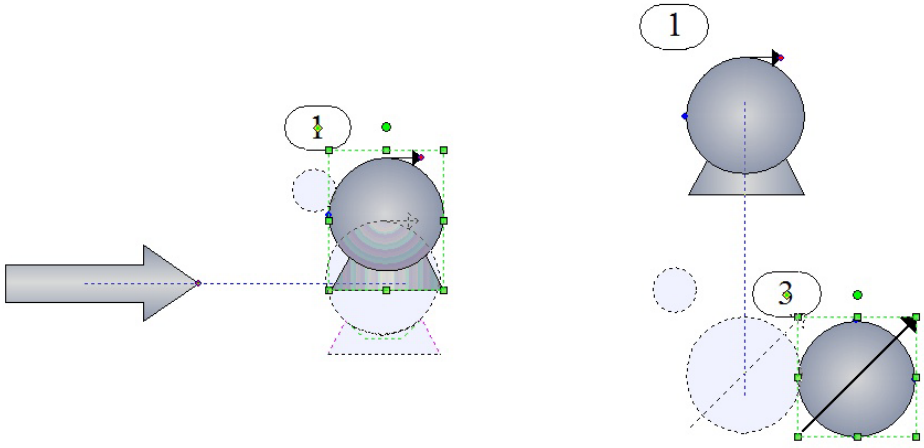


Figure 3-15: The Snap to Center feature in action, showing when objects are centrally aligned

Selecting Change Grid Size brings up the Grid dialog box, which enables you to customize the look and spacing of the grid lines when the visible grid is turned on.

The **Stream Styles** tool enables you to customize the way that stream lines appear on the flowsheet. The Stream Styles dialog includes settings for stream line width and arrow size, as well as for the behavior of stream intersections. A full discussion of stream intersections and the use of the Stream Styles settings is included in Chapter 5, *Building and Using a Basic Simulation*.

The **Font** tool enables you to change the appearance of text on flowsheet objects. If you click **Font** with one or more flowsheet objects selected, the settings you choose for size, style, and so forth will apply only to those objects. If you click **Font** with no

objects selected, the font properties you set will apply to future flowsheet objects that display text.

The Insert Group

The Insert command group provides the tools for adding flowsheet objects beyond UnitOps and streams.

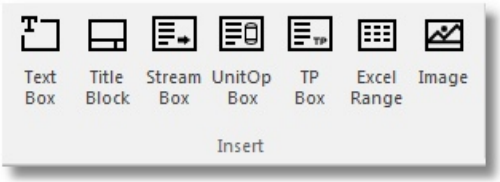


Figure 3-16: The Insert group

The Text Box Tool

To place text on a flowsheet, click **Text Box**. Then move the cursor to the desired location on the flowsheet and click the mouse. When you see "Insert text here," begin typing your text. When you finish, click anywhere in the workspace to turn off the Text Box tool. To add another text block, simply click **Text Box** again.

You can now click and drag your new block of text around the workspace as needed. You can also select the text block and then click **Font** (in the **Workspace** group) to access standard text formatting tools such as font style, size, and color.

If you have formatted a block of text and need to add a similar text block, you can copy the existing block (using the **Copy** and **Paste** commands) and then edit the text in the copy. To change the text attributes for several existing text boxes at once, simply select them all (hold down **[SHIFT]** while you click each one in turn), then click **Font** and choose the desired text attributes. When you click **OK**, all of the selected items will display with matching text formatting.

The Title Block Tool

Use this command to place a pre-formatted title block on your flowsheet. For a complete discussion of title blocks in CHEMCAD, refer to Chapter 8, *Output and Reports*.

The Stream Box, UnitOp Box, TP Box, and Excel Range Tools

Using these commands, you can insert various kinds of customized data boxes, in table form, on your flowsheet. This makes it easy to view current stream, equipment, temperature/pressure/flow rate, or imported Excel worksheet information in the CHEMCAD workspace. For a complete discussion of these tools, refer to Chapter 8, *Output and Reports*.

The Image Tool

This command enables you to place an image file on the flowsheet workspace. When you click **Image**, CHEMCAD displays the Open dialog box, where you can browse for any graphic file (.bmp, .gif, .jpg, .png, or .tga) on a local or networked drive.

Double-click the desired file to return to the main workspace, where the image will appear highlighted with sizing handles.

As with any other flowsheet object, you can click and drag the image on the workspace, use the sizing handles to make the image larger or smaller, align the image with other objects, and even rotate or flip the image.

The Objects Group

The Objects command group provides tools to draw numerous shapes and to arrange flowsheet objects on the workspace.

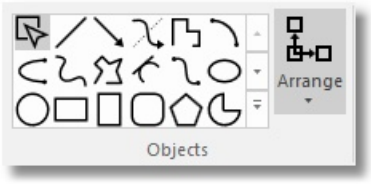


Figure 3-17: The Objects group

Line and Shape Drawing Tools

You can draw various lines and shapes as needed on a flowsheet. The simplest items to draw are straight lines, ellipses, and rectangles. To view the drop-down gallery that displays all available drawing tools, click the down arrow in the bottom right corner of the drawing tools area. In either view, you can hover your mouse pointer over any icon to view the tooltip with the drawing tool's name.

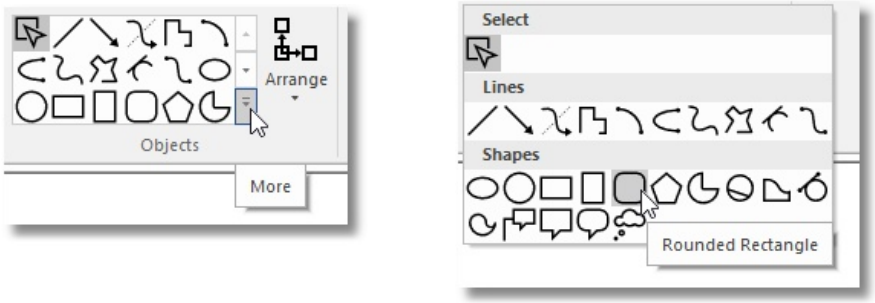


Figure 3-18: Expanding the drawing tool gallery (left), full gallery showing a tooltip (right)

To add any of these items to a flowsheet, start by clicking the corresponding button. Then point to the location where you want to draw and begin.

For many items, you simply click and drag in the workspace to draw the shape, releasing the mouse button when you have achieved the desired size and shape. These drawing tools include:

- Line
- Arrow Line
- Bezier Arrow Line
- Arc
- Free Line
- Ellipse
- Circle
- Rectangle
- Square
- Rounded Rectangle
- Closed Free Line
- Caption
- Rectangular Callout
- Round Callout
- Cloud Callout

For other drawing objects, instead of simply clicking and dragging, you must click multiple times on the workspace to create the line or shape. The following tools can be used to create multi-sided shapes with many mouse clicks; note that you must double-click to complete the drawn object and turn these tools off.

- Pipe Line
- Bezier Line
- Closed Bezier
- Path Line
- Polygon
- Spline Line
- Closed Spline Line

To draw these items, you will need to click and drag to define a shape, then click exactly two points along the shape to complete the drawn object.

- Extend Arc
- Pie
- Chord

After you have drawn a shape on the workspace, the drawing tool is turned off, and the mouse pointer reverts to a selection arrow. To draw another shape, simply click the appropriate shape button again.

To make a line or shape exactly like the first one you drew, click the drawn object to select it, then right-click and use the **Copy** and **Paste** commands to place a duplicate on the flowsheet.

Any drawn object can be easily moved, resized, reshaped, or rotated, using the green sizing and rotating handles that appear when you select the object. You can also change the outline or fill appearance on a selected object, by right-clicking and choosing **Line** or **Fill** from the pop-up menu.

The Arrange Gallery

The **Arrange** drop-down gallery provides tools to help control the exact placement and order of flowsheet objects.

Figure 3-19: The Arrange drop-down gallery

Tools for controlling the relative placement of flowsheet items are located in the Align group. Using these commands, you can align objects in any direction, and distribute a set of selected items evenly within a given space.

To see these tools in action, imagine that you've started a flowsheet by placing three Feed arrows on the workspace, somewhat randomly. You can select them all and click **Align Left** to line them up precisely. Then select them again and click **Space Down** to distribute them evenly within the vertical space.

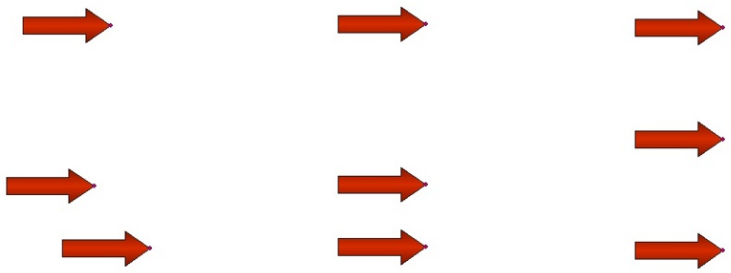


Figure 3-20: Feed arrows (left to right) randomly placed, left-aligned, and evenly distributed

Now that the arrows are arranged the way you want, you can select them one more time and click **Group**; this will ensure that they remain in the same position relative to one another if they are ever moved.

Grouped objects will appear highlighted all together if you click on any object in the group. To separate grouped objects, simply click anywhere on the group to highlight it and then click **Ungroup**.

The **Rotate** and **Flip** commands can be used to change the orientation of single objects, grouped objects, or multiple objects selected using **[SHIFT]-click**.

Other Useful Interface Hints

The following are helpful items that can help to make your CHEMCAD experience easier and more efficient.

Undo and Redo

As with most Windows-based programs, CHEMCAD allows you to "back out" of actions you have just taken while working with a file. You can use the Undo command to reverse the last change you made; simply click **Undo** on the Quick Access Toolbar, or use the key combination **[CTRL-Z]**. You can use the Undo command to retract up to the last 99 actions that you performed since the last time you opened the current simulation file.

To reverse the most recent Undo action at any time, click **Redo** on the Quick Access Toolbar, or use the key combination **[CTRL-Y]**.

Flowsheet Quickview

The Flowsheet Quickview feature is turned on by default when you install CHEMCAD. This handy tool enables you to see a quick data 'snapshot' for any stream or UnitOp on a flowsheet, without even clicking the mouse.

To use this feature, simply hover the mouse pointer over any part of a stream line or UnitOp symbol. This brings up a pop-up window with relevant data for that particular stream or UnitOp.

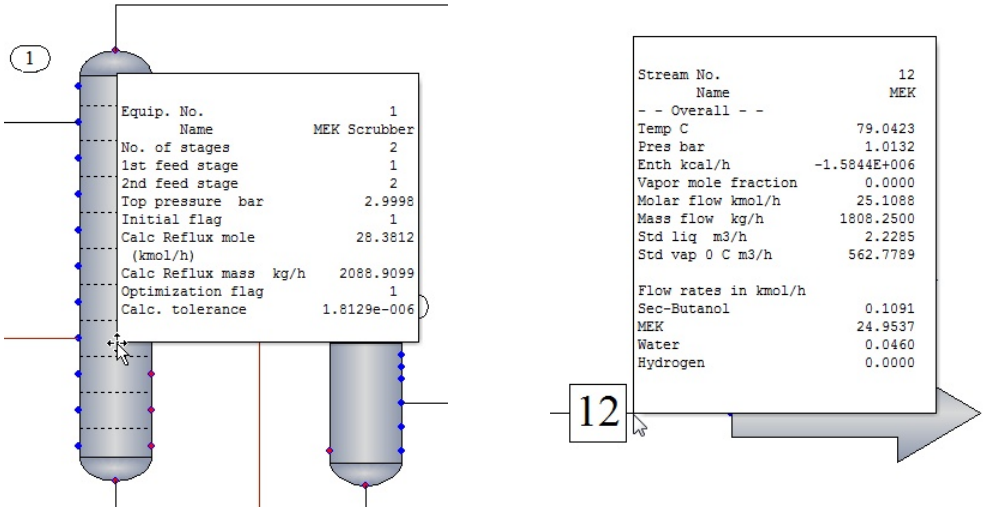


Figure 3-21: Quickview pop-up windows for a distillation column (left) and a product stream

By default, the Quickview window for streams includes temperature and pressure, stream enthalpy, mole vapor fraction, and overall flow rate, plus composition flow rates. You can customize the stream information displayed in the Quickview window using property sets, which are discussed in detail in Chapter 8, *Output and Reports*.

For UnitOps, Quickview displays key parameters about the equipment, and in some cases about the streams entering and exiting the equipment, depending on the UnitOp type.

To turn off the Quickview feature, click the **Home** tab, then click **Quickview** in the Results group. To turn the feature back on at any time, simply click this button again.

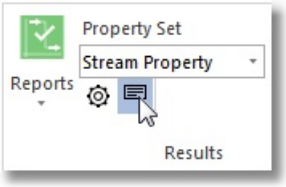


Figure 3-22: Turning off the Quickview option

Adjusting Your View of the Workspace

CHEMCAD offers several options for moving and resizing your view of the workspace. Most of these are available on the status bar, in the bottom right corner of the program screen.

If your computer mouse is equipped with a scroll wheel between the left and right mouse buttons, you can zoom in and out on the CHEMCAD workspace with a touch of your finger. To zoom in, roll the wheel up—that is, push your fingertip

away, toward the top edge of the mouse. To zoom out, roll the wheel down toward the bottom of your mouse, pulling your fingertip toward your palm. When you zoom in and out this way, the focal point for the zoom is the location of the mouse pointer.

You can also click and hold the mouse wheel to pan across the workspace. If your mouse is not equipped with a scroll wheel, click **Auto Pan** on the status bar and then click and drag to pan. To turn off the pan feature, you can either click **Auto Pan** again, right-click the mouse, or press **[ESC]** on the keyboard.

Next to **Auto Pan** are two buttons used to change the zoom level, or magnification, of your workspace view. To center the entire flowsheet at the largest size that will fit in the available workspace Click **Zoom to fit**. To zoom in on a specific area of your flowsheet, click **Zoom rectangle** and then click and drag to outline the area you want.

To the right of these commands is a slider bar with a numeric percentage display. You can click and drag the slider to the left to zoom out, or to the right to zoom in. For small, controlled zoom adjustments, you can click the minus or plus signs on the ends of the slider bar. When you use the slider bar, the zoom action is centered on the current center point of the workspace display.

The final zoom tool is a percentage display. Click the number to bring up a Zoom dialog where you can choose a magnification level or type in a custom zoom percentage.

Figure 3-23: View tools: Auto Pan, Zoom to Fit, Zoom Rectangle, slider bar, zoom percentage

Resetting the User Interface

If at any time you want to return the CHEMCAD interface to its original configuration, with the same color scheme you saw at installation and all panes back to their initial positions and sizes, you can do this with a single menu command.

To perform this reset, first save and close any simulation file you may have open. Then click the **File** tab and select **Reset User Interface**. You will see a message asking you to confirm that you want to proceed; click **Yes** to reset the interface.

Locking Flowsheet Elements

You can lock flowsheet elements in place to prevent unintended movement of your carefully placed UnitOps and streams. Once these objects are in a locked state, they cannot be moved around the flowsheet. You can lock any or all items on a flowsheet with a single click, and then unlock them just as easily.

To access the flowsheet locking commands, click the **View** tab and then find the **Flowsheet** group.

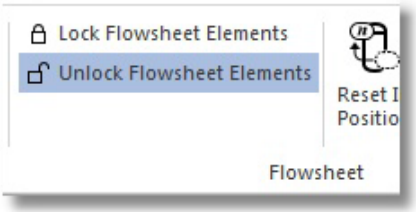


Figure 3-24: The flowsheet locking commands

To lock a specific object in place, click to select that object (a stream, UnitOp, text box, drawn object) and then click **Lock Flowsheet Elements**. Now, when you click the locked object, you'll see small yellow lock icons instead of the usual green sizing handles. To unlock the object, simply select it and click **Unlock Flowsheet Elements**.

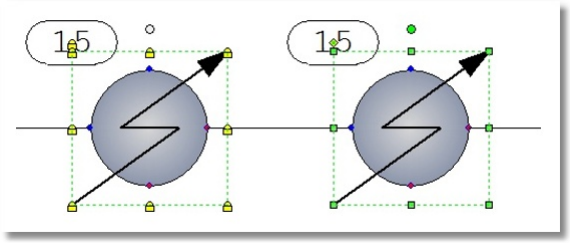


Figure 3-25: A heat exchanger as it appears when locked (left), and when unlocked (right)

You can change the lock status of objects individually, or select a block of items on a flowsheet and change them all with one click of the lock or unlock command.

To lock or unlock the entire flowsheet, simply click into a blank area of the workspace to ensure that no objects are currently selected, then click the desired locking command. This approach affects all items currently on the flowsheet; if you add more items, they are initially unlocked by default.


Chemstations™

Chapter 4

Working with Simulation Files

All the work that you do with CHEMCAD is stored in simulation files. Each discrete simulation is packaged into a single file that is portable and easy to handle. All the details of the simulation—from UnitOp specifications to stream composition to thermodynamics—are included in this file. This chapter describes the various ways that you can access and manage CHEMCAD simulation files.

About CHEMCAD Simulation Files

Simulations created in CHEMCAD use the file extension *.ccsim*, which distinguishes them from other files on your computer, including simulation files created using earlier versions of CHEMCAD. A .ccsim simulation file is as easy to work with, transport, and share as an MS Word document or an Excel spreadsheet.

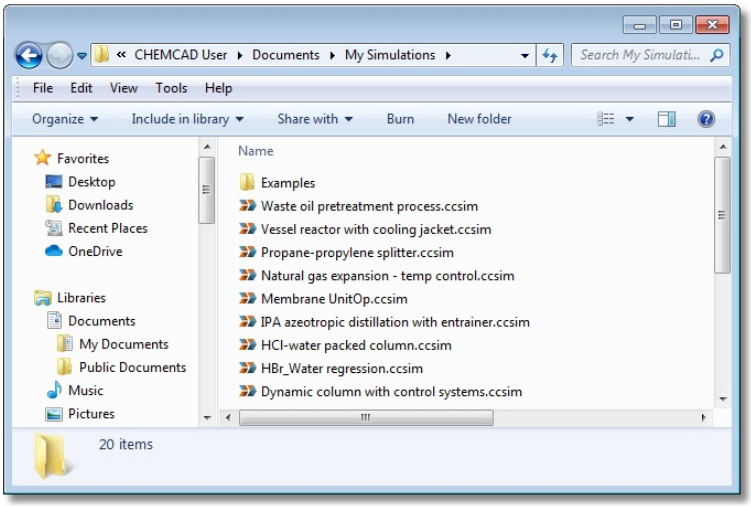


Figure 4-01: CHEMCAD files in the My Simulations directory

User Components in CHEMCAD

CHEMCAD simulations are also self-contained with respect to the data required to run them. Custom components that you create can be stored in a common database so that you can use them in many different simulations. User components are also stored within the simulations that use them, so that those components remain available when simulation files are moved among various directories, drives, devices, or networks.

Each time you open a simulation, CHEMCAD compares any user components in the simulation with the copies of those same components in the database. If the two copies do not match, you will be offered a choice: you can keep using the local copy stored in the simulation, or use the updated copy from the database.

Your installation of CHEMCAD can have multiple user databases, and even share them on networks with other users. To learn more about user components and best practices for managing and securing user component databases, see Chapter 10, *Customizing CHEMCAD*.

Example Files

Especially if you're new to CHEMCAD, it's a good idea to open and practice working with some example files before creating your own simulations. For this purpose, we've created numerous examples of simulations for typical chemical processes. You can open, view, and edit any example file, and even save a copy in another location to jump-start a simulation of your own.

The CHEMCAD example files are automatically copied to your computer with a complete CHEMCAD installation. The examples are organized by process type and located in the **\My Documents\My Simulations\Examples** directory.

Opening an Existing Simulation

To open an existing CHEMCAD simulation, click **Open** on the Quick Access Toolbar, or press **[CTRL + O]** on the keyboard. In the Open dialog, navigate to the folder where the simulation is located, select the appropriate .ccsim file, and click **Open**.

Note: An alternative method for opening a simulation file is simply to drag and drop the simulation's filename from a Windows Explorer window onto the CHEMCAD workspace.

If you use CHEMCAD on a network and share files with other users, it's possible that you could try to open a simulation that is already open for editing by another user. If you should attempt to open a simulation that is unavailable for editing, a message box will appear. You can choose to save the simulation with a new name and/or location, open a read-only copy of the simulation, or cancel the open operation.

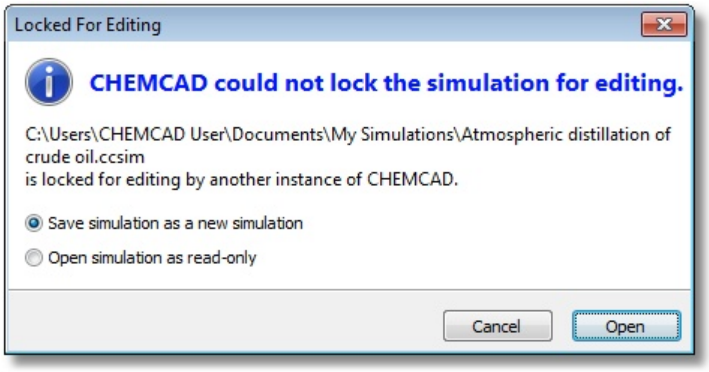


Figure 4-02: Notification that a simulation is already in use

If you should have trouble locating a particular simulation, you can search your hard drive or network for all files with a .ccsim file extension.

Creating a New Simulation

When you first open CHEMCAD, you'll see a blank simulation window and **[Untitled]** in the title bar.

You can begin building your simulation right away, but it's recommended that you save and name the simulation before you proceed very far. The longer you wait to save the simulation, the more you risk losing your work if an unforeseen computer or network problem should occur.

If you already have a simulation file open and want to start a new simulation, first save your work if applicable. Then click **New** in the Quick Access Toolbar to close the current file and bring up a new blank simulation screen. Note that if you have unsaved changes in your existing file, CHEMCAD will ask you to save or discard your changes before opening the new simulation.

Saving a Simulation

To save all changes in a simulation that you have already named, click **Save** on the Quick Access Toolbar, or press **[CTRL + S]** on the keyboard.

> **Note:** In some cases, such as the built-in CHEMCAD example files, existing files may be set as read-only to prevent accidental overwriting. You can save a copy of a read-only file using a different file name and/or file location.

To save a new simulation that you haven't yet named, click the **File** tab and then select **Save Simulation As**. The Save As dialog box appears, with **CHEMCAD simulation (*.ccsim)** as the default file type. Leave the file type as it is, give the file a unique name, and if necessary navigate to a new file location. Click **Save** to close the dialog box and return to the saved simulation.

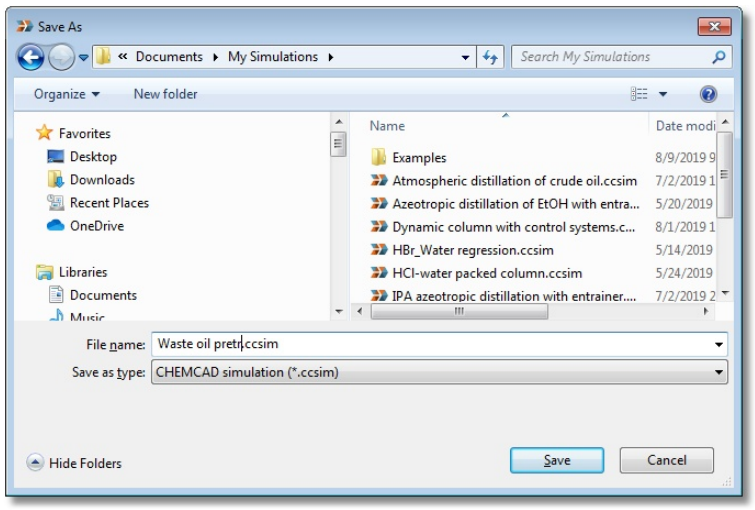


Figure 4-03: Giving a new simulation a unique name

Note: Any changes you make to a simulation are not saved until you use the **Save** or **Save As** command. This enables you to choose which changes to keep or discard.

Saving and storing all your simulations in the same main directory helps prevent the lost time and frustration that can result when files are scattered in different locations. It is recommended that you store your simulations in the **My Simulations** directory, which is created automatically within **My Documents** when you install CHEMCAD.

Saving Different Cases for the Same Simulation

In certain situations, you may need to create a group of simulations that are nearly identical to one another; early versions of CHEMCAD referred to such groups of similar simulations as *cases*. In today's CHEMCAD, each simulation is a free-standing file, but you can still easily "clone" simulations and make minor changes for comparison cases.

To do this, first create a simulation and save it. Then click the **File** tab and use the **Save Simulation As** command to rename the next case. Make the needed changes for that case, save it, and continue in that vein to create as many clones of your original simulation as needed, with whatever differences you require.

E-mailing a Simulation

Sending a simulation file via e-mail is quick and easy. You can either send a simulation from within the CHEMCAD program or attach the simulation file from within an e-mail program.

Sending from Within CHEMCAD

If you are working on a computer that has a default e-mail client program set up, you can e-mail a simulation without ever leaving the CHEMCAD window.

Before you attempt to send, be sure to save any changes to the simulation. Then click the **File** tab and select **E-mail Simulation** from the list of options. Your e-mail program will create a new message with the subject line "CHEMCAD Simulation *[file name]*," and the current simulation included as an attachment.

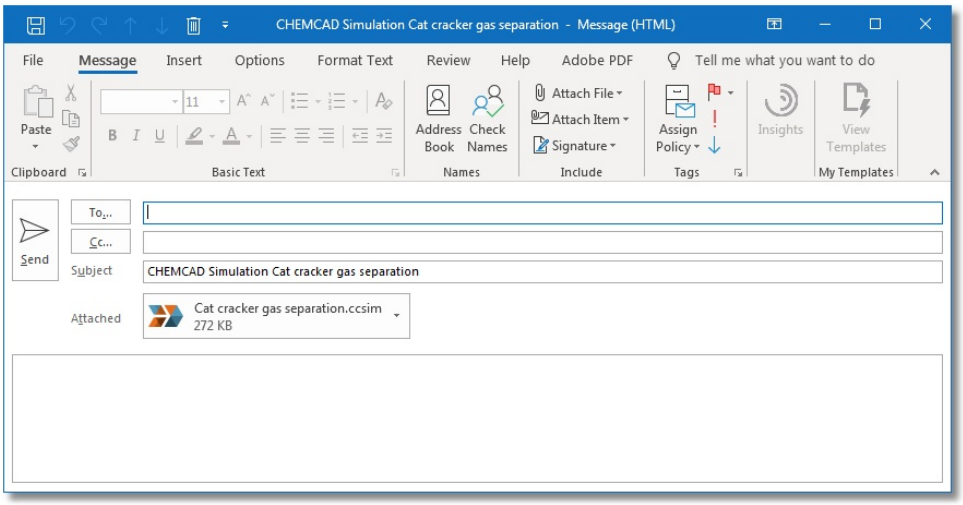


Figure 4-04: E-mailing directly from the CHEMCAD window

You can now enter your recipient information and add any message text, then send the message. It's a good idea to check the attachment information to see the size of the simulation file, as these files can in some cases be quite large.

Attaching to an E-mail

You can also e-mail any simulation that is stored on a local hard drive or network without opening CHEMCAD. This comes in handy if you are working on a computer or other device where you do not have access to a local e-mail program, or one where CHEMCAD is not currently installed.

To do this, simply create a new message, using your web mail or other e-mail account. Then use the e-mail program's command for attaching a file. Navigate to the directory where the simulation is located, select the appropriate file, and add the file as an attachment before sending.

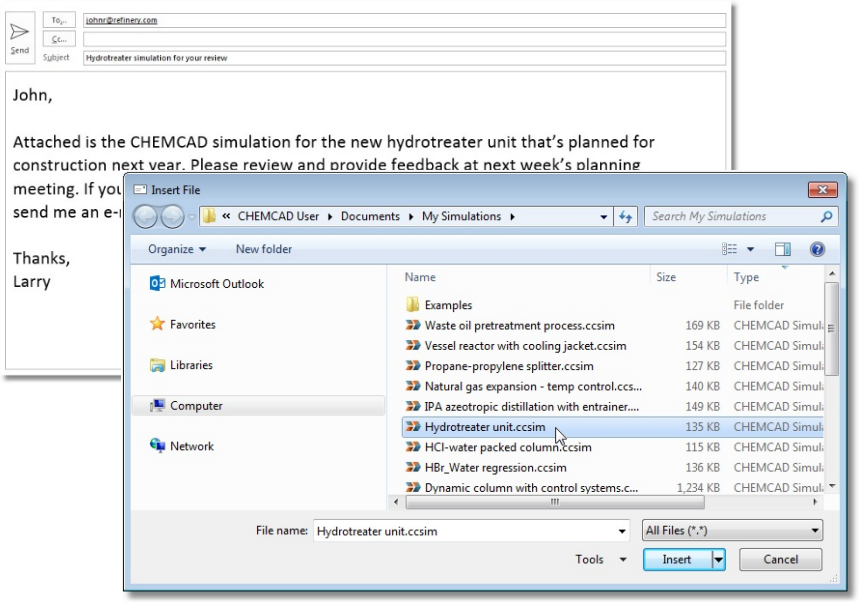


Figure 4-05: Adding a .ccsim file as an attachment in MS Outlook

Working with CHEMCAD Files from Previous Versions

You can use CHEMCAD NXT to open simulations that were originally created with CHEMCAD 7. When you do this, the program creates a copy of the original simulation, and makes that copy compatible with all CHEMCAD NXT functionality. The flowsheet and simulation data in the copy are not altered in any way, and the original file is left intact.

To update an existing CHEMCAD 7 simulation to CHEMCAD NXT format, click the **File** tab, then click **Open**. In the Open dialog box, navigate to the correct directory, select the simulation, and click **Open**. The Update Simulation Format dialog box appears, informing you that you need to save a new copy of the simulation.

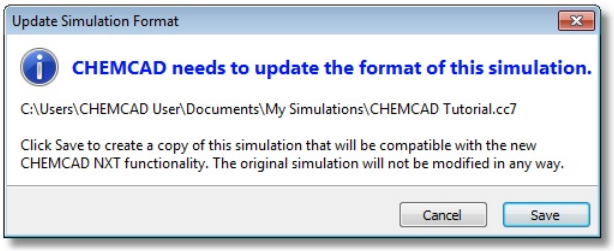


Figure 4-06: Converting a CHEMCAD 7 file to .ccsim format

Click **Save** to bring up the Save As dialog box, where you can either keep or change the file's name and select a location for the new CHEMCAD NXT copy. Click **Save** again to create and open the new file.

To import a simulation file that was created with CHEMCAD 6, you must first open and save that file using CHEMCAD 7, and then bring the file into CHEMCAD NXT using the method described here.

Chapter 5

Building and Using a Basic Simulation

The types of simulations you can create using CHEMCAD are many and varied, but the basic procedure for creating a simulation can be broken down into the following common steps:

1. Start a new simulation.
2. Specify engineering units for the simulation.
3. Select chemical components for the process.
4. Select K-value and enthalpy options for the process.
5. Draw the flowsheet with appropriate streams and unit operations.
6. Define the feed streams used in the process.
7. Enter specifications for the unit operations.
8. Run the simulation.
9. Review the results of the simulation.

Starting a New Simulation

When you launch CHEMCAD, you will see *[Untitled]* in the program's title bar. Click the **File** tab, then select **Save Simulation As**. In the Save As dialog box, specify a name and location for the simulation file.

When you first install CHEMCAD, the default location for saving new simulations is a folder called **My Simulations**, located within your computer's **My Documents** folder. You can save your new simulation to that folder, or to any

accessible directory on your computer or network. As you'll notice in the Save As dialog box, the file extension for CHEMCAD simulation files is **.ccsim**.

Specifying Engineering Units

To specify engineering units for this simulation, begin on the **Home** tab. In the **Setup** group, click **Engineering Units**. This brings up the Engineering Units dialog box, where you can select the units to be used for everything from time and temperature to surface tension.

In this dialog, the available pre-selected sets of engineering units are called *profiles*. The left side of the dialog box lists the built-in *system profiles*: **English**, **Common SI**, **Formal SI**, and **Metric**. If the set of units you prefer to use doesn't match any of these profiles, you can choose the best match and then manually select different units as needed. To save your selections, click **Apply**. If you decide not to save any changes, click **Cancel** to close the dialog.

If you do find yourself customizing your engineering unit selections, you can save them as a *user profile*, which you can then easily apply to future simulations. To do this, first set all the units the way you want them. Then at the top of the dialog, click **Save As** > **New Profile**. Type a name for this profile and click **OK** to save your settings. The name you entered will now appear on the left side of the dialog, under the User Profiles heading.

For full details about how to manage user profiles for engineering units, see the *Engineering Units* topic in the CHEMCAD help file.

Selecting Chemical Components

You can select chemical components for your simulation at any point while creating the flowsheet, or you can wait until you've drawn the entire flowsheet before adding components. Before you can run the simulation, you will need to list every component involved in your chemical process, so that CHEMCAD can work with those components' properties.

These chemical components are pulled from CHEMCAD's *component database*, a master list of thousands of chemicals with their associated properties. When you're ready to add components for your simulation, first select the **Home** tab. Click **Select Components** in the **Setup** group to open the Select Components dialog box.

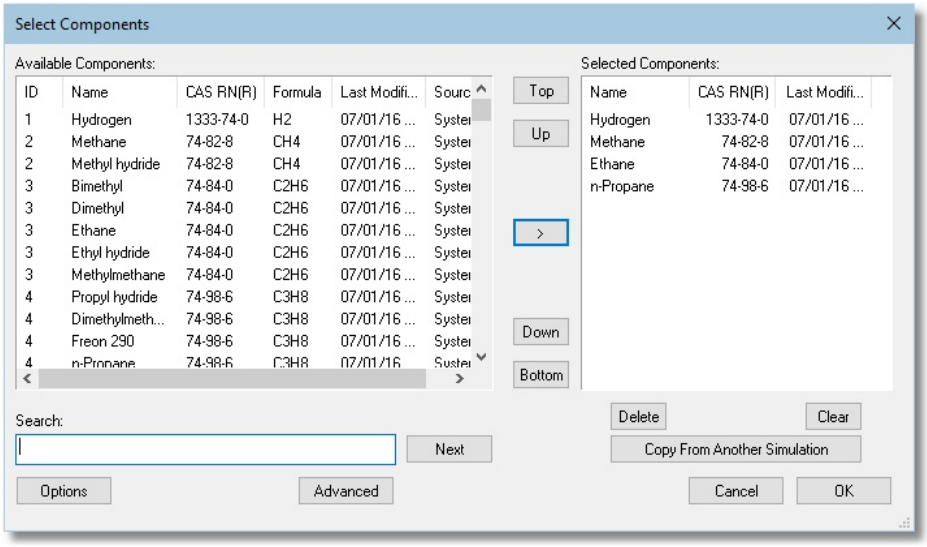


Figure 5-01: The Select Components dialog box

The Available Components column lists the contents of the CHEMCAD component database, while the Selected Components column lists the components currently included in this simulation. For a new simulation, the Selected Components list is empty at first.

Every chemical that will be part of the process, whether it's a feed stream, product, or utility, must be listed on this simulation's component list.

Finding a Component

Because of the large number of components in the CHEMCAD component database, scrolling up and down the list of available components can be time-consuming. To find a specific component quickly, use the Search field at the bottom of the Select Components dialog box.

Type the name of the chemical you want to find in the Search field. With each letter that you type, CHEMCAD suggests possible matches in the Available Components list. In the following example, typing the letters **wa** in the Search field has highlighted the **Water** component.

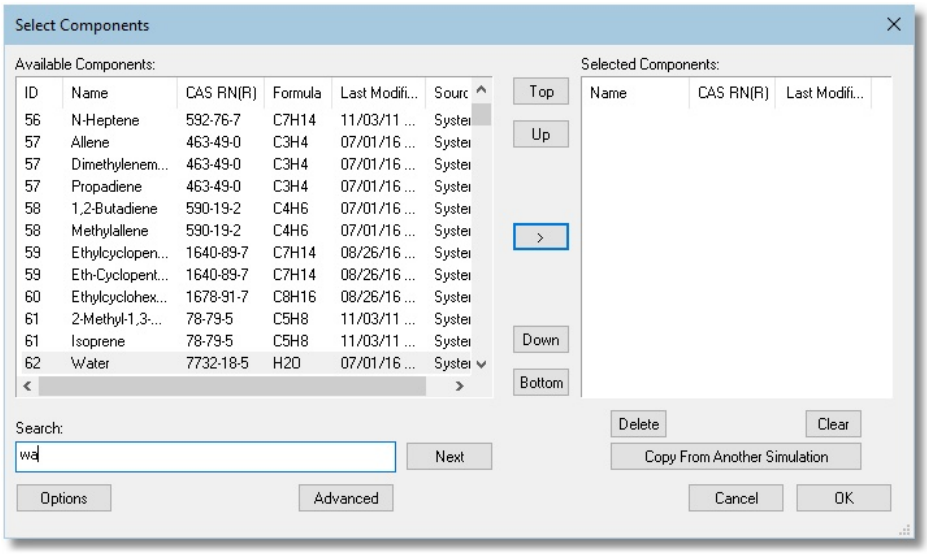


Figure 5-02: Using the Search field to locate the Water component

Note that in some situations, the first result may not be the one you want. For example, typing **ethane** in the Search field brings up the **Methane** component at first. To see the next match for your text, click **Next**; continue clicking this button as needed until you find the desired component.

The Search field accepts both text and numeric entries. By default, CHEMCAD will search for your entry among all chemical names, chemical formulas, and CHEMCAD database IDs; if you like, you can also search by CAS RN® number. To turn any of these search options on or off, click the **Options** button below the Search field. This brings up the Search Options dialog box, where you can specify which data to include in your component searches.

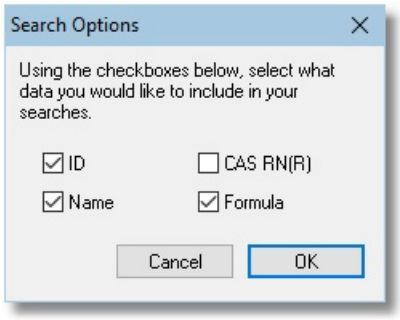


Figure 5-03: Selecting which data to include in component searches

Note: You can add your own custom components to the CHEMCAD component database. For more details about this feature, see Chapter 9, *Customizing CHEMCAD*.

Adding a Component

Once you've located the component you want in the Available Components list, simply double-click the component to add it to the Selected Components list for your simulation.

You can also select multiple components in the Available Components list and then click the right arrow button, located between the two columns, to add all the selected components to your simulation. To select multiple components, use Windows' standard selection methods of holding down **[SHIFT]** to select contiguous items or holding down **[CTRL]** to select non-contiguous items.

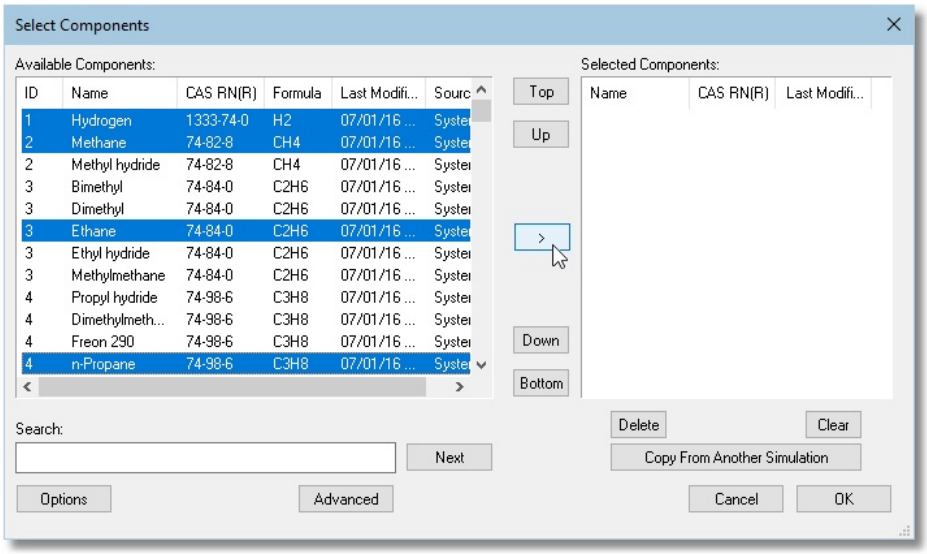


Figure 5-04: Adding multiple components using the right arrow button

If you would like to duplicate the component list from an existing simulation, click **Copy From Another Simulation**. In the resulting Open dialog box, navigate to the desired simulation, select that simulation, and click **Open**. The Selected Components list is now populated with the components used in the simulation you selected; you can add or delete items to customize the list.

Changing the Order of Selected Components

When your Selected Components list for a simulation is particularly long, you may find it helpful to place certain components at either the top or the bottom of the list. You can add components in any order, and then move them around in the list as needed.

To move a component to a new position in the Selected Components list, click the component to select it and then:

- Click **Top** to move it to the first position on the list.
- Click **Up** to move it up one position.
- Click **Down** to move it down one position.
- Click **Bottom** to move it to the last position on the list.

Removing Items from the Selected Components List

To remove a single component from the Selected Components list, click the component to select it and then click **Delete** in the bottom right area of the Select Components dialog box.

To remove all components from the Selected Components list and begin again, click **Clear**, just to the right of **Delete**. If you have changed your mind about adding components at this time, you can simply click **Cancel** to back out of component selection.

When you have added all the desired components to the Selected Components list, click **OK** to load these components into the simulation and return to the main CHEMCAD workspace.

Selecting K-value and Enthalpy Options

The first time you complete the Select Components dialog box, you'll be taken to the Thermodynamic Suggestions dialog box. At this point, you can either click **Cancel** to skip this dialog and select thermodynamics manually, or enter parameters and click **OK** to see which methods the program suggests.

Using the Thermodynamic Suggestions Dialog

Proper selection of thermodynamics is generally the most important step in a process simulation. A poor thermodynamics selection may lead to unrealistic simulation results.

With the Thermodynamic Suggestions dialog, CHEMCAD makes general suggestions, based on your component list and the specified ranges for temperature and pressure.

Selecting Components to Ignore

In the upper portion of the dialog, use the drop-down boxes to indicate any components that CHEMCAD should *not* consider. This may affect the results for model suggestion. For example, if you are using water as a coolant and your other components are alkanes, the program will suggest UNIFAC. If you specify that water should be ignored, the program will ignore water and select SRK.

Specifying Process Conditions

In the lower portion of the dialog, specify the approximate temperature and pressure ranges for this process. Entering accurate information in these fields will help the program return a more useful recommendation.

You can also specify a *BIP data threshold*—a minimum percentage of possible binary interaction parameters (BIPs) which must be present in a BIP activity coefficient model (NRTL, Wilson, etc.). Without BIPs, activity coefficient models simplify to Raoult's law.

How CHEMCAD Makes Thermodynamic Suggestions

The program follows a logic tree to choose a model. The logic tree assumes that all your components are mixed in a vessel, with conditions falling into the specified temperature and pressure ranges.

- If all components are hydrocarbons, CHEMCAD will likely suggest an equation of state.
- If water is present, the program will likely select an activity coefficient model.
- If water and hydrocarbons are present, the likely suggestion will be UNIFAC.
- If water and strong electrolytes (HCl, NaOH, etc.) are detected, the program will suggest electrolyte models.

Temperature and pressure range will affect the selection of model. If pressure is high, CHEMCAD is more likely to suggest an equation of state. If pressure is atmospheric and temperature is below the normal boiling point of all components, the program may choose an activity coefficient model or ideal vapor pressure.

Should the results of the Thermodynamic Suggestions dialog be trusted to make design decisions?

Use this dialog as a starting point for your decision. Proper selection of thermodynamics is the engineer's responsibility. Your simulation may call for the use of a different thermodynamic model than what the program suggests.

Manually Selecting Thermodynamics Settings

When you complete the Thermodynamic Suggestions dialog (or simply click **OK** to accept the default entries), you'll see a pop-up message displaying the selected K-value and enthalpy models for your simulation. Click **OK** again to bring up the Thermodynamic Settings dialog, which enables you to set up thermodynamics for your simulation manually.

If you're happy with the current selections, or you would prefer to address these settings later, you can click **OK** to close the dialog and return to the main CHEMCAD workspace.

To return to the Thermodynamic Settings dialog at any time, start on the **Home** tab and follow these steps:

1. Select **Thermodynamic Settings in the Setup group**.
2. This opens the Thermodynamic Settings dialog box. Start by determining, based on your process knowledge, whether your system has two liquid phases or a single liquid phase. In the **Global K-value Model** field, select a method that can calculate the phase behavior relevant to your system.
3. Based on the specific circumstances of your process, make any needed alterations to the options displayed on the **K-value Models** tab. Note that the

options appropriate to your selected K-value method are displayed in black, while irrelevant options are displayed in gray.

> **Note:** When you change the **Global K-value Model** selection, CHEMCAD may automatically update the **Global Enthalpy Model** setting as appropriate. If this happens, you will see a message on the K-value Models tab. You can change the selected enthalpy model by making a new selection in the Enthalpy Models tab.

4. Click the **Enthalpy Models** tab, select the most appropriate model in the **Global Enthalpy Model** field, and make any other changes to the options on this tab as needed for your process.
5. Click the **Transport Properties** tab and verify that the settings there are appropriate for this simulation. Change any settings as needed and then click **OK** to close the Thermodynamic Settings dialog box.

Drawing the Flowsheet

To create the flowsheet for your simulation, you'll need to add the appropriate unit operation icons to your workspace and connect those UnitOps to one another with streams. This connected group of streams and UnitOps forms the basis for the simulation.

Adding UnitOps

Start by adding UnitOp symbols for the equipment that will be part of your simulation. The tools for adding UnitOps to a flowsheet are located in the Palette pane, which by default displays on the right margin of the CHEMCAD window.

This pane offers specialized palettes for UnitOp categories such as *Heat Exchangers* and *Reactors*, but the default palette view is *All UnitOps*, which displays all the available UnitOp icons at once.

> **Note:** If you do not at first see the Palette pane, it may have been turned off. To restore this pane, click the **View** tab, then click **Palette** in the **Show** group. If the pane is turned on but you only see the word *Palette* sideways in the upper right corner of the screen, the pane is unpinned; see Chapter 3, *The CHEMCAD Interface*, for information about pinning and unpinning panes.

To place a UnitOp icon on your flowsheet, follow these steps:

1. On the All UnitOps palette, find the appropriate UnitOp symbol for the equipment you want to represent. If you are unsure about which UnitOp best fits your purposes, you can see a brief pop-up description of any palette item by hovering your mouse pointer over its symbol.

2. Click the symbol and drag it onto the workspace where you want to place the UnitOp. When you release the mouse button, the UnitOp symbol appears where you clicked.

Using Alternative UnitOp Symbols

Most CHEMCAD UnitOps have alternative symbols that you can use to represent equipment on a flowsheet. You can use those symbols on a case-by-case basis, or change a UnitOp's default symbol to customize your palette.

> **Note:** Items that are already in place on the flowsheet will not be affected when you select a new default symbol for a UnitOp.

To view the symbols available for a given UnitOp, right-click the current symbol on the palette. A subpalette will pop up, displaying all available symbols.

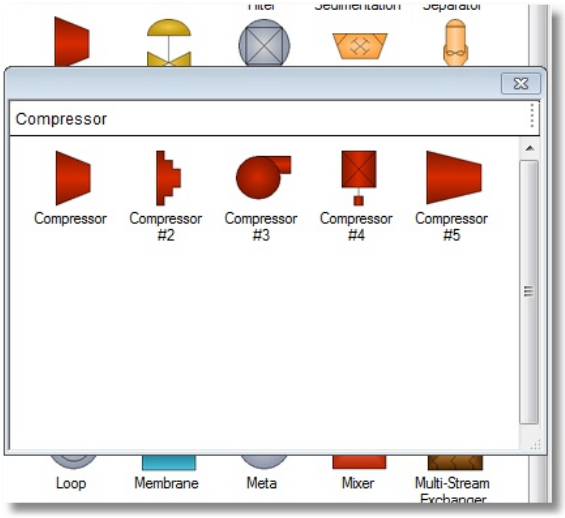


Figure 5-05: Viewing the subpalette for the Compressor UnitOp

From a subpalette, you can drag any symbol onto the flowsheet, just like the symbols on the main palette. When you do this, the selected symbol appears on the flowsheet and the subpalette automatically closes.

To change the default symbol for a UnitOp, first right-click to open the subpalette, then hold down the **[CTRL]** key and click the symbol you want to use. After you do this, the symbol you selected appears on the main palette. You can change the default icon for a UnitOp as often as you like.

Manipulating UnitOp Icons

After drawing a UnitOp symbol on a flowsheet, you can move, duplicate, resize, flip, rotate, or delete the symbol as needed.

1. Click the UnitOp symbol so that you see its sizing handles (green boxes at each side and at each corner). If you click a UnitOp and no handles appear, try zooming in for a closer view.
2. Manipulate the UnitOp icon as needed:
   - To ***move*** a UnitOp, click the center of the symbol and drag it to a new location.
   - To ***duplicate*** a UnitOp, right-click its symbol and select **Copy**. Then right-click anywhere on the workspace and select **Paste**.
   - To ***resize*** a UnitOp symbol, click any sizing handle and drag inward or outward to achieve the desired size. It is recommended that you always use the corner handles for resizing, as this will maintain the symbol's original shape.
   - To ***flip*** a UnitOp symbol, right-click it and then select either **Flip Horizontal** or **Flip Vertical**.
   - To ***rotate*** a UnitOp symbol 90 degrees, right-click it and then select either **Rotate Clockwise** or **Rotate CounterCW**.
   - To ***delete*** a UnitOp, right-click its symbol and select **Delete**, or simply press the **[DELETE]** key on your keyboard.

UnitOp IDs

When you place UnitOps on a flowsheet, CHEMCAD assigns each one an ID number that is unique within the simulation. The UnitOp number is a vital identifier for the unit, as it is used in various reports and charts related to the simulation.

The UnitOp ID is displayed in an oval, easily distinguishable from the rectangular boxes used to display Stream IDs.

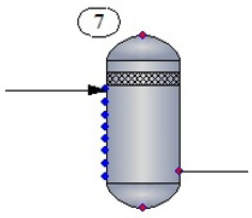


Figure 5-06: A UnitOp symbol with its ID oval

The default position of a UnitOp ID is just above and to the left of the unit's flowsheet symbol. If you subsequently move the UnitOp symbol, its ID remains in the same relative position.

In some situations, you may want to move a UnitOp ID from its default location. To do this, click the UnitOp to highlight it, then move your mouse cursor over the UnitOp ID oval. When you see the cursor change to a curved hand shape, click and drag the ID oval to the desired location.

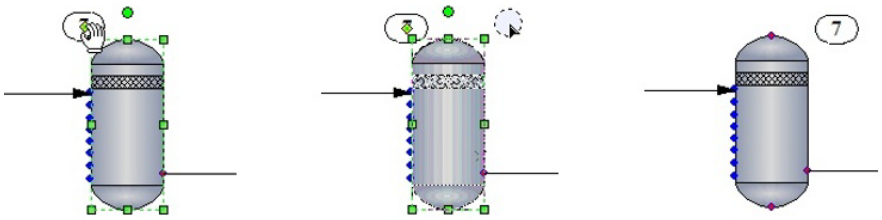


Figure 5-07: The hand cursor for moving a UnitOp ID (left), an ID being moved to the opposite side of the UnitOp symbol, and the ID oval in its new location

UnitOp ID Ranges

When you place UnitOps on a flowsheet, CHEMCAD assigns each one a UnitOp ID number that is unique within the simulation. The UnitOp ID number is an important identifier for the unit, as it is used in various reports and charts related to the simulation. By default, your UnitOps will be numbered, starting at 1, in the order in which you create them; all types of equipment share the same pool of ID numbers.

If you want to group your UnitOps numerically by equipment type, you can use the Starting IDs feature to accomplish this.

Click the **Specification** tab, then in the **Simulation** group, click **Starting IDs**. This brings up the Stream and UnitOp Starting IDs dialog box. Here you will see each type of UnitOp available in CHEMCAD, each with a default Starting ID setting of **1**. This means that any new UnitOp will be assigned an ID from the same number pool—the next number (1 or greater) that has not yet been used in this simulation.

To set up separate ranges of numbers for different equipment types, you can edit the values in the Starting ID column. For example, you could set the Heat Exchanger value to 200, the Pump value to 300, the Pipe value to 400, and so on, using any starting values that are meaningful to you. Any UnitOp type you don't assign a starting value will pull ID numbers from the main pool starting with 1, skipping any numbers that are already assigned.

Click **OK** to put your selected starting IDs into effect.

UnitOp Names

In addition to the assigned ID, you can give a UnitOp a name, using up to 11 alphanumeric characters. This name appears in the UnitOps area of the CHEMCAD Explorer pane, on certain reports, and optionally on the flowsheet with the UnitOp ID.

To add a UnitOp name, right-click the UnitOp on the flowsheet and select **Edit Name**; type the name in the resulting dialog box and click **OK**.

By default, a newly added UnitOp name will appear beneath the number in the UnitOp ID box. To hide a single UnitOp's name, right-click the UnitOp and clear the check mark next to **Show Name**; simply check this menu item again to make the UnitOp name visible.

To view or hide all UnitOp names on the flowsheet at once, click the **View** tab, then in the **Flowsheet** group, either check or clear the **Show UnitOp Names** box.

Feed and Product Arrows

The first two items at the top of every built-in palette in CHEMCAD are the Feed and Product arrows. You will need to place Feed and Product icons on the flowsheet to represent the starting and ending points of feed and product streams, respectively.

- The Feed icon must be placed at the start of any feed stream, i.e., any stream not originating in a flowsheet UnitOp.
- The Product icon must be placed at the end of any product stream, i.e., any stream not terminating in a flowsheet UnitOp.

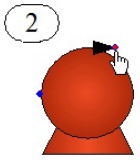
For the color scheme called System Color, the Feed icons are red and the Product icons are blue.

> **Note:** Once a feed or product arrow is connected to a stream, you can double-click the arrow to open the Edit Streams dialog for the associated stream.

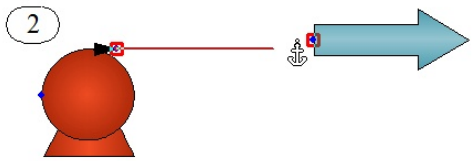
Drawing and Connecting Streams

Before you can add a stream to a flowsheet, you must already have drawn the UnitOps that the stream will connect. Follow these steps to add a stream:

1. Decide which outlet and inlet ports you will use to connect the two UnitOps on the flowsheet. Each UnitOp icon displays its ports as dots: red for outlets and blue for inlets.
2. Move the cursor to the red outlet port you've chosen, until you see the hand cursor appear.



3. Click and drag toward the desired inlet on the downstream UnitOp. When you see the cursor change to an anchor shape, and the inlet port outlined in red, release the mouse button.



4. The stream will appear between the objects you have connected.

> **Note:** You can also click and release at the outlet port, move the mouse pointer wherever you like, and then click and release again when you reach the desired inlet port. There is no need to hold the mouse button down the entire time.

Choosing a Stream Route

When you draw a stream using the basic click-and-drag method described above, CHEMCAD chooses a path for the stream. In some situations, you may want to choose a deliberate route for your stream.

To do this, click the mouse as you move from outlet to inlet, wherever you want the stream to make a turn. Each time you click, the stream freezes in place, and from there you can make a 90° turn to either the left or the right. You can add as many detours as you like to a stream before bringing it into a UnitOp inlet.

Rerouting a Stream

Even after you've completed your flowsheet and added detailed information about your streams, you can still reroute a stream if needed. There are two ways to do this.

The first method is to move the existing stream around using its sizing handles. When you click on a stream to select it, the stream line displays in green, and small green sizing handles appear. Each stream turn will have a sizing box, as well as each stream segment. You can click and drag any of these handles to move the adjacent stream segment(s) to a new location.

If you click a corner sizing handle, you can move the two adjacent stream segments in any direction; this often affects the position of other stream segments as well. If you click a sizing handle in the middle of a stream segment, then you can only move the segment left and right (for a vertical segment) or up and down (for a horizontal segment).

The second method for rerouting a stream is to re-draw it entirely. To do this, click the stream to select it, then right-click and select **Reroute stream**. The old stream disappears, replaced by the beginning of a new stream originating at the same outlet.

You can now click to create 90° turns, the same way you would with a new stream, to route the stream exactly where you want it. After a stream is rerouted, it retains all of the stream detail that you had previously entered.

Stream IDs

When you draw streams on your flowsheet, CHEMCAD assigns each one a stream ID number that is unique within the simulation. The stream number is an important identifier for the stream, as it is used in various reports and charts related to the simulation.

The stream ID is displayed in a rectangular box, easily distinguishable from the ovals used to display UnitOp IDs.

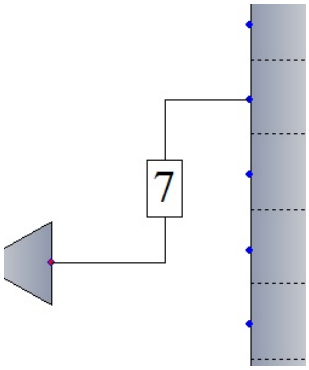


Figure 5-08: A stream ID box

When you draw a stream, the ID box is positioned on the longest stream segment. If you subsequently move the flowsheet objects that contain the stream's end points, or otherwise change the path of the stream, the stream ID box will change its position accordingly.

In some situations, you may want to move a stream ID box from its default location. To do this, click the stream to highlight it, then move your mouse cursor over the stream ID box. When you see the cursor change to a curved hand shape, click and drag the ID box to the desired location.

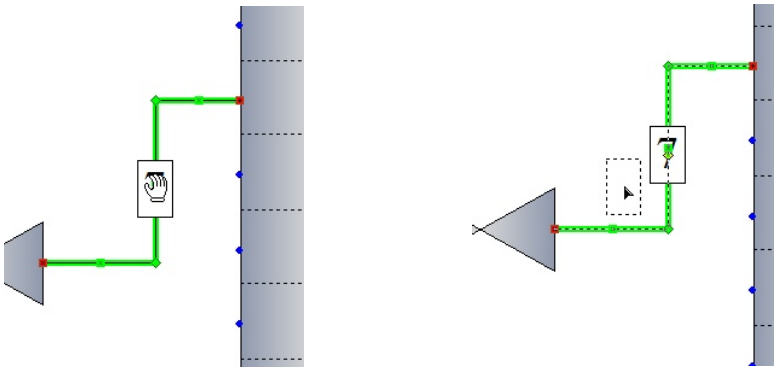


Figure 5-09: The hand cursor for moving a stream ID box (left) and a stream ID box being moved

If you have manually placed a stream ID box, you might later want to restore it to its default location on the stream. To do this, simply right-click the stream or the ID box and select **Reset ID Position**. This returns the stream ID box to its automatic placement on whichever stream segment is currently the longest.

Stream ID Ranges

By default, your streams will be numbered, starting at 1, in the order in which you create them. If you want to create a series of streams with a separate range of ID numbers from the rest of your simulation, you can use the Starting IDs feature to accomplish this.

Click the **Specification** tab, then in the **Simulation** group, click **Starting IDs**. This brings up the Stream and UnitOp Starting IDs dialog box. Scroll down to the Stream option and click the right column. Enter the number that will be the start of your separate stream ID pool and then click **OK**. If you later need to draw more streams with ID numbers in the normal range, you can return to this dialog box and reload the default setting.

For example, to draw a series of utility streams with ID numbers starting at 300, you would set the stream starting ID option to **300** and draw the streams in question. Those streams would be numbered 300, 301, 302, and so forth. After drawing all your utility streams, you would then set the Stream ID option back to **1**, so that the next new stream in the main flowsheet would be assigned the next available stream ID from the regular pool of numbers. You can reset the stream option number as many times as needed while you create and edit your simulation.

Stream Names

In addition to the assigned stream ID, you can give a stream a name, using up to 11 alphanumeric characters. This name appears in the Edit Stream dialog, in the Streams area of the CHEMCAD Explorer pane, on certain reports, and optionally on the flowsheet with the stream ID.

To add a stream name, you can open the Edit Streams dialog and type in the **Stream Name** field. Another way to add a name is to right-click the stream and select **Edit Name**; type the name in the resulting dialog box and click **OK**.

By default, a newly added stream name will appear beneath the number in the stream ID box. To hide a single stream's name, right-click the stream and clear the check mark next to **Show Name**; simply click this menu item again to make the stream name visible.

To view or hide all stream names on the flowsheet at once, click the **View** tab, then in the **Flowsheet** group, either check or clear the **Show Stream Names** box.

Stream Intersections

When streams cross on a flowsheet, a visual indicator can be helpful to show that the streams do not interact with one another. You can set up a default size and shape to show one stream "jumping" over another wherever two streams meet. By default, a stream jump displays as a semicircle.

CHEMCAD offers several other options for stream intersections, including no jump indicator and a dash to break one stream line as it crosses. The figure below shows all of the available stream intersection options.

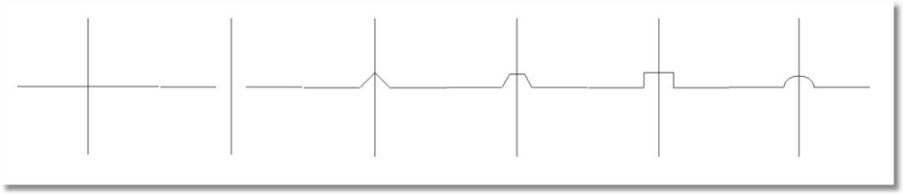


Figure 5-10: Stream intersection options (from left: None, Dash, Triangle, Trapezoid, Square, and the default setting, Circle)

To select a stream intersection option for the *current simulation*, click the **Drawing** tab, then in the **Workspace** group, click **Stream Styles**. In the Stream Styles dialog, drop down the **Style** list under Intersections, and select an option. When you click **OK**, any stream intersections already on your flowsheet will change to the new style; any new intersections that occur will also use that style. This style will continue to be used for new intersections, even after this simulation has been closed and re-opened.

To change the *global style* for stream intersections—that is, to set the default for all future simulations created in your CHEMCAD installation—you can change the setting in a different place. Click the **File** tab, then **Preferences**. In the Preferences dialog, click **Stream Styles** in the left column. This brings up the same list of stream intersection options, but when you select one and click **OK**, the chosen style will become the global default for this CHEMCAD installation.

Note that you can also change the size of the stream jumps in both the local and global settings for stream intersections. The default size is 48, which is well proportioned for use with standard UnitOp sizes.

Defining Streams

At this point, the streams that you have drawn on your flowsheet are still just lines with no data behind them. The next step is to edit these streams as needed, populating them with composition data and other properties.

In most situations, the streams you'll need to define will be the feed streams in your process. Other types of streams, such as recycle cut streams, may also require definition.

You can edit a single feed stream using any of these methods:

- Double-click the stream.
- Right-click the stream line and select **Edit Stream**.
- On the **Home** tab, in the **Specification** group, click **Edit Streams**. Enter the stream number you want to edit and then click **OK**.
- On the Explorer's **Simulation** tab, expand **Flowsheet** and then **Streams**, right-click the stream in question, and select **Edit Stream**. (This is a useful approach for especially large and complex flowsheets.)

To edit multiple streams at once, you can use the following methods:

- Hold down **[SHIFT]** and click to select multiple streams on the flowsheet, then right-click and select **Edit Stream**.
- Click **Edit Streams** in the **Home** tab's **Specification** group, then either type the stream numbers into the Select Streams dialog box or click the streams on the flowsheet to add them to the list. Click **OK** when finished.
- To edit all the feed streams in the flowsheet at once, click the **Edit Streams** drop-down (**Home** tab, **Specification** group) and select **Edit Feed Streams**. Similarly, to edit all the cut streams in the flowsheet, select **Edit Cut Streams** from the same drop-down.

The Edit Streams dialog box displays with either a single column of data (for one stream) or a column for each stream that you have selected. Use this dialog box to specify properties for each feed stream listed.

Thermodynamic Properties

You must specify exactly two of the following three variables:

- Temperature
- Pressure
- Vapor fraction

CHEMCAD will calculate the third variable and enthalpy, based on the two variables you specify and the thermodynamic method you've selected, once the stream composition data has been entered.

Note: In the Edit Streams dialog box, the user-specified values for feed streams will display in green, differentiating them from calculated values.

Stream Composition

To define the stream composition, you'll need to specify a composition unit and the amount of each component that is present in the stream.

Select a unit from the **Comp unit** drop-down list, and then based on that selection, populate the field for each component with the appropriate amount, percentage, or fraction.

For stream compositions expressed as a percentage or fraction, you can enter values that do not total 100%. In this case, CHEMCAD will normalize the composition to fractional values that total 1. To preview the normalized values that CHEMCAD assigns to the components, click **Flash**.

Total Flow Properties

If the component flow engineering unit used for a stream is dimensionless (i.e., mole fraction, weight fraction, or volume fraction), you must specify the following flow properties:

- Total flow
- Total flow unit

If you enter composition amounts using quantitative flow units, CHEMCAD calculates the total flow rate for you.

Specifying Equipment Parameters

Once you have specified the necessary stream properties for your simulation, the next step is to enter specifications for the UnitOps. You can edit the parameters of a UnitOp using any of the following methods:

- Double-click the UnitOp icon on the flowsheet.
- Click the UnitOp icon (or hold down **[SHIFT]** and click to select multiple UnitOp icons) and then click **Edit UnitOps** in the **Home** tab's **Specification** group.
- On the Explorer's **Simulation** tab, expand **Flowsheet** and then **UnitOps**, right-click the UnitOp in question, and select **Edit UnitOp Data**. (This is a useful approach for especially large and complex flowsheets.)

The dialog box that displays when you go to edit a UnitOp's specifications will depend on the type of UnitOp. The Stream Mixer UnitOp, for example, has only one specification that you can set, while the SCDS Distillation Column UnitOp has five tabbed pages of detailed settings.

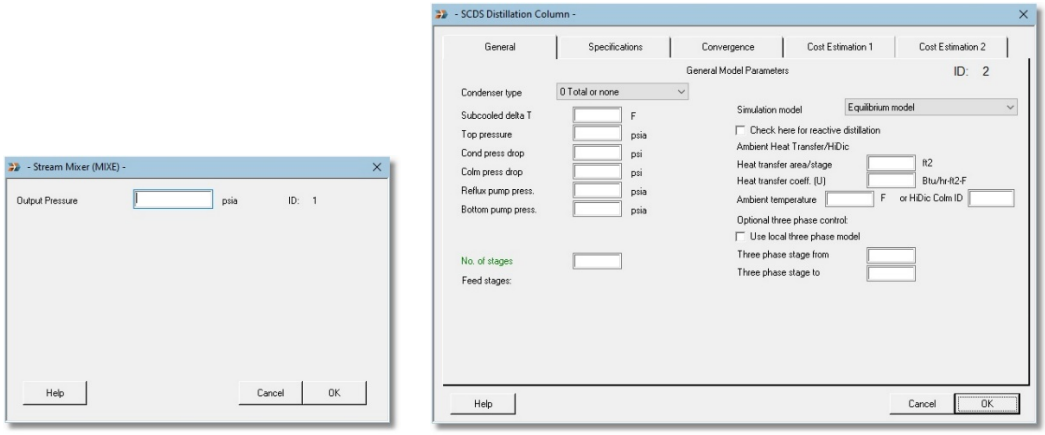


Figure 5-11: Two UnitOps that require very different amounts of input

The detailed information about the specifications for each type of UnitOp is contained in the CHEMCAD Help system, which you can access from any CHEMCAD screen by pressing the **[F1]** key.

These specification screens do, however, have certain rules in common:

- Items with green text labels are required entries.
- All other entries are optional.
- Clicking **OK** saves your specification changes; clicking **Cancel** discards them.

After you click **OK**, CHEMCAD checks your data for internal consistency and then returns errors or warnings as warranted. These items display in the Messages pane in the CHEMCAD window.

Running the Simulation

> **Note:** The steps for running a simulation are different if you are using CC-DYNAMICS for dynamic calculation. See Chapter 7, *Building and Using a Dynamic Simulation*, for information about setting up and running dynamic simulations.

Now that you've drawn the flowsheet and added detail to the streams and UnitOps that make up the flowsheet, you can run the simulation. To do this, simply click **Run All** in the **Home** tab's **Run** group.

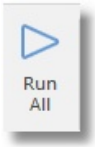


Figure 5-12: The Run All command

When you run a simulation, CHEMCAD calculates material and energy balances throughout the entire flowsheet and returns any errors or warnings discovered in the flowsheet. If the run completes successfully, a *Run finished* message appears at the far left of the status bar, at the very bottom of the CHEMCAD window.

If the flowsheet run has converged, the message *Flowsheet calculation has converged* will appear in a pop-up message window, as well as in the Messages pane. The word *Converged* will also appear near the center of the status bar; this message will continue to display until you make changes to the flowsheet or the simulation models that could affect convergence, and it will reappear after each successfully converged run.

For preliminary checks of individual UnitOps or groups of UnitOps, you can click **Run Selected** instead of **Run All**; either highlight the relevant UnitOps on the flowsheet before invoking this command or select them afterward in the Select UnitOps dialog box. You can also right-click any UnitOp on the flowsheet and select **Run This UnitOp**.

Reviewing the Results

After a simulation has run, you can call up any number of individual text-based reports or graphical charts, either for on-screen viewing or for printing. Reports can provide data on any single stream or UnitOp, or any group of streams or UnitOps, in a steady-state or dynamic simulation. You can also request a consolidated report that provides comprehensive data on the streams and UnitOps you select.

> **Note:** CHEMCAD reports, plotting, and chart printing are covered in detail in Chapter 8, *Output and Reports*.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Chapter 6

Using CHEMCAD for High-fidelity Modeling

Simulations created in CHEMCAD vary greatly in detail, from vague and conceptual to extremely specific and realistic. Depending on the demands of your process and what you're trying to achieve with your simulation, you may work with what we call *low-fidelity modeling*, *high-fidelity modeling*, or both.

This chapter addresses CHEMCAD's capacity for high-fidelity modeling and how to achieve a high level of realism with your UnitOps.

What is high-fidelity modeling?

With low-fidelity modeling, you specify what you want, or what you have observed, and CHEMCAD makes its calculations based on the assumption that you can achieve what you've specified. It's common to specify observed properties such as temperature and/or pressure coming out of a UnitOp, or component purity coming out of a separation unit. Specifying temperature coming out of a heat exchanger is an example of low-fidelity modeling.

High-fidelity modeling, on the other hand, requires that you enter numerous extensive variables. CHEMCAD calculates the resulting conditions based on these detailed entries. With high-fidelity modeling, you're often required to specify geometry-related variables for a UnitOp so that CHEMCAD can calculate precise conditions at the equipment's outlet.

Here's the key distinction between low-fidelity and high-fidelity modeling in CHEMCAD:

- **Low-fidelity:** You specify the desired results and CHEMCAD assumes that you can achieve those results with the equipment you have.

- **High-fidelity:** You specify energy and equipment parameters and CHEMCAD calculates the actual results.

Criteria for High-fidelity Modeling

To take advantage of CHEMCAD's high-fidelity modeling capabilities, you must provide detailed specifications for your equipment. To do this, most UnitOps require that you select a calculation *mode* that allows for entry of high-fidelity-caliber detail.

For example, if you have a pump that is set to the default mode of *Specify outlet pressure*, you'll get a low-fidelity result from this pump—that is, the simulation will use the outlet pressure that you specify, but without consideration for the size of the pump, the amount of fluid entering the pump, or inlet pressure.

If you switch the pump to *Specify performance curve*, a high-fidelity mode, you'll need to enter data points from the pump's performance curve, either for a single speed line or for multiple speed lines. Using this mode, CHEMCAD will calculate the change of pressure head based on the performance data and the inlet volumetric flow rate. This provides a realistic pressure increase for the actual pump that your process uses.

Not every type of CHEMCAD UnitOp lends itself to high-fidelity modeling. The following sections discuss various types of UnitOps that do offer high-fidelity calculation modes, and provide some basic information about how to use those modes.

Introduction to Equipment Sizing

Equipment sizing in CHEMCAD is optional. It entails using the **Sizing** tab commands, generally after running a simulation, to calculate approximate sizes for pipes, vessels, valves, orifices, and other equipment.

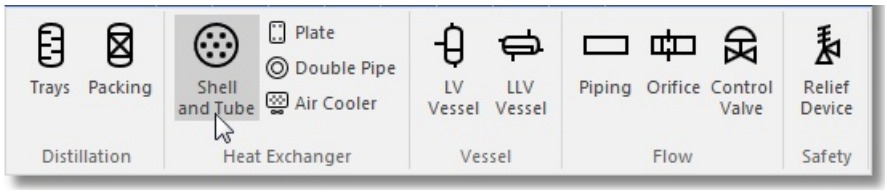


Figure 6-01: Commands for sizing various UnitOps, accessed via the Sizing tab

Equipment sizing can complement low-fidelity results, and often provides an excellent starting point for high-fidelity modeling. You can use certain sizing results as input for high-fidelity models of UnitOps in your simulation. Specifying geometric parameters for UnitOps can help you obtain more realistic results.

Note that for low-fidelity modeling, sizing does not change converged flowsheet results. Also, for some UnitOps, certain geometry parameters must be entered regardless of the selected calculation mode.

High-fidelity Modeling and Sizing for Common UnitOps

High-fidelity modeling does not apply to all CHEMCAD UnitOps. This section summarizes those UnitOps for which you can use high-fidelity modeling, and compares that approach for each UnitOp type to low-fidelity modeling. Where applicable, UnitOp sizing is also discussed as it relates to low-fidelity versus high-fidelity modeling of these UnitOp types.

Piping

You can use either low- or high-fidelity modeling for piping in your simulation. Pipeline sizing is done based on the composition of a selected stream.

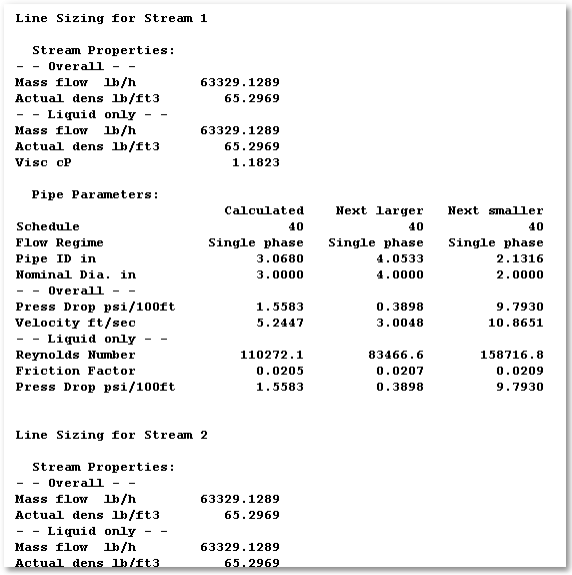
Low-fidelity

For low-fidelity modeling of piping, you are required to specify pipe diameter and length in most modes; design modes that calculate diameter are the obvious exception to this. The pressure drop through the pipe is calculated based on diameter, length, and flow rate through the pipe.

Sizing

To perform sizing calculations, first click the **Sizing** tab. In the **Flow** group, click **Piping**, and then select the relevant stream or streams. In the Pipe Sizing dialog box, select a sizing option and click **OK** for line sizing results. You can use these results, such as suggested pipe thickness and diameter, to specify geometry for a Pipe UnitOp, or simply review them for the information you need.

Note: You can also click to select the relevant stream on the flowsheet (hold down **[SHIFT]** to select multiple streams), then right-click and select **Line Sizing** to access the Pipe Sizing dialog box.



Line Sizing for Stream 1

Stream Properties:

- - Overall - -	
Mass flow lb/h	63329.1289
Actual dens lb/ft3	65.2969
- - Liquid only - -	
Mass flow lb/h	63329.1289
Actual dens lb/ft3	65.2969
Visc cP	1.1823

Pipe Parameters:

	Calculated	Next larger	Next smaller
Schedule	40	40	40
Flow Regime	Single phase	Single phase	Single phase
Pipe ID in	3.0680	4.0533	2.1316
Nominal Dia. in	3.0000	4.0000	2.0000
- - Overall - -			
Press Drop psi/100ft	1.5583	0.3898	9.7930
Velocity ft/sec	5.2447	3.0048	10.8651
- - Liquid only - -			
Reynolds Number	110272.1	83466.6	158716.8
Friction Factor	0.0205	0.0207	0.0209
Press Drop psi/100ft	1.5583	0.3898	9.7930

Line Sizing for Stream 2

Stream Properties:

- - Overall - -	
Mass flow lb/h	63329.1289
Actual dens lb/ft3	65.2969
- - Liquid only - -	
Mass flow lb/h	63329.1289
Actual dens lb/ft3	65.2969

Figure 6-02: Line sizing results from the Pipe Sizing dialog box

High-fidelity

In high-fidelity piping models, Pipe UnitOps interact with Node UnitOps to balance pressure and flow rates hydraulically among connected pieces of flow-based equipment. Nodes must be placed on both sides of all Pipe UnitOps to be included in hydraulic balance; pressure and flow constraints are set at the nodes, not in the pipes.

A high-fidelity piping model can show changes in flow rate based on back pressure where two pipes mix, whereas a low-fidelity model would simply assign the lower of two specified pressures to the outlet without consideration for back pressure.

Pumps, Compressors, and Expanders

You can create pump, compressor, and expander UnitOps using either low-fidelity or high-fidelity modeling.

Low-fidelity

For these equipment types, CHEMCAD calculates power usage and thermal effects on the fluid, based on specified output pressure or pressure increase. Other parameters, such as efficiency, are optional but do affect results.

High-fidelity

To produce a high-fidelity model for these equipment types, you must select the operation mode in which you specify performance curves—that is, pressure change as a function of volumetric flow rate. This performance information is generally available from the equipment vendor. Based on the volumetric flow entering the UnitOp, CHEMCAD calculates outlet pressure.

As with piping, high-fidelity modeling for pumps, compressors, and expanders can be used with nodes as part of a hydraulic flow balanced network.

Vessels and Tanks

You can add vessels and tanks to your simulations using high-fidelity modeling, or perform limited approximation of these equipment types with low fidelity in steady state. Sizing is available for certain types of vessels.

Low-fidelity

With low-fidelity modeling of a vessel or tank, a stream enters the Flash UnitOp and separates into vapor and liquid; CHEMCAD does not consider hold-up or liquid level in the tank. If you want to take a steady-state snapshot of the vessel, you can manually adjust the flow rate and/or thermal conditions to make volumetric flow rates match the volume of the vessel.

Note: The Batch Tank UnitOp is specifically intended for use with the Batch Distillation Column UnitOp. It does not represent a standard storage tank for general purposes.

Sizing

To calculate sizing for a vessel, first select a Flash UnitOp, then click the **Sizing** tab. In the **Vessel** group, click either **LV Vessel** (liquid-vapor vessel) or **LLV Vessel** (liquid-liquid-vapor vessel), depending on your needs. In the resulting dialog boxes, enter the appropriate values for your vessel and click **OK**.

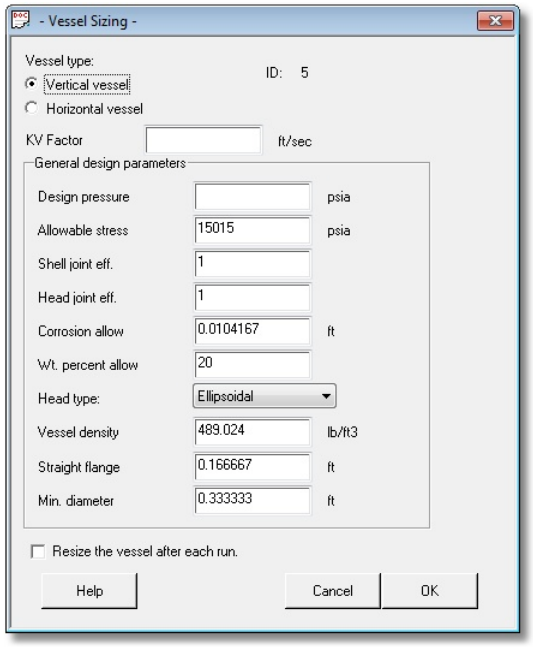


Figure 6-03: Sizing a vessel in CHEMCAD

The results that CHEMCAD returns include basic vessel geometry such as height and diameter.

You can also perform vessel sizing on a converged distillation column to calculate geometry for a reflux drum or similar piece of equipment.

High-fidelity

You can perform high-fidelity modeling only on vessel reactors and dynamic vessels, and only with a CC-DYNAMICS license (for dynamic vessels, a CC-SAFETY NET license will suffice). If you specify the geometry of your vessel and use CHEMCAD's dynamics mode, you can study what happens in the vessel over time as material is added or withdrawn.

Unlike simple flash vessels, vessel reactors and dynamic vessels do consider hold-up, liquid level, and variable pressure over time.

Valves

Valve modeling in CHEMCAD can be either low-fidelity or high-fidelity. You can size a control valve based on any flowsheet stream.

Low-fidelity

The Valve UnitOp is used for low-fidelity modeling of a valve. For this type of UnitOp, you specify outlet pressure or pressure decrease through the valve.

Sizing

To size a control valve, first click the **Sizing** tab. In the **Flow** group, click **Control Valve**, then select a stream. In the Control Valve Sizing dialog box, specify the outlet pressure for the theoretical valve, and enter other specifications as appropriate. When you click **OK**, CHEMCAD returns information such as capacity coefficient (Cv) and valve size.

Note: You can also click to select the relevant stream on the flowsheet, then right-click and select **Control Valve Sizing** to access the Control Valve Sizing dialog box.

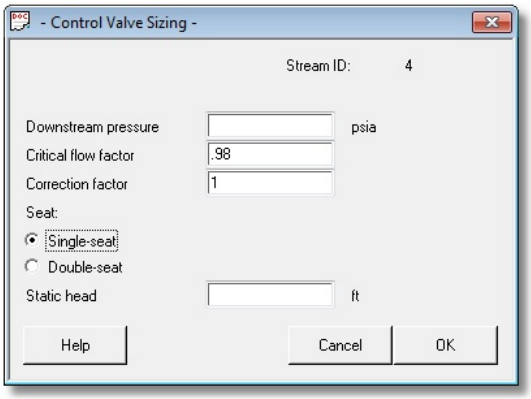


Figure 6-04: The Control Valve Sizing dialog box

High-fidelity

The CVAL UnitOp is used for high-fidelity valve modeling. Decide which values you will provide and which values CHEMCAD will calculate, and select the appropriate operating mode in the Control Valve dialog box. Provide the valve's Cv value, and any other specifications as needed.

Control valves can be used with nodes as part of a hydraulic flow balanced network.

Columns

Columns in CHEMCAD can be modeled as either low-fidelity or high-fidelity. You can perform sizing on any converged column.

Low-fidelity

For low-fidelity modeling of columns, use the Tower, Tower Plus, or SCDS UnitOps. Specify ideal stages and the conditions at the reboiler and condenser, as applicable. A low-fidelity column model does not consider mass transfer effects or column internals.

Different column specifications can provide more realism without taking geometry into account. Specifying top purity is a very low-fidelity model, while specifying reflux ratio or condenser duty can bring your results closer to reality.

Sizing

After running your simulation, first select the UnitOp representing the distillation column, then click the **Sizing** tab. In the **Distillation** group, click either **Trays** or **Packing**, based on the type of column.

The resulting dialog boxes prompt you to enter information about your trays or packing and the calculation methods you want to use for column sizing. You will generally need to enter some geometry and hydraulic parameters to complete column sizing.

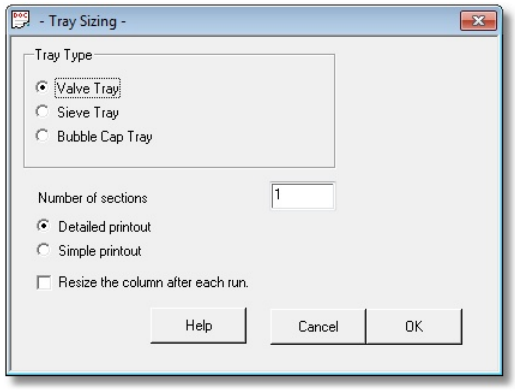


Figure 6-05: Specifying high-level tray data for distillation column sizing

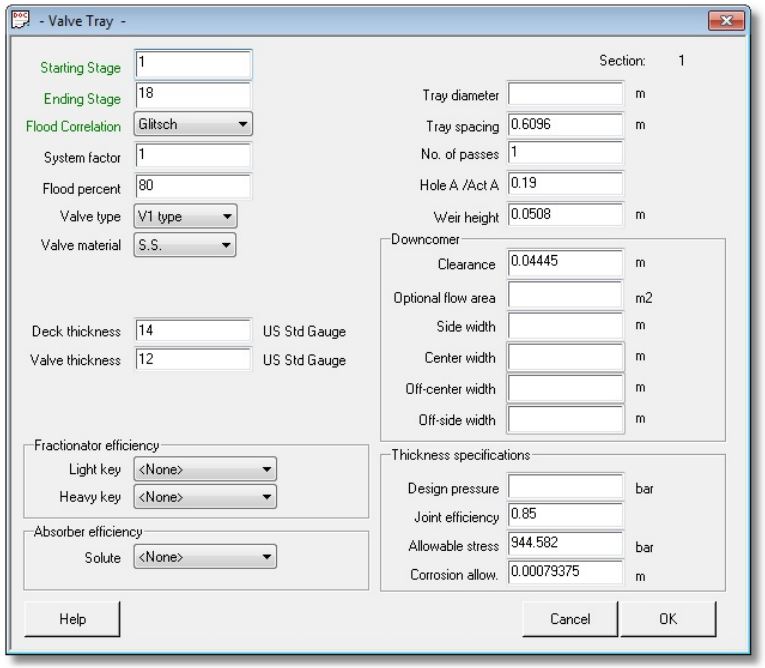


Figure 6-06: Specifying detailed tray data

Based on flowsheet values and your sizing input, CHEMCAD returns column geometry information such as height and diameter. It also provides hydraulic performance information such as predicted amount of flooding.

High-fidelity

To perform high-fidelity modeling of a distillation column in steady state, use the SCDS UnitOp and select either of the mass-transfer simulation models for the column.

You will need to specify geometry for the column and choose a calculation method for the selected mass-transfer model. CHEMCAD calculates column performance based on your packing or tray specifications.

For columns, mass transfer-based modeling performs rigorous non-equilibrium mixing of vapor and liquid, whereas low-fidelity modeling assumes ideal mixing.

To perform high-fidelity modeling of a distillation column in dynamics, specify the geometry of the column and details about the control system. This dynamic distillation can consider column hold-up and the effect of variables changing over time.

Note: The Shortcut Column UnitOp is *not* a rigorous calculation model. Unless your system satisfies the constant molar underflow assumption, you should consider using a different type of distillation column.

Heat Exchangers

When specifying a heat exchanger in a simulation, you can use either low- or high-fidelity modeling as well as sizing, depending on the type of heat exchanger involved.

Low-fidelity

When creating a simulation, you can use a low-fidelity approach by simply specifying the thermal conditions coming out of the exchanger. Specifying heat duty instead of merely an outlet temperature brings your results closer to reality, but this approach still doesn't consider geometry.

Sizing

You can use the CC-THERM module for rigorous calculation of heat transfer coefficient (U) based on heat exchanger geometry. In rating mode, CC-THERM determines whether the user-specified heat exchanger is capable of the flowsheet heat exchanger performance. In design mode, CC-THERM calculates an exchanger design that is capable of the flowsheet performance.

High-fidelity

For some exchanger categories—specifically shell-and-tube and double-pipe—you can use the rigorous CC-THERM model to calculate heat exchanger performance. The flowsheet results are based on rigorously calculated U value and the specified exchanger geometry. You can also determine approximate fouling of a unit if actual outlet temperatures are known.

Summary

Geometry Data		
Exchanger Class		R
Exchanger Type		AEL
Shell I.D.	ft	6.00
Shell in Series		1
Shell in Parallel		1
Number of Tubes		4000
Tube Length	ft	25.00
Tube I.D.	ft	0.05
Tube O.D.	ft	0.06
Tube Pattern		TRI60
Tube Pitch	ft	0.08
Number of Tube Passes		1
Number of Baffles		11
Baffle Center Spacing	ft	2.0718
Baffle Cut, %	Diameter	35
Baffle Type		SSEG
Baffle spacing definition		Edge-Edge

Fluid Dynamics Data		
Shell Side Pressure Drop	psi	12.5667
Tube Side Pressure Drop	psi	4.8009
Average Shell Side Velocity	ft/sec	15.33
Average Tube Side Velocity	ft/sec	23.82

Heat Transfer Data		
Effective Transfer Area	ft2	19347.88
Area Required	ft2	13023.75
Excess %		48.56
COR LMTD	F	44.68
Overall Coefficient (Calculated)	Btu/hr-ft2-F	122.57
Overall Coefficient (Service)	Btu/hr-ft2-F	82.50
Heat Calculated	MMBtu/h	105.95
Heat Specified	MMBtu/h	71.32
Shell Side Film Coefficient	Btu/hr-ft2-F	1201.71
Tube Side Film Coefficient	Btu/hr-ft2-F	251.74
Shell Side Fouling	hr-ft2-F/Btu	1.0000E-03
Tube Side Fouling	hr-ft2-F/Btu	1.0000E-03
Tube Wall Resistance	hr-ft2-F/Btu	3.2735E-05
Fin Resistance	hr-ft2-F/Btu	

Thermodynamics and Others	
K model	UNIFAC
H model	SRK
Data Source	Library
Number of Components	2
Calculation Mode	Rating

Figure 6-07: Heat exchanger summary report generated as an Excel worksheet

Relief Devices

For relief devices, sizing is not necessarily distinct from low-fidelity modeling. To model dynamic relief of a vessel, you can instead use high-fidelity modeling.

Low-fidelity

To model a steady-state snapshot of a relief device, first click the **Sizing** tab. In the **Safety** group, click **Relief Device** to bring up the DIERS for Relief Device Sizing dialog. Here you can specify a rating or design mode and select the appropriate options for your relief scenario. When you click **OK**, CHEMCAD returns a relief device calculation summary.

High-fidelity

If you select the *Rigorous integral analysis* design method when sizing a relief device, you will obtain a results based upon the changing latent heat of the liquid as it changes over time.

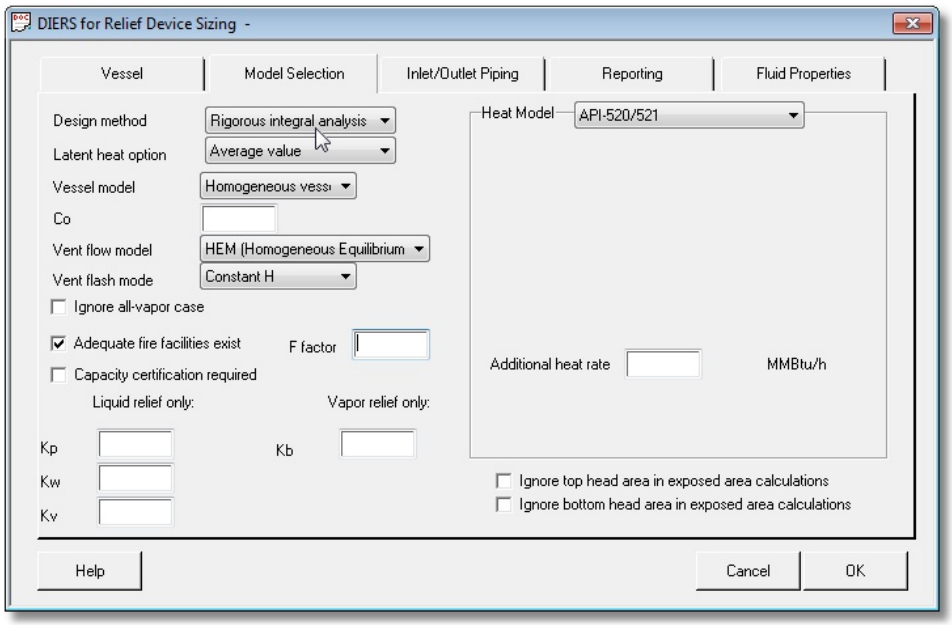


Figure 6-08: Selecting the rigorous integral analysis method for relief device design

You can also perform high-fidelity relief device modeling for the Vessel Reactor and Dynamic Vessel UnitOps. You can specify the relief device nozzle area, as well as other specifications for your relief scenario. This enables you to study the dynamic relief of the vessel.

Licensing Considerations for High-fidelity Modeling

To use the heat exchanger sizing functionality, you must have a valid license for the CC-THERM module of CHEMCAD. To use vessel reactors, you'll need a valid license for the CC-DYNAMICS module. For dynamic vessels, a license for either CC-DYNAMICS or CC-SAFETY NET is required.

Each of these modules is licensed independently. To view or change the disposition of your various product licenses, see the CHEMCAD License Monitor screen (**File** tab, then **Licensing)**.

If you don't currently have access to the heat exchanger sizing or dynamics features and want to add any of these modules to your installation of CHEMCAD, contact the person within your organization who handles software licensing, or if appropriate, you can contact Chemstations or a CHEMCAD distributor directly. For a complete list of Chemstations contacts worldwide, see our website (www.chemstations.com).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Chapter 7

Building and Using a Dynamic Simulation

While steady-state modeling can provide all the information you need for many purposes, it's often informative to look closely at the changes over time that affect your streams and equipment. CHEMCAD's CC-DYNAMICS module makes it possible to simulate a process over time.

What do we mean by dynamics?

We use the term *dynamics* to describe modeling a chemical process over a set period of time. During the course of a real-world chemical process, factors such as utility temperature, feed composition, and liquid levels tend to change. Modeling the response of your process to these changes can help you understand and predict what happens with your process over time.

Given a flowsheet, a length of time to run, and the calculation interval to use, CHEMCAD can return detailed results that take into account these types of changes. The program can consider the material holdup within process equipment such as tanks, reactors, and pipes. It also enables you to model control systems such as PID controllers.

Licensing Considerations

To use the functionality described in this chapter, you must have a valid license for the CC-DYNAMICS module of CHEMCAD. To view or change the disposition of your CC-DYNAMICS product license, see the CHEMCAD License Monitor screen (**File** tab, then **Licensing**).

If you don't currently have access to the dynamics features and want to add CC-DYNAMICS to your installation of CHEMCAD, contact the person within your organization who handles software licensing, or if appropriate, contact Chemstations or a CHEMCAD distributor directly. For a complete list of Chemstations contacts and CHEMCAD distributors for all parts of the globe, see our website (www.chemstations.com).

Additional Input for Dynamic Operation

Before you create a dynamic simulation, you'll need to gather the relevant information about your UnitOps and streams, as you would with any simulation. In addition, you need to be able to answer the following dynamics-specific questions:

- How long will the simulation run?
- What will be the interval (delta time/step size) between calculations?
- What is the change that you want to study over time?
- If applicable, what is the initial composition and charge of any dynamic vessels or vessel reactors?
- Which streams or UnitOps will be recorded for later analysis?

The basic steps for a dynamic simulation are largely the same as those for a steady-state simulation, with a few vital differences:

1. Create a new simulation.
2. Select engineering units.
3. Select components.
4. Select thermodynamic options.
5. Draw the flowsheet.
6. Specify feed streams and initial stream conditions.
7. Set specifications for UnitOps.
8. Run the simulation in steady state to obtain time-zero values.
9. Switch the simulation to dynamics.
10. Specify dynamics settings, such as run time and initial charge(s), and indicate which streams and/or UnitOps to record.
11. Reset the simulation to its initial state.
12. Run the simulation in dynamics.
13. Review the results.
14. Re-run or extend the simulation as needed.
15. Generate charts and reports as needed.

Before you start working on a dynamic simulation, it's important to have as much information about your process as possible, a clear idea of what you want to find out, and a strategy for producing the results you need.

Strategies for Dynamic Simulations

When you start planning a dynamic simulation, it's vital that you know what question or questions you are trying to answer. To get useful, informative results, you should start with a simple question and then refine the simulation and run it again.

For example, to discover how heat affects a vessel's temperature over time, you might start by applying constant heat to the vessel for the duration of your dynamic simulation. You can then save a copy of that simulation, change it to use variable heat, and review the results to see how they differ from the original. Based on that second simulation, you can make another copy, and this time try variable heat with a control system to attempt to maintain a consistent temperature. Each of these dynamic simulations would bring you closer to what you want to discover. Each subsequent simulation requires more information from you to run and return the results you want.

While there is no requirement that you approach dynamics problems this way, it's a sound practice that will save you time and frustration in the long run.

Setting up Dynamic Operation

Before you can run a dynamic simulation, you need to provide parameters such as run time and step size. First, however, you must activate CHEMCAD's dynamics mode.

Switching to Dynamics

To switch to dynamics, first open the simulation. On the **Home** tab, simply click the word **Dynamic** in the **Run** group.

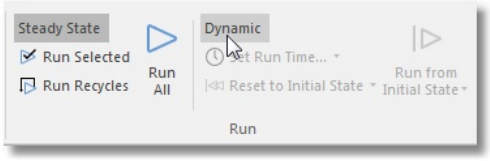

Figure 7-01: Switching to dynamics

After you do this, you'll notice that a few things have changed on the CHEMCAD screen:

- The status bar at the bottom of the main CHEMCAD window changes. A few inches from the left edge of the screen, instead of the words *Steady State*, you'll now see *DTime* and a time counter displaying the number of minutes your simulation has run. Before you run the simulation, the *DTime* setting displays **0:00 min**.

- The steady-state commands on the **Home** tab's **Run** group are now unavailable, and the dynamics commands are activated.

Setting the Run Time

The next step is to set the run time for the simulation. First decide whether your run will require a single step or multiple steps.

A step in this case refers to a time period during which CHEMCAD will capture data from the simulation at uniform intervals. For example, you might set up a single-step dynamic run of 60 minutes, with a step size of one minute, for a total of 60 data points for the run. If this is all that you need to do, your run can be accomplished in a single step.

If, on the other hand, you need to run your process for 60 minutes capturing data at one-minute intervals, and then switch to capturing data every 30 seconds for the next 20 minutes, you'll need to use two steps. If you want to record data every five minutes for the first hour, every minute for the second hour, and every 30 seconds for the third hour, you'll need to use three steps.

The step size that you select will have an impact on the accuracy of the results and the speed of the calculation. Smaller time steps produce more precise results, but also require more time to make the run. Smaller isn't always better, however, as extremely small time steps can lead to significant round-off error.

Once you know how many steps you need to use and what your data-capture interval will be for each step, follow these steps to set the run time parameters:

1. In the **Home** tab's **Run** group, click **Set Run Time**. This brings up the Dynamic Run Time Schedule dialog box.

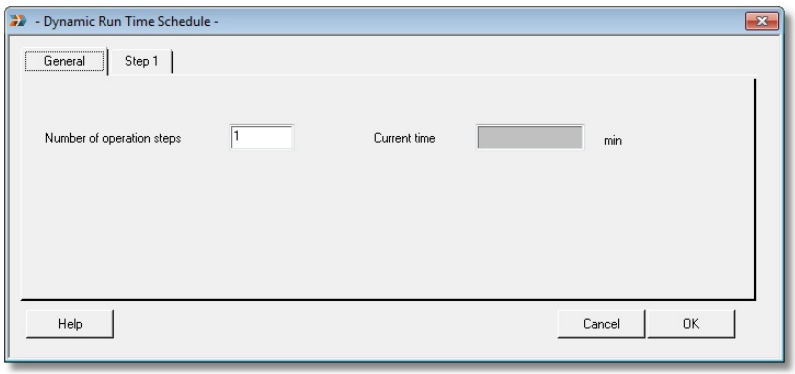

Figure 7-02: The General tab on the Dynamic Run Time Schedule dialog box

2. On the **General** tab, set the number of operation steps you plan to use, or leave the default setting of **1**. The maximum number of steps that you can specify is 10.

Note: When you initially set up dynamics for a simulation, the **Current time** display field on this tab will be empty. After the simulation has run, this field displays the total time of a completed run, or the current time of an interrupted run.

3. Now click the **Step 1** tab and specify the parameters for this portion of the dynamic run. Enter the total time for this dynamic step in the **Run time** field, and the interval in minutes in the **Step size** field.

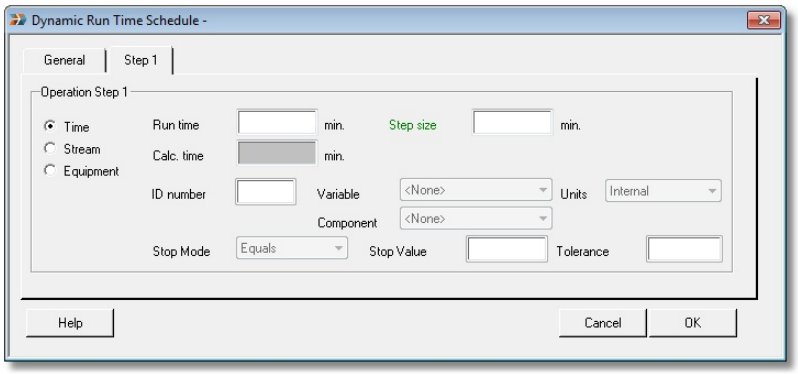

Figure 7-03: The Step 1 tab on the Dynamic Run Time Schedule dialog box

4. If you have other steps to specify, click each tab in turn and enter the **Run time** and **Step size** information.

5. When you have specified all steps, click **OK** to return to the main CHEMCAD workspace.

The Dynamic Run Time Schedule dialog box also allows for conditions other than time to determine the duration of a dynamic operation step. If you select **Stream** or **Equipment** instead of the default **Time** option, you can specify a stream or UnitOp parameter that will trigger the end of this step, if that parameter is reached before the step's run time is up.

Selecting Streams and UnitOps

Now that you have specified how long your dynamic process will run, you need to tell CHEMCAD what stream and UnitOp data to record during the run.

1. On the **Home** tab, in the **Run** group, click the **Set Run Time** drop-down and select **Record Streams**.

2. In the Record Streams dialog box, do one of the following:

   - Check the **Select streams from flowsheet** box, click **OK,** and then use the mouse to add streams to the **Select Streams** dialog box.

   - Type the numbers of the streams you want to record in the **ID** boxes.

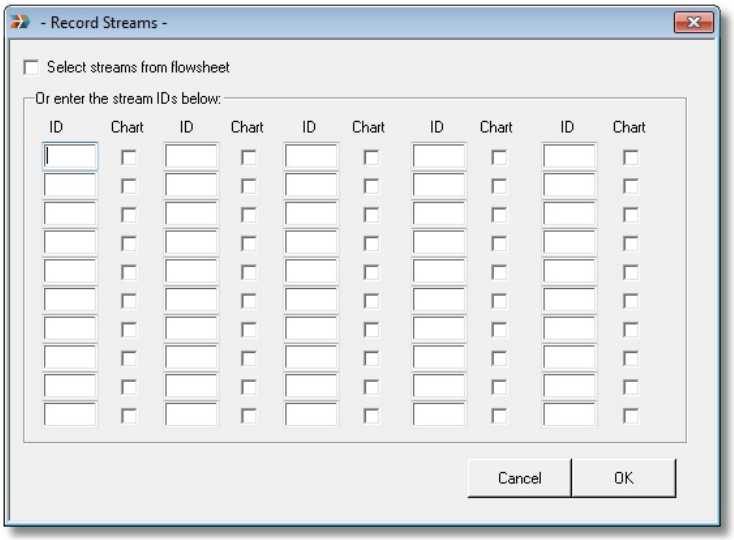

Figure 7-04: The Record Streams dialog box

3. When you have selected all the streams you want to record, click **OK** to return to the main workspace.
4. Now click the **Set Run Time** drop-down again, and this time select **Record UnitOps**. In the Record UnitOps dialog box, select UnitOps in the same way that you selected streams in step 2.
5. Click **OK** to return to the main CHEMCAD workspace.

> **Note:** In both the Record Streams and Record UnitOps dialog boxes, you can use the **Chart** check boxes to include selected items in a real-time chart. Selecting items for runtime plotting leads to another dialog box (either Dynamic Stream Chart Options or Dynamic Equipment Chart Options), where you can select chart specifics for each stream or UnitOp. It is recommended that you use runtime plotting in moderation, as too many streams and UnitOps can become visually confusing and slow down calculations considerably.

6. Before proceeding, click **Save** in the Quick Access Toolbar to ensure that the current settings are used as the simulation's initial state.

Initial State Settings

In addition to the options for setting up and running a dynamic simulation, the **Home** tab's **Run** group offers two other dynamic commands: **Save as Initial State** and **Reset to Initial State**. It's important to understand what these commands do before you begin to work with dynamic simulations.

Save As Initial State

The **Save as Initial State** command sets the current conditions of the dynamic run as the new initial state. It discards all parameters from the previous initial state, and makes it impossible to recover the previous initial state data.

An example of a dynamic run can illustrate the usefulness of this command. Suppose that you run a simulation for five minutes and the temperature in a vessel increases from 50 °C to 70 °C. You decide that 70 °C is a better starting point for this vessel, and you want to capture all the other values that correspond to that temperature in this vessel. You can achieve this by saving the current conditions as the initial state.

To do this, click the drop-down arrow to the right of the **Reset to Initial State** command, then select **Save as Initial State**. You will see a message warning you that you will lose the original state conditions if you continue. If you are prepared to do this, click **Yes**. For our example, this would mean losing the first five minutes of your previous run, along with the 50 °C starting temperature for the vessel.

After you save a new initial state, the **Run from Initial State** and **Reset to Initial State** commands both reference your new initial state settings.

Reset to Initial State

In a dynamic simulation, you can change stream and UnitOp specifications only when the dynamic time is set to zero. During or after a run, if you attempt to edit the specification dialog box for a UnitOp, you will find the **OK** button disabled and a message instructing you to restore the simulation to its initial state.

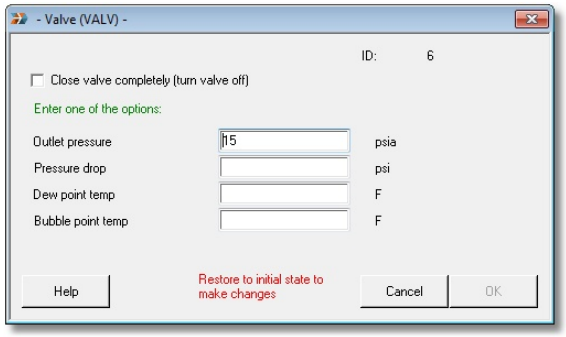

Figure 7-06: A UnitOp specification dialog box after a dynamic run

To return the simulation to its initial state—also known as *time zero*—simply click **Reset to Initial State**.

Note: An advanced feature to allow specification editing at any time is available, but should be used with extreme caution to avoid confusion and unintended results. This feature is controlled by a check box on the Convergence Parameters dialog box.

Running a Dynamic Simulation

Now that you have set the run time and recording parameters, you can run the simulation. When you run a dynamic simulation in CHEMCAD, a calculation of the entire flowsheet runs for each step in the time range that you select.

In dynamics mode, you have three options for running a simulation: run from the simulation's initial state, run from the simulation's current state, or manually advance the simulation one interval at a time.

Note: At any point during a dynamic run, you can press the **[ESC]** key on your keyboard to stop the run after the current calculation. When you do this, you will see a *Program interrupted* message. Click **OK** to close the message box, and then either inspect your run results or select a run command to continue.

Run from Initial State

This option resets the flowsheet to its initial conditions and begins the dynamic simulation. When you run a simulation this way, all results from previous simulations are discarded.

To choose this option, simply click **Run from Initial State** in the **Home** tab's **Run** group. This is the default dynamic run mode each time you open CHEMCAD.

Run from Current State

When you use this option, the dynamic run begins from the current conditions. Those conditions might be the initial state of the flowsheet, the end of a previous run, or the middle of an interrupted run. Selecting this option continues the simulation from the current state, i.e., from the last calculated result.

You can use this option only when some calculations remain to be run. This means that unless you have interrupted the run using **[ESC]** or the step-by-step method described in the next section, you must schedule one or more additional steps using the **Set Run Time** command before continuing.

To run the simulation starting from current conditions, click the **Run from Initial State** drop-down (**Home** tab, **Run** group) and select **Run from Current State**.

Run One Step at a Time

If you want to get a detailed view of your dynamic run as it unfolds, you can choose to run one interval at a time. With this option, the dynamic run will stop after each discrete time step. To run the next time step, you will need to either direct CHEMCAD to run the next step or use the **Run from Current State** command.

To use this frame-by-frame approach to dynamics, click the **Run from Initial State** drop-down (**Home** tab, **Run** group) and select **Run One Step**.

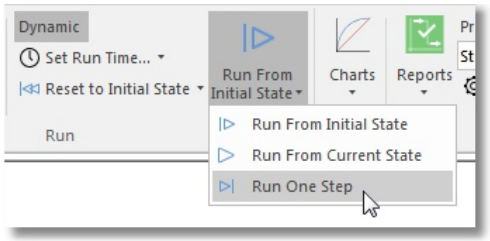

Figure 7-05: Selecting the command to run one interval in a dynamic simulation

Output from Dynamic Simulations

The results from dynamic simulations are markedly different from those produced by steady-state simulations, primarily in that they record data trends over time instead of a static snapshot of a fixed process. With dynamic simulations, comparisons of slightly different process specifications, and of the same process at different points during a run, can be very useful.

For this reason, you may find that graphical reports provide the most useful information when you're working with dynamic simulations. CHEMCAD provides a series of dynamics charting options to meet this need; you can also generate various text-based reports, and view calculated flowsheet values at any point during a dynamic run or after a run is complete.

Reviewing the Flowsheet Specifications

A snapshot of flowsheet values from a dynamic run doesn't provide as much value as it would for a steady-state run, but it can come in handy in many situations.

After running a dynamic simulation, you can view the data behind any flowsheet stream or UnitOp to see the effects of the run calculations. Double-click any stream or UnitOp on the flowsheet to review its end-of-run values.

You can also stop to review flowsheet data in the middle of a run, either by using the **Run One Step** option or by pressing **[ESC]** to pause a run. While the run is stopped, you can click the flowsheet tab and then double-click any stream or UnitOp to review its current values. To resume running after pressing **[ESC], click Run from Current State on the Home tab.**

Plotting Dynamic Results

Dynamic charts display selected values over time. You can plot the results of dynamic simulations using the **Charts drop-down gallery on the Home tab**. The following dynamic charts are available:

- **Stream History:** This chart displays selected stream properties from any recorded stream.
- **UnitOp History:** This chart displays selected UnitOp parameters from any recorded UnitOp.
- **Column History:** This chart displays selected values for a dynamic column, including composition of trays, distillate, and bottoms.
- **Vessel Reactor:** This chart displays selected values for a Vessel Reactor UnitOp, including composition of the contents over time.
- **Dynamic Vessel:** This chart displays selected values for a Dynamic Vessel UnitOp, including composition of the contents over time.
- **Batch Column: This chart displays values for a Batch Column UnitOp, which requires a license for the CC-BATCH module.**

Note: For the Stream History and UnitOp History charts, be sure to record the streams and UnitOps that you want to study. You can only request these charts for recorded streams or UnitOps.

Text-based Dynamic Reports

Based on the graphical results of your dynamic simulation run, you may decide to make changes to your process, run parameters, or both, and then re-run the simulation. When you have fine-tuned your simulation and obtained satisfactory results, you can view those results in tabular form, for a more detailed look at exact values.

To access text-based dynamic reports, click **Reports** on the **Home** tab and then select one of the following reports from the **Dynamic** section of the gallery:

- **Stream History**: This report provides stream histories for a specific stream that you select, based on the interval that you specify and including the compositions, components, and stream properties that you select.
- **UnitOp History:** This report provides detailed information about a dynamic UnitOp in the simulation, based on the interval that you specify and including the UnitOp parameters that you select.
- **Column History:** This report provides dynamic column results for a selected column. The Dynamic Column: Print Options dialog box offers the most relevant items for dynamic column reporting.

Note: For the Stream History and UnitOp History reports, be sure to record the streams and UnitOps that you want to study. You can only request these reports for recorded streams or UnitOps.

Chapter 8

Output and Reports

One of CHEMCAD's greatest strengths is its capacity to provide detailed, customized information about equipment, streams, and processes. The program can display a customizable snapshot of current data for any stream or UnitOp at any time. You can also create custom reports, spec sheets, and databoxes for process flow diagrams, and you can view data in the most appropriate chart or report format.

The charts and reports described in this chapter, along with the tools to customize and format your simulation data, are all accessible from the **Home** tab, using commands found in the **Results** group.

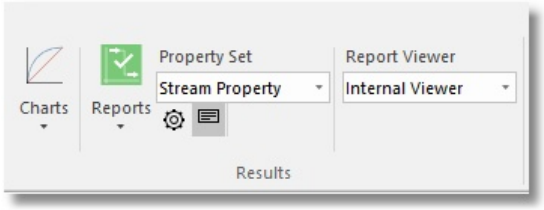

Figure 8-01: The Results group on the Home tab

The Basics: Generating Individual Charts and Reports

CHEMCAD makes it easy to generate a wide range of data charts and reports that reflect the current state of your process simulation.

Clicking the drop-down arrow for either **Charts** or **Reports** brings up a *gallery* view, displaying all the available chart or report selections. When a gallery is open, you can point the mouse to any item to see a pop-up description of that chart or report. To proceed, simply click the item you want.

When you make a valid selection, CHEMCAD brings up a dialog box where you can specify what to include in the requested chart or report. (If you choose a selection that is not valid—for example, a chart type that is not compatible with your current thermodynamic settings—you will see a message box explaining the error.) After you specify the parameters for the chart or report, the results will display.

Charts and reports always display in their own tabs on the main CHEMCAD workspace. Whenever a chart or report tab is selected, the ribbon displays commands specific to charts or reports, respectively.

Note that there are also large icons above both the **Charts** and **Reports** commands. When you first launch CHEMCAD, the icons displayed match the first items in the respective galleries. When you select a different chart or report from a gallery, you will see that item's icon display on the command ribbon. If the next chart or report you want to generate next is the same as your last selection, you can simply click the icon to choose that item without opening the gallery. This can save time whenever you find yourself generating the same chart or report repeatedly.

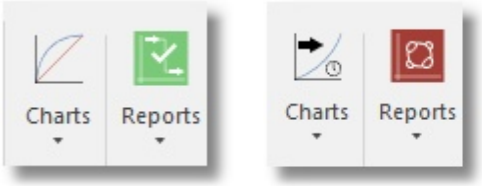

*Figure 8-02: Icons above the **Charts** and **Reports** drop-down commands: defaults (left) and examples of "last used" items (right)*

The Charts Gallery

CHEMCAD offers a wide variety of charts—reports in graphical format—that you can view onscreen or print for review. The Charts gallery displays the available charts in groups according to their type or purpose.

Depending on the type of chart you select, you may need to specify relevant streams or UnitOps or select other options in a dialog box before the chart can be generated. Detailed information about chart generation options is available in the CHEMCAD help system, which you can access by clicking a dialog's **Help** button.

The available charts are listed and described below, according to the group headings displayed in the Charts gallery.

Thermodynamic

CHEMCAD offers several charts that relate specifically to a simulation's selected components and thermodynamic options. To access any of these items, click **Charts** to view the gallery, then select the appropriate item under the **Thermodynamic** heading.

TPXY

This selection generates vapor-liquid equilibrium curves between any two components, with an optional third component. You can include TPXY, TXY, activity coefficient, and fugacity coefficient curves.

Binary LLE

This selection generates liquid-liquid equilibrium curves between any two components.

Binodal Chart

This selection generates a ternary phase diagram showing the distribution of three selected components in two liquid phases, including tie lines and plait point.

Residue Curves

This selection generates and plots a graphical display of distillation zones, azeotropes, and residue curves associated with a user-specified ternary mixture.

Binodal/Residue Curves

This selection creates a plot that combines the curves from a binodal plot and a residue curve plot. This is useful when working with heterogeneous azeotropic distillation.

Binary SLE

This selection displays solid-liquid equilibrium curves for binary mixtures.

Stream

CHEMCAD offers several charts that display data for selected streams on a flowsheet. To access any of these items, click **Charts** to view the gallery, then select the appropriate item under the **Stream** heading.

For any of these charts, you can choose the streams to include by typing in their ID numbers in the Select Streams dialog; click the streams on the flowsheet to add them to the stream ID list; or use **All Streams**, **Feed Streams**, **Product Streams**, or **Cut Streams** to add groups of streams with a single click.

Stream Properties

This selection plots one selected stream property for any or all streams on the flowsheet.

Phase Envelopes

This selection plots a phase envelope for a selected stream, highlighting the critical point of the mixture. This chart can include plots at vapor fractions other than 0 (bubble point curve) and 1 (dew point curve).

Petroleum Assay

This selection displays a chart of one or more distillation curves for a stream.

UnitOp

CHEMCAD offers several charts that display data for a single UnitOp. To access any of these items, click **Charts** to view the gallery, then select the appropriate item under the **UnitOp** heading.

Column Profiles

This selection plots compositions, temperature, and flow profiles for distillation columns.

Heat Curves

This selection plots heating and cooling curves for a selected heat exchanger.

Composite Curves

This selection plots composite heat curves for the entire flowsheet, as well as optional heat curves for individual UnitOps.

Plug Flow Reactor Profile

This selection plots the temperature or composition profiles along the axial length of a kinetic plug flow reactor.

Pipe Profile

This selection plots fluid properties for pipe UnitOps along the axial length of the pipe. This chart requires that the pipe contain multiple segments.

Controller Convergence

For controllers that have not converged, this chart enables you to diagnose the controller behavior that is preventing convergence. The chart shows how the controller error function changes with iteration.

Dynamic

CHEMCAD offers a series of charts for use with dynamic, or non-steady-state, operations. (For more on dynamic process simulation, see Chapter 7, *Building and Using a Dynamic Simulation).*

To access any of these charts, click the **Charts** gallery, then select the appropriate item under the **Dynamic** heading.

Stream History

This chart displays stream data recorded over the course of a dynamic run. Before requesting this chart, you must first use the **Record Streams** command to select streams to include, and then run the dynamic simulation.

UnitOp History

This chart displays UnitOp data recorded over the course of a dynamic run. Before requesting this chart, you must first use the **Record UnitOps** command to select UnitOps to include, and then run the dynamic simulation.

Column History

This chart displays selected data for a single dynamic run of a column. Note that in the Dynamic Column Chart Options dialog, if you choose to plot a variable for a specific stage, that stage must have been recorded during the dynamic run as part of the column's specifications.

Vessel Reactor

This chart displays selected data over time for a single dynamic run of a Vessel Reactor UnitOp. In the Vessel Reactor Chart Options dialog, you can select various equipment parameters to chart, and choose whether to include reactor composition over time.

Dynamic Vessel

This chart displays selected data over time for a single dynamic run of a Dynamic Vessel UnitOp. Composition over time can be displayed or excluded, and you can single out a specific phase to appear on the chart.

Batch Column

This chart displays selected data over time for a single run of a Batch Distillation UnitOp. In the Batch Column Chart Options dialog, you can choose to plot all operation steps or specify a single step to include.

User

If you have customized CHEMCAD using VBA, C++, or other programming languages, you can save chart data into a text file and use this feature to display that data as a curve.

To access this feature, click **Charts** and then select **User-specified** at the bottom of the gallery. This brings up a message box that provides instructions on how to format the text file. Click **OK** to continue to an Open dialog box, where you can select the text file you want to use. When you click **Open**, the curve is plotted and displayed.

Chart Tab Commands

After you request a chart, CHEMCAD generates the graphic and displays it in a separate workspace tab. If multiple charts were generated, each chart displays in its own tab. The simulation tab, all open chart tabs, and all open report tabs can be seen and selected at the bottom of the main workspace.

Whenever you are viewing a chart, the top of the CHEMCAD window displays the **Chart** tab, beneath the title *Charting Tools*. On this tab, you will find specialized commands that control the appearance of the current chart's data and labels.

The **Chart** tab commands are described below.

Edit Group

Close All Charts

This command closes the current chart, along with every other chart that is currently open. To close only the current chart, simply click the **x** on the chart's tab at the bottom of the workspace.

Save

This command enables you to save a chart within the simulation. Saved charts are listed in the Explorer pane under **Saved Charts**, where you can re-open them for later reference. This command is also used to save any changes you may have made to a re-opened chart.

Save As

This command is much like **Save**, except that it brings up a Save As dialog that requires you to provide a name for the chart that you are saving. You can also use it to make a copy of a re-opened chart under a different name, so that you can change the new copy's settings or labels while keeping the original copy.

Export Chart

You can use this command to export the current chart data, either as an Excel .csv file or as a semicolon-delimited table.

User Series

The User Series feature enables you to add a data point or series of points to an open chart in a CHEMCAD simulation. This information appears alongside the chart's calculated results. This feature is discussed in greater detail later in this chapter.

Chart Settings Group

Title

This field displays the default title of the chart. To change the title that appears above the chart, type new text here.

Type

This setting determines whether the chart displays both data markers and connecting lines (the default setting), only lines, or only markers.

Legend

This setting determines the location of the chart's legend. The default location is to the right of the chart; you can also choose to display the legend above or below the chart, to the left of the chart, or not at all.

Fixed Axis

By default, CHEMCAD charts place the X and Y axis lines at the edges of the display area. In cases where the range of data spans the positive and negative number space, you may prefer to see the lines drawn at X = 0 and Y = 0 for easier reference. Clear this check box to show the labeled axis lines intersecting at the point of origin. Note that this option is not available for use with ternary charts.

Spline

Check this box to produce a display where data points are connected by smooth, curved lines instead of straight lines.

Display Tie Lines

Check this box to hide or display the tie lines in a ternary (triangle) chart. These lines connect the two liquid phases in equilibrium.

X Axis, Y Axis, Secondary Y Axis, and Tertiary Y Axis Groups

These four groups of commands, found on the **Charts** tab for all XY charts, are nearly identical. They control the way data appears on each of the axes that can be displayed in various CHEMCAD charts.

Label

This field displays the default label for the relevant axis. To change the axis label, type new text here.

Formatting

Use this drop-down set of options to customize the numbers and lines that make up the relevant axis. The **Numerical Display** commands (**Format Type**, **Format Digits**) control the way grid numbers display on the axis, and the **Axis and Grid** commands (**Axis Color**, **Grid Fade**) determine the color and visibility of the axis' grid lines.

Log Scale

Check this box to switch from linear to logarithmic scale for the relevant axis.

Assigned Series

This control is available for all but the X axis. Click the drop-down control to view the available data series. Check or clear the box next to a series name to turn that series on or off for the relevant axis.

A Axis, B Axis, and C Axis Groups

These command groups, used with ternary charts, resemble the axis groups described above for XY charts. Each axis has an editable **Label** field, and the **Formatting** drop-down offers settings for **Axis Color** and **Grid Fade**.

Window Group

These commands offer a quick way to place all open tabs in view at the same time. Click **Tile Horizontally** to arrange items across the width of the workspace, or **Tile Vertically** to arrange them next to one another.

Adding Chart Data Manually with the User Series Feature

You can add one or more data points to display on any open chart in a CHEMCAD simulation. This feature, called *User Series*, is accessible from the **Edit** group on the **Chart** tab.

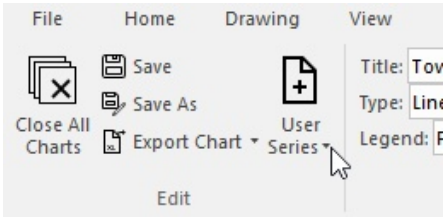

Figure 8-03: The User Series command on the Chart tab

When you add a user series, it becomes available for use in all current chart tabs, as well as in all future charts that you generate for the current simulation.

Adding a New User Series

On the **Chart** tab, in the **Edit** group, click the **User Series** drop-down and select **New**. This brings up the Add User Series dialog.

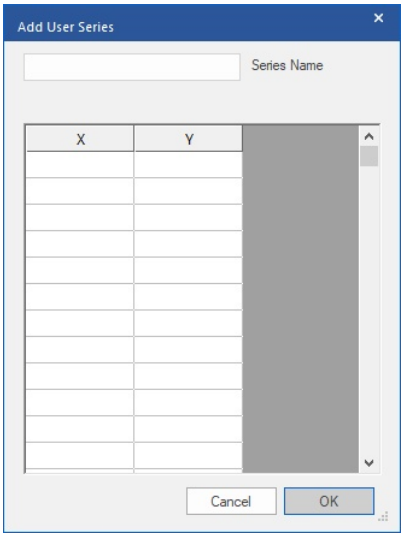

Figure 8-04: The Add User Series dialog

First type a descriptive name in the **Series Name** field, then enter the desired data points in the **X** and **Y** columns. (Note that you can paste numerical values here from the Windows Clipboard; simply right-click in the cell where you want the first copied value to appear and select **Paste**. See the full description below for more detail.)

To save the new user series and return to your chart, click **OK**.

Displaying a User Series on a Chart

Creating a user series does not automatically place the series on the chart. To plot the values from a user series on the current chart, click **User Series**, then choose the desired series name and select **Add to Chart**.

Once you have added a user series to a chart, it displays alongside the existing chart data, and its name and line color appear in the chart legend.

By default, the data points in a user series display on the primary Y axis. If you prefer, you can choose to display them using the chart's secondary or tertiary Y axis. To do this, click the **Assigned Series** drop-down for the desired Y axis and then click the user series name.

If you want to hide a user series from view once you have added it to a chart, click the **Assigned Series** drop-down in the relevant Y Axis group, then clear the check box next to the series name. To view the user series on the chart again, simply return to this drop-down and check the box again.

Editing User Series Values

To review or change the values in a user series, click **User Series**, then choose the series name and select **View/Edit**. This brings up the View/Edit User Series dialog.

In this dialog, you can change or add any values to update the current user series. After you have made any desired changes, click **OK** to save the changes.

Note that the series will not update automatically on the chart. To replace the previous series with the updated version, click the **User Series** drop-down again, select the series name, and click **Add to Chart**.

Importing Values for a User Series

If you already have the desired X and Y values in a spreadsheet or other table format, you can copy them from that location and then paste them into the Add User Series dialog from the Windows Clipboard.

To do this, first copy the desired values from their source location using the program's **Copy** command or the **[CTRL-C]** keyboard shortcut. Then, in the appropriate CHEMCAD chart, create a new user series as described above. After you provide a series name, right-click the cell directly below the **X** column heading and

select **Paste**. The values you copied from another source will populate the cells of the dialog.

Note that if you copy a block of cells that consists of more than two columns, only the leftmost two columns will be pasted into the Add User Series dialog.

Adding Data Points to a Ternary Chart

For a ternary chart, such as a residue curve map, you can use the User Series feature to place data points of interest on the chart.

On a tab displaying a ternary chart, when you click **User Series** and select **New**, the Add User Series dialog displays **A** and **B** columns, representing the A and B axes on the chart. To plot a point on the chart, enter values in a single row of this dialog. Be sure to assign a name, then click **OK** to return to the chart window.

As with other chart types, the new user series will not appear automatically on the ternary chart. Click the **User Series** drop-down, select the series name, and choose **Add to Chart** to view the point of interest on the ternary chart.

Deleting a User Series

To delete a user series from a simulation, click **User Series**, then choose the series name and select **Delete**. A message box will appear, asking you to confirm that you want to delete the series. Click **OK** to confirm and return to the chart tab.

After you delete a user series, it no longer appears on the **User Series** drop-down list, but it does not automatically disappear from the chart. If the deleted series is displayed on the chart, you can remove it by going to the **Y Axis** group (or other Y axis controls, as applicable) and clicking the **Assigned Series** drop-down. Clear the check box next to the name of the deleted series to remove it from the chart and the legend. You can also simply close the chart tab, as the deleted user series will not appear the next time you generate the chart.

Note: To remove a point of interest that you have added to a ternary chart, first delete the applicable user series and then close the chart tab. When you return to the same chart (**Home** tab, **Results** group, then click the ternary chart icon above the **Charts** drop-down), the point of interest will no longer be displayed.

The Reports Gallery

CHEMCAD can produce a wide array of customizable text reports, which you can view, save, and print. The Reports gallery displays the available reports in groups according to their type or purpose.

Depending on the report you select, you may need to specify relevant streams or UnitOps or select other options in a dialog box before the report can be generated.

The available reports are listed and described below, according to the group headings displayed in the Reports gallery.

Stream

You can run stream property reports for any grouping of streams from your simulation, as well as specialized stream-based reports for particle size distribution and petroleum assays.

Select

Choose the streams you want to include in the Select Streams dialog box, either by typing in the stream numbers (one per line) or by clicking on streams in the flowsheet. Click **OK** to close the dialog box and display the report.

All

This report displays stream property data for every stream on the flowsheet. No further input is required after you click **All** in the Reports gallery.

Feed

This report displays stream property data only for streams issuing from a Feed icon on the flowsheet. No further input is required after you click **Feed** in the Reports gallery.

Product

This report displays stream property data only for streams terminating in a Product icon on the flowsheet. No further input is required after you click **Product** in the Reports gallery.

UnitOp

This report displays property data for all inlet and outlet streams connected to a specified UnitOp on the flowsheet. If no UnitOp icon is selected when you run the report, you'll see the Select UnitOps dialog box; type the UnitOp ID or click the UnitOp on the flowsheet and then click **OK** to display the data. If you select a UnitOp icon before running the report, the data will display without further input.

Note: You can also generate a stream report from the flowsheet. To do this, click the applicable stream (or **[SHIFT]**-click to select multiple streams), then right-click to bring up the stream menu. Select **Stream Reports** and then choose a property set from the menu flyout to generate the stream report.

PSD (Particle Size Distribution)

For a particle size distribution report, select **PSD** from the **Reports** gallery. In the Select Streams dialog box, choose one or more streams for which a particle size distribution exists, then click **OK** to display the report.

Petroleum Assay

For a text report on pseudocomponent curves (also known as distillation curves), select **Petroleum Assay** from the **Reports** gallery. Select one or more streams containing hydrocarbons, then click **OK** to display the report.

UnitOp

CHEMCAD can also run reports to analyze UnitOp data. The results will display in either WordPad or Excel, depending on how you have configured CHEMCAD to handle text reports.

To access any of these items, click **Reports** to view the report gallery, then select the appropriate item under the **UnitOp** heading.

Select

To run a report that covers just the Unit Ops you specify, choose **Select** from the Reports gallery**.** In the Select UnitOps dialog box, specify the UnitOps you want to include in the report, either by typing in the UnitOp IDs (one per line) or by clicking on UnitOps in the flowsheet. Click **OK** to close the dialog box and display the report.

If you select one or more UnitOp icons before running the report, the data will display without further input.

Batch Results

This report summarizes the results of a batch distillation column simulation at the end of each operating step.

Spec Sheet

This command exports detailed information about a UnitOp into a preformatted Excel file. This report is useful for tasks such as soliciting a manufacturing quote for a piece of equipment.

When you select **Spec Sheet** from the Reports gallery, the Select UnitOps dialog appears. You can type in a single UnitOp ID or multiple IDs, click the desired UnitOp icons on the flowsheet, or click **All UnitOps** in the dialog to create a spec sheet for all units on the flowsheet. If you request spec sheets for more than one UnitOp, the resulting Excel file will include a separate worksheet for each UnitOp's data.

For a single UnitOp spec sheet, you can select the UnitOp icon before requesting the spec sheet, and Excel will open and display the data without further input.

Distillation

CHEMCAD offers several reports that focus on distillation data. To access any of these items, click **Reports** to view the report gallery, then select the appropriate item under the **Distillation** heading.

Column Profiles

Generates a report detailing temperature, pressure, and flow rate for a distillation column

Tray Composition

Creates a report that shows the vapor flow rate, liquid flow rate, and K-value of each component on each stage of a distillation column

Tray Properties

Reports on currently selected stream properties for each stage of a distillation column

Mass Transfer

For an SCDS distillation column that uses a mass transfer model, provides mass transfer coefficients, height of transfer units, and estimated height of theoretical plates (HETP)

Column Diagnosis

For columns that have not successfully converged, provides recommendations for changing column settings to achieve convergence

Flowsheet

In addition to reports that focus on particular UnitOps and streams, CHEMCAD offers text reports that provide information about the simulation as a whole. To access any of these reports, select the appropriate item from the **Reports** gallery.

Topology

This report provides a listing of all UnitOps in the flowsheet, as well as all stream origins and destinations.

Thermodynamics

This report lists all components used in the simulation and provides vital information about the thermodynamics methods used.

User Component

This report lists the physical properties of all user-added components in the simulation.

Mass and Energy

In addition to mass and energy balances, this report gives the order in which UnitOps are calculated, calculation modes used, and information about recycle loops, cut streams, and convergence.

Dynamic

This group of reports is used to obtain data about dynamic, or non-steady-state, processes. Dynamic process simulation is addressed in Chapter 7, *Building and Using a Dynamic Simulation*.

Stream History

This report provides stream information recorded over the course of a dynamic run. Before running this report, you must first use the **Record Streams** command to select streams to include, and then run the dynamic simulation.

UnitOp History

This report provides UnitOp information recorded over the course of a dynamic run. Before running this report, you must first use the **Record UnitOps** command to select UnitOps to include, and then run the dynamic simulation.

Column History

This highly customizable report details the data from a single dynamic run of a column.

UnitOp and Stream Groups

You can create custom groups of streams or UnitOps within a simulation to streamline your report and chart requests.

For example, if you have a process that involves ten different utility streams, and you frequently run reports or charts including all these streams, you can set up a group consisting of just those streams. Then, whenever you want to obtain composition or property data for those streams, you're just a few clicks away anytime the simulation is open.

Similarly, for UnitOp reports or charts, you can create custom UnitOp groups within a simulation. Much like their stream-based counterparts, UnitOp groups can save you time and effort when requesting reports or charts; in addition, you can use these groups when running your simulation, to isolate and run only selected UnitOps for diagnostic or other reasons.

Note: Because of this other functionality of UnitOp groups, the order in which you list UnitOp IDs when setting up these groups is important.

Creating a Group

The quickest way to set up any group is to use the Explorer pane on the left side of the CHEMCAD screen. Follow these steps to create a stream or UnitOp group:

1. In the Explorer pane, find the top-level item called Groups. Click the triangle next to **Groups** to expand this item.

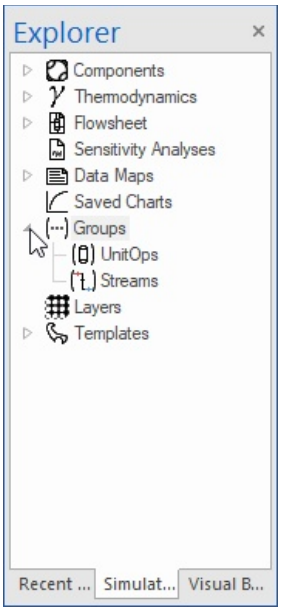

Figure 8-05: Expanding the Groups item in the Explorer pane

2. Now click either the **Streams** item or the **UnitOp** item under **Groups**, to bring up the New Group dialog. Replace the default name (such as **Group 1**) with a descriptive name for your group, then click **OK**.

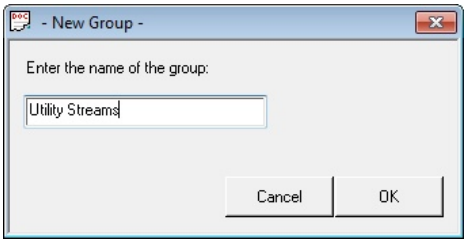

Figure 8-06: Naming a new stream group

3. In the next dialog box, select the streams or UnitOps for this group, either by typing in their flowsheet ID numbers (one per line) or by clicking on objects in the flowsheet. Click **OK** to close the dialog box.

UnitOp and Stream Group Commands

As soon as you finish creating the group, its name appears under **UnitOps** or **Streams** in the Groups area of the Explorer pane. From here, you can right-click the group name and select any of the following:

- **View/Edit:** Open a dialog box where you can add or delete stream or UnitOp numbers to include in the group.
- **Select Group/Select Streams:** Highlight the group's UnitOps or streams on the flowsheet.
- **Rename:** Open a dialog box where you can type a new name for the group.

- **Copy:** Open a dialog box where you can type a new group name to make an exact copy of the group. After you click OK, you can then edit the new copy of the group to fit your needs.
- **Delete:** Remove this group from the simulation. If you're sure about deleting the group, click Yes in the dialog box that appears.

The following specialized items appear on the right-click menu only for UnitOp groups:

- **Run:** Run the simulation only for those UnitOps included in this group.
- **View:** Display a summary report of the UnitOps included in this group.
- **Specifications:** Bring up the UnitOp specification dialog boxes for each item in the UnitOp group, starting with the first UnitOp listed.

The following specialized items appear on the right-click menu only for stream groups:

- **Composition:** Run a stream composition report for the streams in the group, using the Stream Composition property set.
- **Properties:** Run a stream properties report for the streams in the group, using the currently active Report property set.

Note: The commands to view, edit, select, rename, copy, and delete stream and UnitOp groups are also offered in the command ribbon, on the **Specification** tab. Click the **Stream Groups** drop-down in the **Streams** group, or click the **UnitOp Groups** drop-down in the **UnitOps** group, to see a list of existing groups. Hover over a group name to see the available commands. The same areas of the command ribbon also offer the **Add Stream Group** and **Add UnitOp Group** options.

Choosing Groups in the Select Streams and Select UnitOp Dialogs

Once you have set up stream or UnitOp groups, you can save time in the Select Streams and Select UnitOp dialogs when you request a chart or report. When one of these dialogs displays, the relevant group names are listed in the lower portion of the dialog, under the Groups heading.

Selecting a custom group is as easy as choosing a built-in category such as **Feed Streams** or **All UnitOps**—with a single click, you select the group, close the dialog, and generate the report or chart.

Report Viewer Setup

By default, individual text reports are sent to CHEMCAD's internal report viewer, which displays report data in a separate tab within the program. If you prefer, you can instead display report data in one of the following formats:

- Microsoft Excel

- Microsoft Word
- Microsoft WordPad
- CSV format

To change your report viewer option, go to the **Results** group on the **Home** tab and choose an item from the **Report Viewer** drop-down list.

Note: You can also determine the location of the date/time stamp that appears on your reports, and if needed, specify a path to your copy of WordPad. Start by clicking the **File** tab and then selecting **Preferences**. In the Preferences dialog, click **Report Viewer**. In the Report Viewer preferences, you can specify a path to WordPad if necessary, and choose either **Footer** or **Header** as the date/time stamp location for your reports.

Printing CHEMCAD Reports and Charts

You can print any CHEMCAD report or chart from within the program that displays the data.

For charts and reports displayed in workspace tabs, you can print directly from CHEMCAD. With the chart or report tab selected, click the **File** tab and then choose **Print**. The preview of your chart or report shows how it will look on the printed page; if you prefer to change the paper direction, you can select either **Portrait Orientation** or **Landscape Orientation** in the **Settings** area. Click **Print** when the data is displayed the way you want it.

For reports displayed in programs outside of CHEMCAD, the specific printing options differ somewhat from one program to another. Bring up the main Print dialog box in Word, WordPad, or Excel by selecting **File**, then **Print**. Each of these programs also offers a **Print** button on the command ribbon.

Consolidated Reports and the CHEMCAD Report Writer

You can run any combination of the text-based reports described above as a single operation by using CHEMCAD's Consolidated Reports feature.

Start by opening the Reports gallery. Then click **Report Writer** at the bottom of the gallery and select **Consolidated** from the fly-out menu to the right of the gallery. This brings up the Report Writer dialog box.

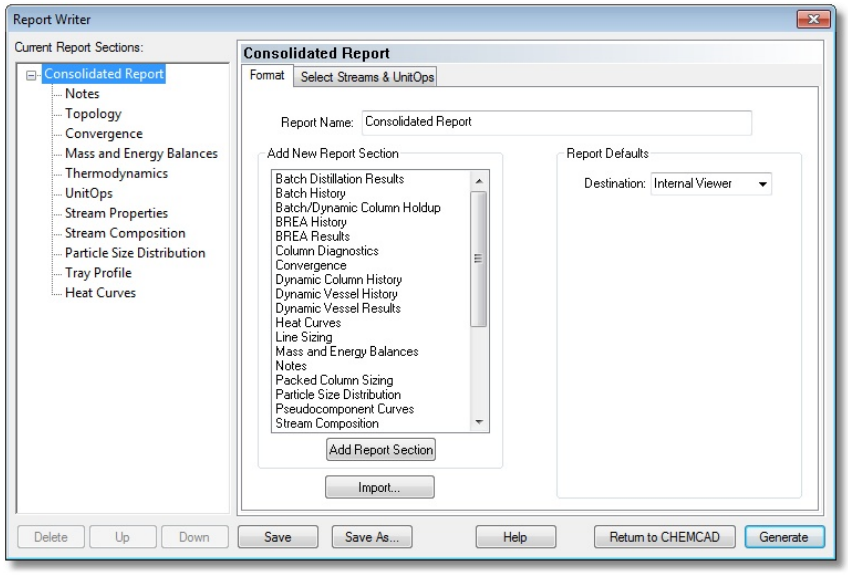

Figure 8-07: The CHEMCAD Report Writer

From here, you can click **Generate** to create a default consolidated report that includes topology, convergence, mass and energy balances, and the other reports listed in the dialog box's left column. If this report is adequate to your needs, simply click **Return to CHEMCAD** after generating the consolidated report, to close the Report Writer dialog box.

If you want something other than the default consolidated report, you can also use the Report Writer to customize which individual reports to include, what order to put them in, which flowsheet elements to include, and much more. You can fine-tune your report settings without closing this dialog box, and then save your report configuration with a new name so that you can run it again in the future.

Choosing and Ordering Report Sections

To customize your consolidated report, first decide which report sections you want to include. The **Current Report Sections** area (on the left side of the dialog) lists items in the order they will appear when you run the consolidated report.

If your preferred list of report sections looks largely like the default list, you can begin with that list and make some changes; if not, you can start with a blank slate and build your consolidated report one section at a time.

You can do any of the following to alter the existing section list:

- Add a section by double-clicking any item in the **Add New Report Section** area of the **Format** tab. The new item appears at the end of the report list.
- Remove a section by selecting it in the **Current Report Sections** list and then clicking **Delete**.

- Move a section to a different position within the Consolidated Report by selecting it in the **Current Report Sections** list and then clicking the **Up** or **Down** button as needed.

If you prefer to build the section list yourself, you should access the Report Writer by selecting **Report Writer** and then **New** from the bottom of the **Reports** gallery. This brings up the Report Writer screen with a blank left column, ready for you to add just the report sections that you want in whatever order you choose.

Selecting Flowsheet Elements

To select flowsheet elements for inclusion in a consolidated report, click the **Select Streams & UnitOps** tab within the Report Writer. This tab, like the **Format** tab, is visible only when **Consolidated Report** (or the report name) is selected in the left column of the Report Writer screen.

Initially, the **Select Streams** and **Select UnitOps** check boxes on this tab are cleared, and the **All Streams** and **All UnitOps** check boxes are checked and disabled.

To exclude streams or UnitOps from your report, first check the appropriate box at the top of the tab; this enables the other options. You can click **Select From Flowsheet** to select streams or UnitOps using your mouse, or clear the **All Streams** or **All UnitOps** box to access options for selecting flowsheet items by types or user-created groups.

Formatting Report Sections

Certain report sections that you can include in a consolidated report have formatting options that you can change before running the report. These options include:

- For **UnitOps**, a section-specific UnitOps selection tab and the option to limit the number of columns for Excel report output
- For **Stream Properties**, a section-specific stream selection tab and the option to change the default list of stream properties to include in the report
- For **Stream Composition**, a section-specific stream selection tab, the option to change the default flow options, and alternative settings for composition data format and precision
- For **Particle Size Distribution**, a section-specific stream selection tab
- For **Tray Profile**, a section-specific UnitOp selection tab and an option to change the default flow units
- For **Heat Curves**, a section-specific UnitOp selection tab and the option to choose a cutting method and number of cut points

Naming the Report and Choosing a Destination

When you finish customizing a consolidated report—particularly if you've done a significant amount of customization, or if you expect to run the same report parameters again—you should consider saving the report for future use.

To do this, first give the report a distinctive name using the **Report Name** field. This field is visible in the right portion of the Report Writer dialog box when you click the top-level item under Current Report Sections.

Note that **Consolidated Report** is the default report name; when you type a new name as shown below, both the top-level item on the left and the title over the right portion of the dialog box change to reflect the report name.

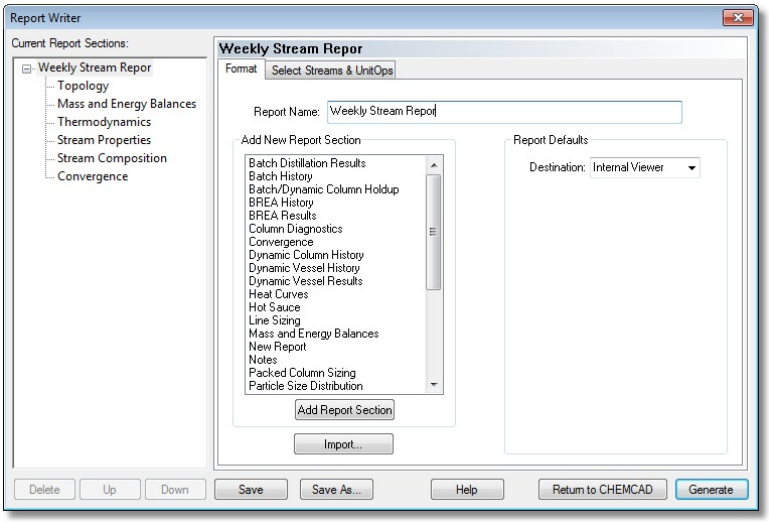

*Figure 8-08: Typing a new name into the **Report Name** field*

Once you have named the report, you can click **Save** to save the report locally (that is, only for this simulation), or click **Save As** to save the report under **My Simulations\My Reports\Global Reports**. Saving in the Global Reports directory makes the report available to any simulation you may open in the future.

To generate a report that you have saved locally, return to the Report Writer fly-out menu at the bottom of the Reports gallery. Select **Simulation** > **[Report Name]** > **Generate Report**. Other options here are **Edit** to open the report in the Report Writer, **Export** to copy it to a global location, or **Delete** to remove it from the menu.

Figure 8-09: Generating a consolidated report that has been saved locally

Similarly, to generate a report that you've saved globally, return to the Report Writer fly-out menu and select **Global** > **[Report Name]** > **Generate Report**. As with local reports, you can use this menu to edit, export, or delete a global consolidated report.

Selecting a Report Viewer for Consolidated Reports

For Report Writer consolidated reports, you can choose from the same list of programs used for other CHEMCAD reports. To select a program to display and print this type of report, click the **Reports** drop-down (**Home** ribbon, **Results** group), and at the bottom of the gallery select **Report Writer** and then **Format**. Make your selection in the **Destination** field and then continue customizing your report; when you finish and click **Generate**, the report will display in the program you selected.

Property Sets

CHEMCAD calculates and stores a large number of data points about the process streams in your simulations. Some of these items will be of great interest to you, while others may be useful only in rare situations. A customization feature called ***property sets*** enables you to choose exactly what information to display about your process streams in the various types of reports.

A property set is a collection of physical data to display about a stream (or a group of streams). It could include very few items—for example, only temperature and pressure—or it could show in-depth details about the stream and all of its components. For every type of text report in CHEMCAD, you can choose a property set that best fits your needs.

Built-in Property Sets

When you first install CHEMCAD, three property sets are available for your use: Quickview, Stream Composition, and Stream Property.

The Quickview and Stream Composition property sets are essentially the same; they produce data views that are informative, but brief. This view is ideally suited for CHEMCAD's Quickview feature, which displays a pop-up window when the mouse pointer hovers over any process stream, and for stream reports displaying important properties of multiple streams. The Stream Property set is more comprehensive, incorporating details about liquid and vapor phases of the stream.

User-created Property Sets

You can create your own property sets, either from the ground up or by copying and editing an existing set. Doing this enables you to leave the built-in property sets as they are, and apply your custom sets as appropriate for certain simulations or situations.

Different Sets for Different Purposes

By default, the built-in property sets are linked to the types of reports for which they were designed. They are intended to serve specific purposes:

- The **Quickview** property set is designed for use with the Quickview pop-up tooltips that appear when you hover the mouse over a stream.

- The **Stream Composition** property set is meant for generating stream reports. By default, this property set displays basic stream properties and stream compositions.
- The **Stream Property** property set is meant for generating stream reports. By default, this property set displays full liquid and vapor phase properties, but it does not display stream compositions.

You can set a default property set for use with most stream reports, using the **Property Set** drop-down list (**Home** tab, **Results** group). This list initially offers the three built-in property sets, but it will also include any custom property sets that you create.

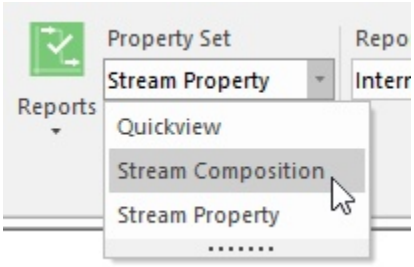

Figure 8-10: Changing the selection in the Property Set drop-down

The Property Set Preferences Dialog

The dialog box where you can view, edit, and save information for property sets is called Property Set Preferences. Various versions of this dialog can be accessed from multiple locations in the program, but the central functions of selecting properties and managing sets are the same in all versions.

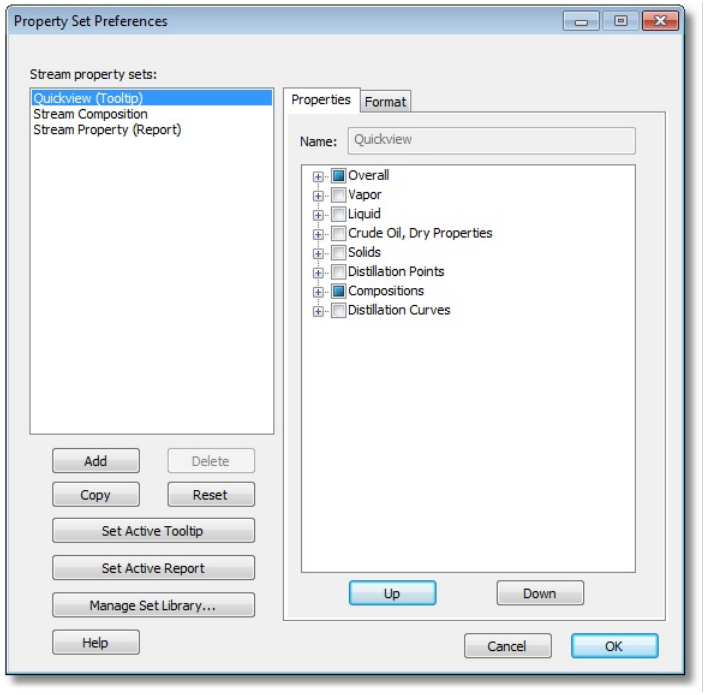

Figure 8-11: The Property Set Preferences dialog box

Active Set Designations

The left column of this dialog lists the available stream property sets, including any that you may have created. At any given time, one of these property sets will be designated as the active tooltip set, and one will be designated as the active report set. As shown in the figure above, the names of the active sets are marked with ***(Tooltip)*** and ***(Report)*** for easy identification.

Note: A single property set can be assigned to both of these designations, if desired.

The active tooltip set will determine the contents of the stream tooltips that appear any time you hover the mouse over a stream. The Quickview property set is assigned as the tooltip set by default.

The active report property set will be used to determine which stream properties are included in standard stream reports. The Stream Property set is the active report set by default.

To change the active tooltip or active report designation, select the property set name and then click either **Set Active Tooltip** or **Set Active Report** in the area below the list of sets. When you do this, the ***(Tooltip)*** or ***(Report)*** designation will switch to the property set that you had selected.

Editing a Property Set

In the Properties tab at right is a list of stream property categories; click the plus sign next to any category to expand its list of properties. A property set can include any combination of the items in these property lists, which will display in the order you specify.

If you want to change the properties included in a property set, or re-order the properties, first click the desired set name in the left-hand column. You can now add or remove check marks for properties as appropriate, to include or exclude those properties.

To change the order of items in the property list, use the **Up** and **Down** buttons at the bottom of the right-hand column. Simply select any first- or second-level item on the Properties tab and click either **Up** or **Down** to move that item to a new place in the list of properties. All selected properties will display in reports according to the order you choose here.

Clicking **OK** saves all changes that you have made to property sets since opening the Property Set Preferences dialog.

Creating a New Property Set

To start a new property set and add all selections yourself, click the **Add** button. This creates a completely empty property set, with the name ***New Set***. On the Properties

tab, in the Name field, type a meaningful name and then click into the properties list. The new set's name is now listed in the left-hand column.

To add properties to your new set, start by expanding the various first-level options such as *Overall*, *Vapor*, and *Liquid*. Simply click the plus sign next to an item to expand it and view the second-level options.

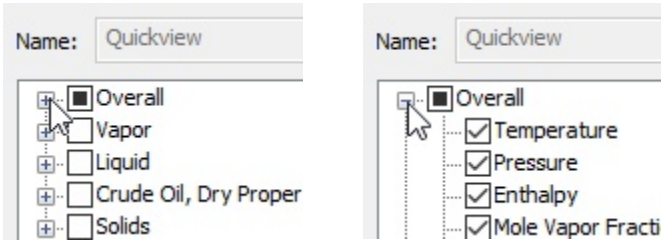

Figure 8-12: Expanding a first-level item to view a list of properties

Note that when you check the box by a first-level item, you select all the items in that category. Similarly, clearing a first-level box removes all its second-level items from the property set. A solid check box indicates that some, but not all, second-level items are currently checked.

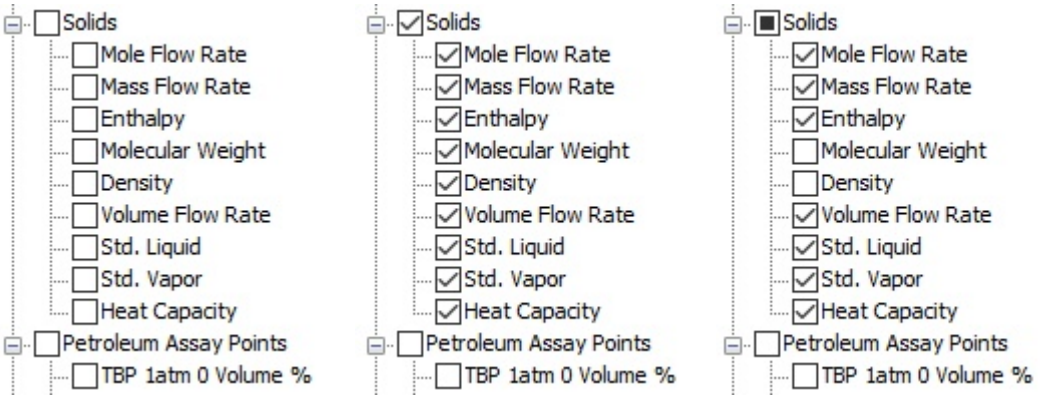

Figure 8-13: Property categories with no options selected (left), all options selected, and mixed selections

As you saw with editing a built-in property set, you can use the **Up** and **Down** buttons to move properties into the desired order. When you have finished, click **OK** to save your changes.

Copying an Existing Property Set

To add a custom property set that uses an existing set as a starting point, select the desired set in the left column and then click **Copy**. The new set will have the same name as the set you copied, with the designation ***(Copy)*** at the end.

In the Name field, give your copied set a unique descriptive name, and then make any needed changes to the property selections. Use **Up** and **Down** to put the selected properties into the desired order, then click **OK** to save your changes.

Format Tab Options

The Property Set Preferences dialog has a second tab called **Format**. The options on this tab affect the way stream data is displayed in reports, Quickview windows, and stream databoxes for the selected property set.

Check the **Display streams by phase** box to display separate columns of data for vapor, liquid, and solid phases. When *not* displaying data by phase, you can type a numeric entry in the **Max. number of streams per row** field (default value is 4), to limit the width of the report display. When a report includes more streams than are allowed on a single data row, the remaining stream data will be displayed in additional rows below the first.

The **Ignore max. streams per row setting** check boxes allow you to customize the display of stream data. By default, these boxes are checked so that Excel reports and stream databoxes will display data for all selected streams in a single row. You can clear the check marks to apply your maximum streams per row setting to these types of reports.

Resetting Built-in Property Sets

For the three built-in property sets, a reset option is available. If you should ever want to revert one of these sets to its original configuration, simply select the set and then click **Reset**. This option is not applicable for custom property sets.

Deleting a User-added Property Set

You can remove a user-added property set that you no longer need. First, make sure that no reporting function is currently using the set in question. Then open any version of the Property Set Preferences dialog, select the set name in the left column, and click **Delete**. The selected property set will disappear from the list. Be sure to click **OK** to save your property set updates.

Using the Property Set Library

A user-created property set remains with the simulation in which it was created, even when that simulation is shared with another user on a different installation of CHEMCAD. If you want a property set that you've created to be available for other simulations on your CHEMCAD installation, you can add it to your *property set library*. This repository enables you to share user-added property sets with any simulation.

The property set library is accessed from the Property Set Preferences dialog. Click the **Manage Set Library** button to bring up the Property Set Library dialog.

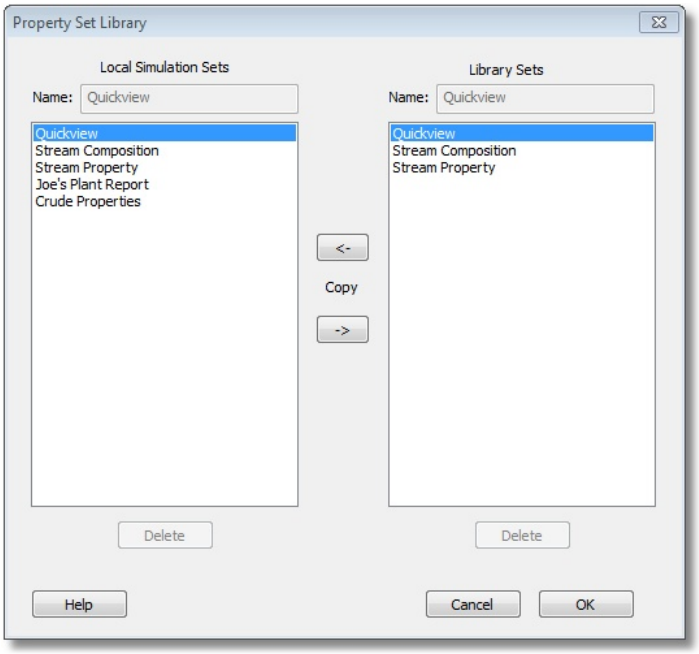

Figure 8-14: The Property Set Library dialog, showing built-in and custom property sets

The left side of this dialog lists local property sets—that is, all property sets that are available in the current simulation. This includes the three built-in property sets (Quickview, Stream Composition, and Stream Property), plus any sets you have created in the current simulation.

If you want to make a custom property set available in the future for simulations that you open on this installation of CHEMCAD, add the set to the Library Sets list on the right.

To do this, select the desired set in the Local Simulation Sets list on the left side of the screen, then click the right arrow between the two lists. The selected set will now appear under Library Sets, with the designation ***(Copy)*** at the end of the set name.

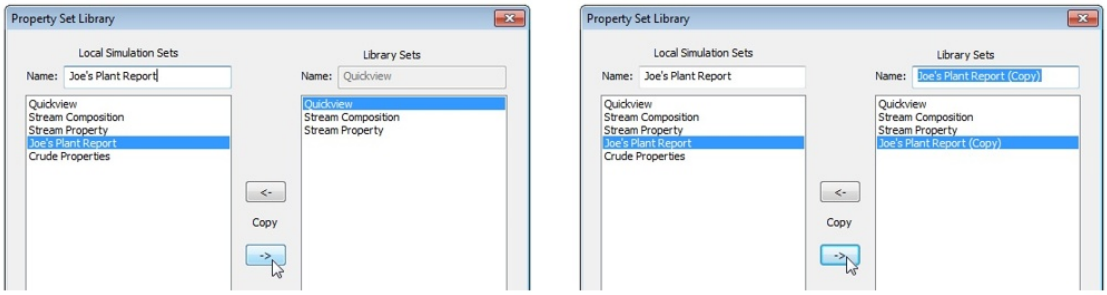

Figure 8-15: Before and after copying a property set to the Library Sets list

It's recommended that you give the library copy of the property set a unique name, to avoid confusion. When you have finished, click **OK** to return to Property Set Preferences, and **OK** again to return to the CHEMCAD workspace.

> **Note:** Changes to the Library Sets list will be saved after you click **OK**, even if you then close the simulation without saving it. You must save the simulation file, however, to keep any changes you have made to the Local Simulation Sets list.

The Library Sets list works as a global repository for a given CHEMCAD installation. Once a property set is designated as a library set, it is available to use in any new or existing simulation.

- When you create a new simulation, all library sets will automatically appear in the local list of stream property sets.
- For an existing simulation, open the Property Set Library dialog box, select the desired property set in the right column, and click the left arrow to copy it to the left column.

Sharing Property Sets with Other CHEMCAD Users

The Property Set Library feature enables you to share property sets with other users, or in other installations of CHEMCAD that you use.

After creating a property set, send a copy of a simulation that contains the set to another user (via e-mail or a network share, for example). When the simulation is opened on that user's CHEMCAD installation, the property set will be listed in the Local Simulation Sets list.

Simply copy the property set to the Library Sets list for that copy of CHEMCAD, making sure to save the change by clicking **OK** in both property set dialogs. From that point onward, the shared property set is available to existing simulations via the Property Set Library, and to all new simulations automatically.

Creating Process Flow Diagrams

CHEMCAD provides easy-to-use tools for creating printed process flow diagrams. You can add various types of databoxes to accompany your flowsheet, and then selectively view and print groups of items, including databoxes.

Adding Flowsheet Databoxes

CHEMCAD offers four types of databoxes that display on the flowsheet and appear on printed diagrams:

- **Stream Box:** Lists the streams that you select in a single table, along with the stream properties that you choose to include
- **UnitOp Box:** Generates a separate databox for each selected UnitOp
- **TP Box:** Generates separate summary databoxes for selected streams
- **Excel Range:** References a range of cells from an Excel worksheet

The commands to insert these items are located on the **Drawing** tab, in the **Insert** group. For each kind of databox, you will need to make specifications to determine which data is included and how it is displayed.

Stream Boxes

To create a stream databox, start by clicking the **Drawing** tab. In the **Insert** group, click **Stream Box**. In the Select Streams dialog, you can choose **All Streams**, **Feed Streams**, **Product Streams**, or **Cut Streams**, or you can list the specific stream IDs to include in the stream box and click **OK** to continue.

The Select a Property Set dialog box displays next. The property set you choose here (along with any changes you make to that property set) determines which properties are included in the resulting stream databox.

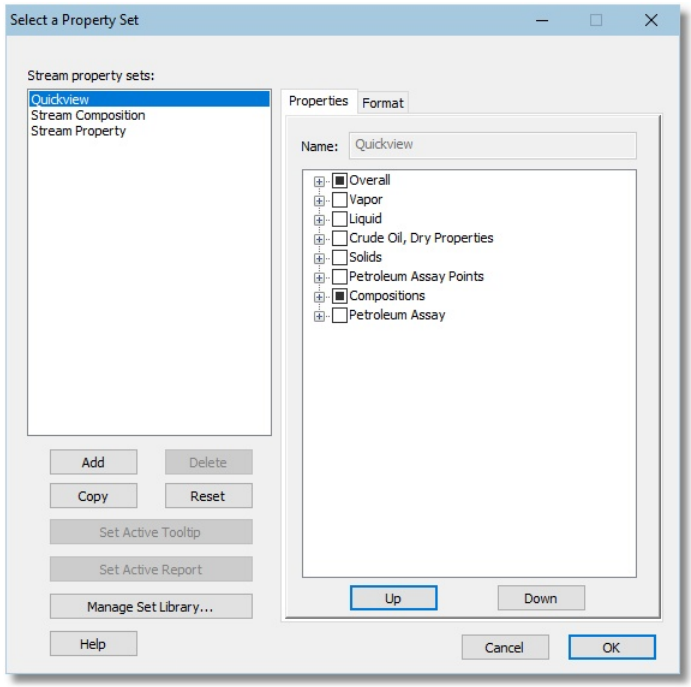

Figure 8-16: The Select a Property Set dialog box

In this standard property selection dialog, you can add, copy, or edit a property set, or simply select an existing set from the list at left. When you click **OK**, the stream databox with the selected streams and properties displays on the flowsheet.

Once you have created a stream databox, you can move, stretch, or resize it using your mouse. You can also edit the contents of the databox by right-clicking the box and selecting **Edit Databox**.

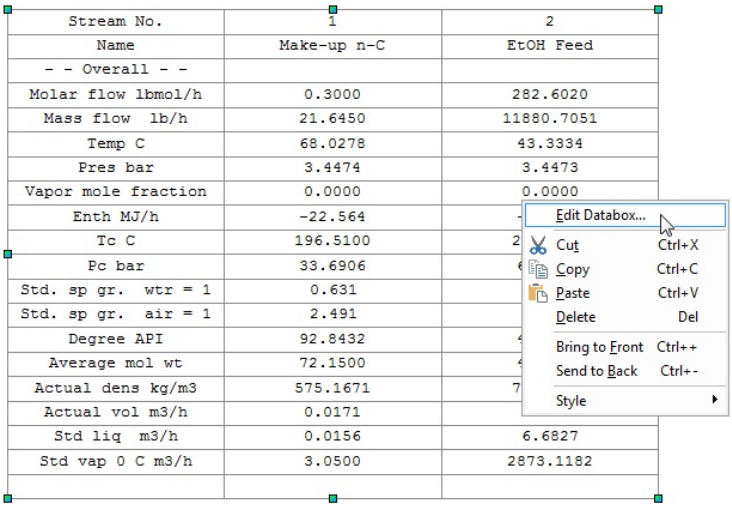

Figure 8-17: Using the Edit Databox command to change stream box contents

This brings up a property selection dialog much like the one you used to create the databox, with the title *Select New Set or Edit Current Databox Set*. Simply add or delete properties here as appropriate, then click **OK** to return to the flowsheet and see your stream databox updated.

UnitOp Boxes

To create a UnitOp databox, click the **Drawing** tab, then in the **Insert** group, click **UnitOp Box**. Then either type UnitOp IDs in the Select UnitOps dialog box or click the desired UnitOp symbols on the flowsheet. To include every UnitOp on the flowsheet, click **All UnitOps** in the lower portion of the dialog, or click anywhere in the workspace and then press **[CTRL-A]**.

When you complete your selections and click **OK**, the UnitOp databox appears on the flowsheet.

TP Boxes

CHEMCAD can create databoxes called *TP boxes* that display any combination of temperature, pressure, and flow rate for all streams or selected streams on a flowsheet.

To add TP databoxes, click the **Drawing** tab, then in the **Insert** group, click **TP Box**. In the TP Box Settings dialog box, first select an option at the top, to determine whether to add TP boxes for all streams or only for the streams you select.

In the **Display** column, select items from the drop-down list in each field to determine which stream properties to display and in what order. Use **No selection** as appropriate if you want to display fewer than four properties.

In the **Number format** column, make a selection in each field to determine how numbers will display in the TP boxes. In the **Digits** column, type the number of

digits to display after the decimal point. You can also choose whether to display stream IDs (enabled by default) and engineering units.

The **Preview** box displays a dynamic sample of how the items you've selected will appear in the TP boxes. Note that the preview area does not reflect any changes you may have made to your default font size or style.

When you finish making your selections in the TP Box Settings dialog box, click **OK**. If you've chosen to make TP boxes for all streams, the TP boxes will appear on the flowsheet right away. If you've opted to select the streams from the flowsheet, you'll see a Select Streams dialog box; type the stream numbers (one per line) or click on the stream lines in the flowsheet to select streams, then click **OK** to create the TP boxes.

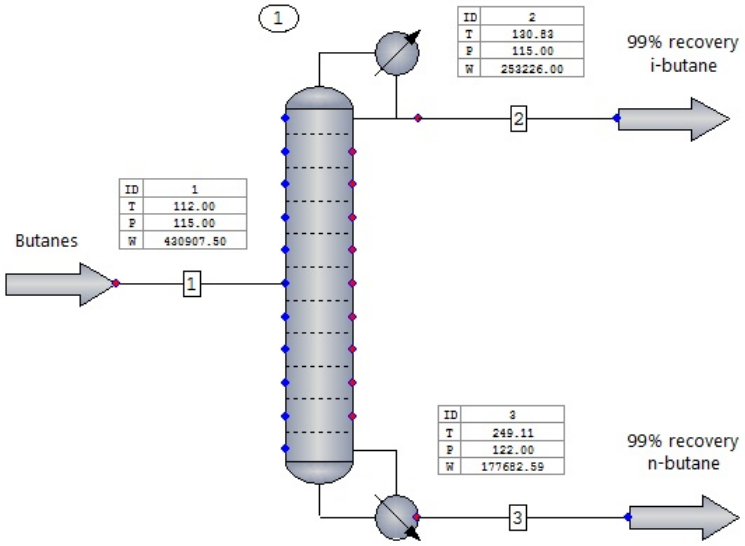

Figure 8-18: TP boxes added to a simple flowsheet

Excel Range Boxes

An Excel range box displays dynamic data from a specified cell range in a specified Excel worksheet. To create an Excel range box, follow these steps:

1. Click the **Drawing** tab, then in the **Insert** group, click **Excel Range**. This brings up the Excel Databox Settings dialog box.
2. Click **Browse** to navigate to the folder where the Excel workbook resides, then highlight the name of the workbook you want and click **Open**.
3. In the *Worksheet name* field, type the name of the relevant worksheet within the workbook that you've indicated.
4. In the *Cell range to display in CHEMCAD* area of the dialog box, specify the starting and ending column and row coordinates that you want to reference within the selected worksheet.

An Excel range box is a dynamic link between CHEMCAD and the Excel worksheet. As data is updated and saved in the selected cell range, the range box can automatically update to reflect those changes. To view the most up-to-date data in your Excel range boxes at any time, click the **View** tab and then select **Data Boxes** in the **Refresh** group.

Using Title Blocks

If your printed process flow diagram requires a title block, you can add one to your simulation, customize its text, and add a logo or other image.

Adding a Title Block

To place a title block on your flowsheet, open the simulation file and click the **Drawing** tab. In the **Insert** group, click **Title Block**. This brings up the Select Title Block dialog box, where you can choose any file with the extension **.tbd**. Your CHEMCAD installation includes several .tbd files, which you can copy and change to create your own reusable custom title blocks.

Double-click the .tbd file you want to use, or select it and then click **OK**. The selected title block now appears on the flowsheet.

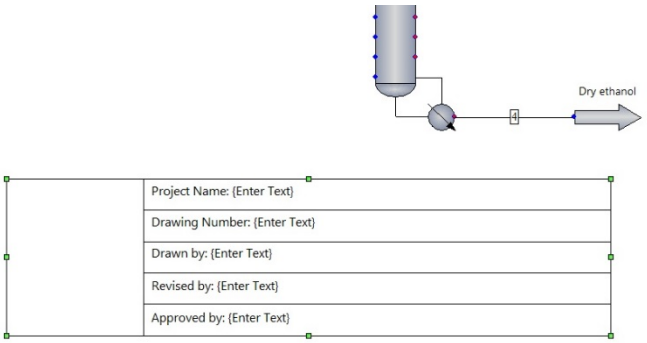

Figure 8-19: Newly added title block

Click and drag the title block to move it to the desired location on the workspace.

Changing Title Block Text

CHEMCAD's built-in title blocks contain text "placeholders," where the phrase **{Enter Text}** stands in for the title block information. The labels provided (such as **Project Name** and **Revised by**) are suggestions, which can also be changed to fit your specific needs.

To enter your own information, first double-click an existing section of text to highlight it. Then simply start typing to replace the entire section of text, or click and drag to select only the portion of the text that you want to replace.

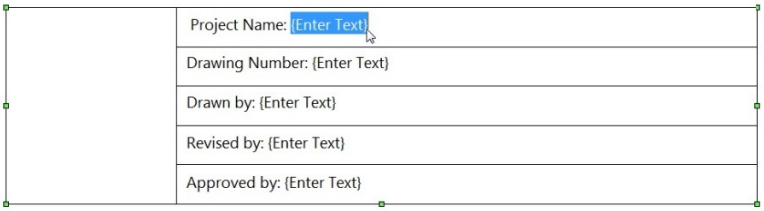

Figure 8-20: Selecting a portion of the text to edit

Adding an Image to a Title Block

To insert a logo or other image in your title block, click the **Drawing** tab, then click **Image** in the **Insert** group. This brings up an Open dialog, where you can navigate to the directory where your image file is stored. When you locate the file, double-click it, or select it and then click **Open**.

This returns you to the workspace, with the newly imported image highlighted. You can now drag the image onto an open area on the title block, and use the green sizing handles on any corner to resize the image as needed.

Note: Be careful to use *only* the corner handles when resizing an image. Using the handles along the sides of the box will distort the image, whereas using the corners will preserve the image's original shape as you scale it to a larger or smaller size.

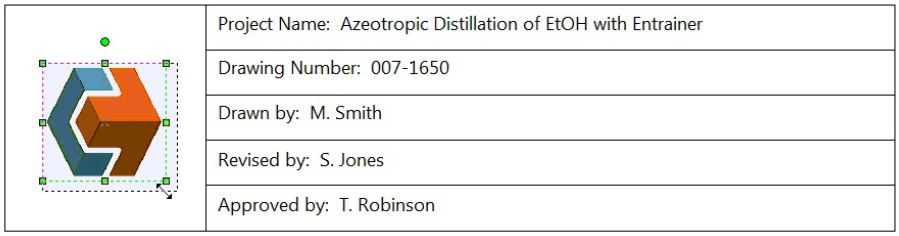

Figure 8-21: Resizing an imported image

You can group the image and the title block together so that they will behave as a single unit. To do this, first click the image, then hold down **[SHIFT]** as you click anywhere on the title block. Then with both items selected, click the **Arrange** drop-down on the Drawing toolbar and select **Group**.

Now when you drag the title block to a different location, the image will move along with it. If you ever want to remove or replace the image, you can select the title block and then use the same method with the **Ungroup** command. Once the items are ungrouped, you can select the image independently from the title block and delete it.

Creating a Custom Title Block

After you have customized the content of a title block with your own field labels and image, you may want to save time by making this title block available for other flowsheets. To do this, use the Title Block Designer tool.

If you already have a custom title block, start by selecting it on the flowsheet. Right-click and select **Copy** from the pop-up menu. Then go to the **Tools** tab and click **Title Block Designer** in the **Flowsheet** group.

In the Select Title Block dialog, choose the .tbd file that you used to start your customized title block, or any of the other .tbd options, and click **Open**. This brings up a new tab on the CHEMCAD workspace, called **Title Block 1**. The title block you chose is displayed in its own workspace tab. At the top of the screen, a special **Title Block Designer** tab now displays, offering drawing objects and other items specific to customizing a title block.

If you were starting a new customized title block, you could begin changing the text and adding an image, as discussed before. But if you have copied in a title block with your custom content, you can simply right-click in the workspace and select **Paste**. This places your customized title block on the tab; you can now select and delete the title block with the placeholder text.

You will probably want to delete some of the specific text that you copied in with the title block, such as a date, title, or drawing number. You could choose to add your own placeholder text, for example to suggest a standard date format, or you may simply leave a character such as **X** to provide a place for users to begin typing.

To make your title block available for future use, you must save it as a .tbd file. In the **Title Block Designer** tab's **Workspace** group, click **Save As**, and then provide a unique name. When you click **Save**, the workspace tab will display your new title block name.

Close the tab to return to the main CHEMCAD workspace and the open simulation. To test your new custom title block, click the **Drawing** tab, then in the Insert group, click **Title Block**. Choose your new .tbd file and click **Open**. The custom title block will appear on the workspace.

Using the Layers Feature for Selective Viewing and Printing

A *layer* is a group of objects in a simulation file—any combination of databoxes, drawn shapes, text labels, streams, and UnitOps—that you can view or hide with a single click. You can create one or more layers, define which objects belong to each layer, and then toggle any layer either on (visible) or off (hidden). The commands for layers are available both on the command ribbon and in the Explorer pane's **Simulation** tab.

Note: Turning off a layer only hides its assigned flowsheet objects from view. Having a layer hidden does not in any way affect the way the simulation runs, nor does it change any stream or UnitOp properties.

Finding the Layer Commands

On the ribbon, the **Layers** command is located on the **View** tab, in the **Flowsheet** group. When you click this command, a drop-down menu displays the layer commands that are currently available. Before you have created any layers, the only available command is **New Layer**.

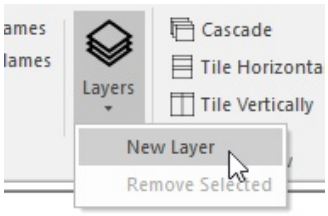

*Figure 8-22: Clicking the **Layers** drop-down on the **View** tab*

The Explorer pane also includes a top-level item called *Layers*, which lists any layers that you have created in the current simulation. On this list, you can see at a glance which layers are currently visible ( ) and which are hidden ( ).

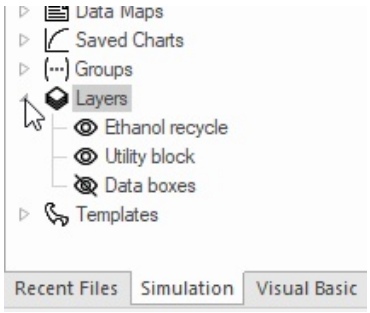

*Figure 8-23: The **Layers** entry on the Explorer pane, listing visible and hidden layers*

Creating a New Layer

Before you can assign objects to a layer, you must first create a new layer to use. You can do this in either of two ways:

- On the **View** tab, click **Layers** and then select **New Layer**.
- On the Explorer pane, right-click the **Layers** item and select **New**.

In the New Layer dialog, type a descriptive name for the new layer and then click **OK**.

The new layer name now displays both on the Explorer pane and in the **Layers** drop-down menu. New layers are visible by default.

Note: To change the name of a layer you have created, either select it in the **Layers** drop-down menu or right-click it in the Explorer pane list, then choose **Rename**. In the New Layer dialog, type the new name and click **OK**.

Assigning Objects to a Layer

As soon as you have a layer, you can assign objects to it. Start by clicking an object to highlight it; you'll see the small green boxes that define its outer edges.

With the object selected, you can assign it to a layer using either of two methods:

- On the **View** tab, click **Layers**, then select the desired layer from the drop-down list and click **Add Selected**.
- In the Explorer pane, right-click the name of the desired layer and choose **Add Selected**.

To save time, you can add multiple objects to a layer at once. Just hold down the **[SHIFT]** key as you click each object in turn, then use the **Add Selected** command as you did for a single object.

Hiding and Viewing Layers

As soon as you have added at least one object to a layer, you can test the layer by hiding it and watching what happens. You can use either of these methods to hide or view a layer:

- On the **View** tab, click **Layers**, then select the desired layer from the drop-down list and click **Show/Hide**.
- In the Explorer pane, simply click the layer name.

Each time you open a simulation file, CHEMCAD displays or hides its layers according to the way they were set the last time you saved the simulation. The status of all layers can be seen in the Explorer pane (the eye icon indicates a visible layer, while the eye with a slash indicates a hidden one), or in the drop-down menu when you click the **Layers** command (a check mark on the list indicates a visible layer).

Removing an Object from a Layer

If you no longer want a specific object or group of objects to be assigned to a given layer, first ensure that the layer in question is visible. Then select the relevant objects and do either of the following:

- On the **View** tab, click **Layers**, then select the desired layer from the drop-down list and click **Remove Selected**.
- In the Explorer pane, right-click the name of the desired layer and choose **Remove Selected**.

Now when you hide the layer, the object or objects you removed should remain in view.

If you want to ensure that an object is not assigned to any layer, click to select the object and then do either of the following:

- On the **View** tab, click **Layers**, then select **Remove Selected**.

- In the Explorer pane, right-click the top-level **Layers** item and choose **Remove Selected from All**.

Deleting a Layer

To remove a layer from the simulation, do either of the following:

- On the **View** tab, click **Layers**, then select the desired layer from the drop-down list and click **Delete**.
- In the Explorer pane, right-click the name of the desired layer and choose **Delete**.

When you delete a layer, it disappears from the Explorer pane and the drop-down layer list. If the deleted layer had been hidden, the objects assigned to it now reappear.

Printing a Process Flow Diagram

When you use the **Print** command on the main CHEMCAD screen, the result is a verbatim reproduction of your visible workspace.

If you're zoomed close in to one portion of your flowsheet when you print, you'll get a close-up printout that does not include the rest of the flowsheet. If you've hidden all your stream and UnitOp IDs to keep them out of your way while you fix a problem, those items will not appear on the printout.

For this reason, the first thing you should do when you're ready to print a process flow diagram is to decide what needs to be included on the printout. If you need the entire flowsheet to appear on the printed diagram, click the **View** tab, then in the **Zoom** group, click **Zoom to Fit**. (You can zoom manually if you prefer.) You may want to hide or unpin one or more panes as well, to give yourself more workspace while you prepare to print.

Next, consider whether your process flow diagram should display UnitOp or stream databoxes, text notes, or other items in addition to the flowsheet itself. If you have already created the needed items, make sure that they are placed where you want them. If you have items that you do not want to include in the print-out, you can add them to a layer and hide that layer from view while you print.

When all the items you want to print are in place, check once more to ensure that everything falls within the currently displayed CHEMCAD workspace. Then click the **File** tab and select **Print**. This brings up the Print dialog box, which displays a preview of how the flowsheet will look on paper. You can select printing options here, or simply click **OK** to print the process flow diagram.

Chapter 9

Customizing CHEMCAD

As you become more familiar with the way that CHEMCAD works and the various options and tools that are available, you may want to make your own additions—either for specialized items or for those you use frequently. You can customize CHEMCAD in several ways that save you time by streamlining and simplifying your workflow. These include:

- Creating and using stream and UnitOp templates
- Adding custom components to CHEMCAD's component database
- Defining custom thermophysical rules
- Customizing UnitOp palettes and color schemes
- Making your own UnitOp symbols to add to existing or custom palettes
- Building custom UnitOps
- Creating custom dialog boxes for UnitOp settings
- Customizing costing calculations

This chapter discusses all these types of customization, starting with the simplest procedures and then moving on to more complex customizations that require some programming experience.

Flowsheet Templates

One of the most effective ways to save time when creating CHEMCAD simulations is to make use of stream and UnitOp templates. A *template* is simply a set of characteristics, which you assign a name and save for later use. When you set up stream or UnitOp specifications that you know you'll need to recreate in the future,

you can create a template of that stream or UnitOp. You can then duplicate that item within the same simulation—or in any other simulation—with just a few mouse clicks.

Creating a Template

To create a stream template, first create the stream you want to clone and give it all the characteristics you want to include in the template.

Then find this stream on the Explorer pane's **Simulation** tab. Expand the **Flowsheet** item, then expand the **Streams** item, and finally double-click the applicable stream ID. This brings up an item called **Save**. Click the word **Save** to display the Enter Template Name dialog box, then type a name for your new stream template and click **OK**. The new template name is now listed beneath the **Save** item.

To create a UnitOp template, select the appropriate UnitOp ID in the Explorer pane, and then follow the same procedure used to create a stream template.

Viewing a Template's Properties

To see what specifications an existing template includes, look it up in the Explorer pane.

First expand the **Templates** item at the bottom of the Explorer pane list. For a UnitOp template, expand the **UnitOps** item, then expand the name of the relevant UnitOp type. For example, if you're looking up a template that you created for a type of pump that you frequently use, expand the **Pump** item in the Explorer pane.

Use the same procedure to look up a stream template, except that these templates are listed all together, not grouped according to type.

When you find the template you want, simply click the template name to view its stream or UnitOp specifications.

Applying a Template

To apply a stream template, first expand the main Flowsheet item for the stream to be affected, either by clicking the triangle icon to its left or by double-clicking the stream name.

When the stream item is expanded, you'll see the **Save** item below it, followed by the names of all the stream templates that you have created. Click the name of the template you want to apply, then choose **OK** to confirm that you want to apply this stream template.

Use the same procedure to apply a UnitOp template. Select the UnitOp to be affected and then expand it in the Explorer pane to apply the desired template. Bear in mind that for a given UnitOp, only templates for the relevant UnitOp type will be listed.

Renaming or Deleting a Template

To rename a template, simply find it under **Templates** in the Explorer pane, right-click the template name, and select **Rename**. Type the new name and click **OK**. This changes the template name throughout the Explorer hierarchy.

The procedure for deleting a template is similar to renaming a template. Again, find the template you want under **Templates**, right-click its name, and select **Delete**. Click **OK** to confirm that you want to delete this template. When you do this, the template name disappears from the Explorer, but streams or UnitOps that were specified using the template are not affected in any way.

Note: Any stream or UnitOp template that you create will be available for use with all other simulations on the same installation of CHEMCAD, until and unless you delete the template.

Creating Custom Components

The CHEMCAD component database places detailed information about thousands of chemicals at your fingertips. If for any reason you find that you need to use a chemical component that does not match any item currently in the CHEMCAD database, you can create your own component for use with your simulations.

You can create a single component, define a range of pseudocomponents, or import a component's physical properties from an external source. These procedures have similar aims, but differ significantly from one another.

Adding a Single Component

Creating a pure component in the CHEMCAD component database is a two-part task. You must first create the component and then regress data into the component.

Creating the Component

To create a new custom component, you can use any of five different estimation methods:

- **Create a hydrocarbon pseudocomponent.** This is treated like a pure component in that certain aspects of how it behaves or reacts are known.
- **Use the Joback/Lydersen method.** With this method you indicate basic characteristics, and select molecular groups (known as Joback groups, called Group Assignments in CHEMCAD) from a list, to indicate how many of each molecular group are present in the component.
- **Use the UNIFAC method.** This method is similar to Joback/Lydersen, except that the group list is more specialized toward organic components.
- **Create a combustion solid.** This method is used to simulate solid components for which an elemental analysis and heating value are known, e.g., coal.

- **Create an electrolyte component.** This method creates a component that you can subsequently use in an electrolyte simulation.

The procedure for creating a pure component is as follows:

1. Click the **Component Database** tab, then in the **User Components** group, click **New**. This brings up the New Component dialog box.

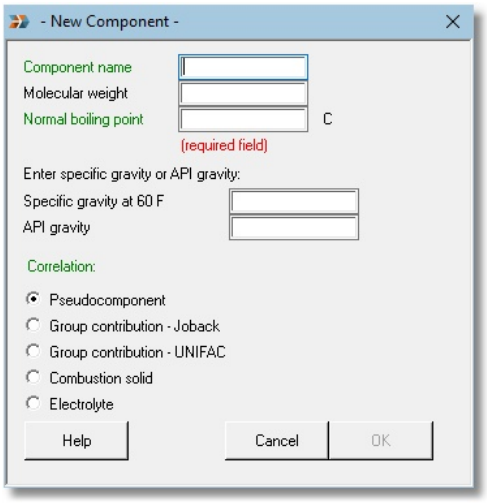

Figure 9-01: The New Component dialog box

2. Give the new component a descriptive name; it is strongly recommended that you make this name unique. All other characteristics here are optional, except for normal boiling point, which is required for the pseudocomponent method.
3. Select a **Correlation** option to indicate which of the above methods you will use, and click **OK** to continue.
4. The dialog box that appears next depends on the correlation that you selected:
   - *Pseudocomponent* brings up the Hydrocarbon Correlation dialog box.
   - *Group contribution – Joback* brings up the Group Assignments dialog box.
   - *Group contribution – UNIFAC* brings up the New Component UNIFAC Groups dialog box.
   - *Combustion solid* brings up the Combustion Solid dialog box.
   - Electrolyte brings up the Electrolyte Data dialog box.

   Select the appropriate options for your new component and specify as many characteristics as you like, as accurately as possible. Click **OK** to continue.
5. In the Select Destination Database dialog box, you will see no databases listed if this is your first time to add a component. If this is the case, click **New** to bring up the Manage Component Databases dialog box.

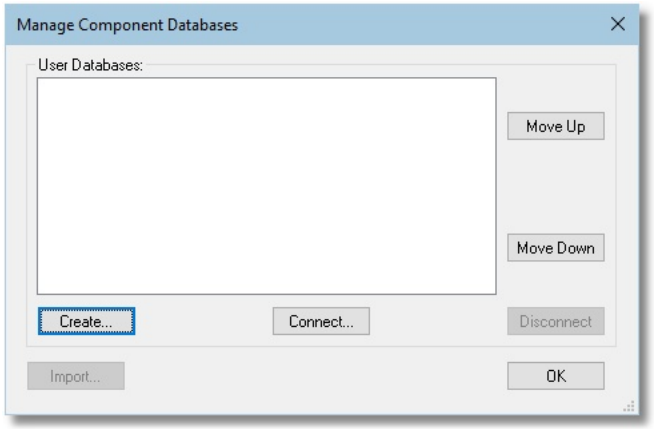

Figure 9-02: The Manage Component Databases dialog box

6. Normally, you'll need to click **Create**, which brings up the Save As dialog box. Navigate to the location you want for your custom component database, give the database a name, and click **Save**. If you want to add a database that someone else has created (generally in a network location), you can click **Connect**, which brings up an Open dialog box; navigate to that database's location, highlight the database, and click **Open**.
7. The Manage Component Databases dialog box now lists the database that you created or selected. Click **OK** to continue.
8. In the Select Destination Database dialog box, the new database you have just named is now listed; highlight it and click **OK**.
9. The View/Edit Component Data menu now appears. Click any item on the menu to access a dialog box with options for defining your new component. After defining as many characteristics as possible, click **Exit** to close the menu.

The new component is now available to add to your current simulation and all future simulations. To return at any time to make changes to a user-defined component, go to the **Component Database** tab and do one of the following:

- In the **System Database** group, click **View/Edit Component** to bring up the Select Single Component dialog box, which lists all available components. Highlight the component you want in the list and click **OK** to bring up the View/Edit Component Data menu.
- In the **Simulation Database** group, click **View Components** to bring up the list of components in the current simulation. Double-click the component you want in the list (or highlight the component and click **View/Edit**) to bring up the View/Edit Component Data menu.

Regressing Data into the Component

Data regression is the process of fitting experimental data points to a polynomial equation form, so that the individual error of each data point is minimized.

Data regression is only relevant to temperature-dependent properties such as heat capacity, density, and vapor pressure. CHEMCAD uses these polynomial equation fits to calculate the properties of a component at any given temperature.

To regress data into a component that you have created, follow these steps:

1. Click the **Component Database** tab, then in the **User Components** group, click **Property Regression**. This brings up the Select Regression Data Set dialog box.

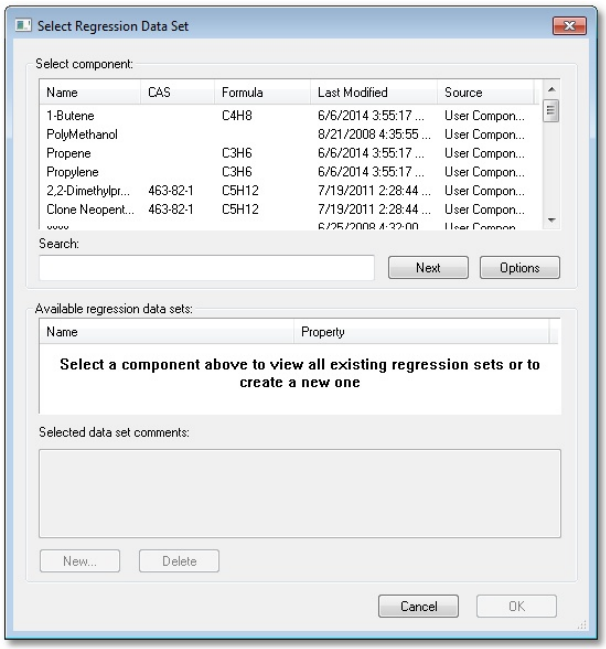

Figure 9-03: The Select Regression Data Set dialog box

2. Select the user-added component that you want to regress and click **New**. This brings up the Edit Regression Set dialog box.

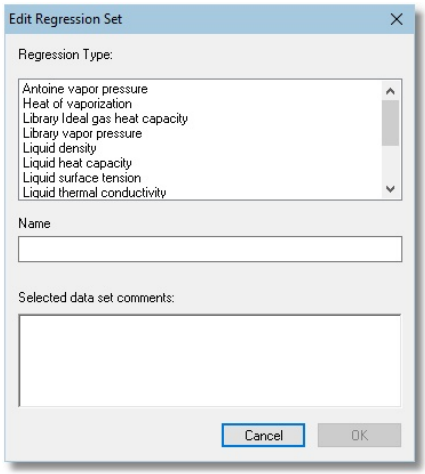

Figure 9-04: The Edit Regression Set dialog box

3. Select a regression type and provide a descriptive name for the data regression, then click **OK**. This brings up a dialog box that displays parameters for the selected regression type.
4. Verify the data on this dialog box, making additions or changes as necessary, and then click **OK**. This brings up a dialog box for data entry.
5. Enter your experiential data points in the cells provided. You can enter a value in the **Weight_factor** column to weight the regression toward one or more data points. When you have entered all of your data points, click **OK**.

Note: You can paste a contiguous range of cells from an Excel worksheet into the cells in this dialog box.

6. The regression data is displayed in a tab in the main CHEMCAD window. Another tab displays the regression results in graphical format. Review the data and chart, and decide whether the regression adequately represents your experimental data.
7. A dialog box appears, asking how you would like the changes to be applied to existing simulations. Choose an option and then click **OK**.
8. Repeat this procedure as needed to regress other properties for your component.

Defining a Petroleum Assay Range

Using a *petroleum assay*—another term for a distillation curve—you can cut a hydrocarbon stream into pseudocomponents, or fractions. A pseudocomponent represents a group of components that boil within a narrow temperature range. Pseudocomponent ranges are used in CHEMCAD to model hydrocarbons.

When you define a petroleum assay for a stream, CHEMCAD creates entries in the component database for each hydrocarbon cut, and assigns these components' compositions to the stream.

Note: Before you define a petroleum assay, make sure that you have specified in your component list, as appropriate, water and any light ends that exist in the assay.

1. Click the **Thermophysical** tab, then in the **Petroleum Assay** group, click **Initialize**.
2. In the Select Streams dialog box, enter the appropriate stream number(s) and click **OK**.
3. In the Hydrocarbon Correlation dialog box, select the appropriate correlations for your curve, or use the default selections and click **OK**.
4. This brings up the Curve Temperature Cut Ranges dialog box. For each cut range that you want to define, provide a beginning and ending temperature,

and enter the number of points that you want to define as discrete pseudocomponents within that range. Click **OK** to continue.

5. In the Bulk Properties dialog box, specify a petroleum assay type and enter a total flow rate and bulk gravity for the stream. You can make other entries here as needed, but only these three items are required. Note that if you have viscosity data that you want to use, you must check the **Viscosity** box here. Click **OK** to continue.
6. In the resulting dialog box, enter the data from your assay, specifying the volume percentage and boiling temperature for at least five data points. Click **OK** to continue.
7. The next dialog box is optional. Enter a gravity curve from your assay, listing the volume percentage and specific gravity for at least five data points. Click **OK** to continue.
8. The next dialog box is also optional. If you have light ends and water defined in your assay, enter volume percentage data here for all relevant components. Click **OK** to continue.
9. If you checked the **Viscosity** box on the Bulk Properties dialog, you will now see the Viscosity Data dialog box. Enter your viscosity data and click **OK**.
10. The pseudocomponent properties now display in a tab in the main CHEMCAD window. You can review and print these results, and leave the tab open as long as you like. To return to the main workspace and your flowsheet, simply click the far left tab, which displays the name of your simulation.
11. To see the list of pseudocomponents that you have created, edit the properties for the stream you selected. The pseudocomponents will be listed after pure components, with names that begin with **NBP**.

Importing a Neutral File

You can also add a component to the database by importing its physical properties from an external data source. This procedure is known as *neutral file import*.

For detailed information about importing and using a neutral file, see the CHEMCAD Help system.

Customizing Thermodynamics

Occasionally, you may find that none of the thermodynamic models built into CHEMCAD serve your needs for a particular simulation. If this should happen, you can take one of two approaches to handling thermodynamics for the simulation: either create your own K-value or enthalpy model or create your own mixing rule.

Creating a Custom K-value or Enthalpy Model

The K-value for any component is a ratio that reflects the amount of that component present in vapor and liquid phases under given conditions. CHEMCAD uses K-values to calculate vapor-liquid equilibrium in streams and in UnitOps.

An enthalpy model calculates the heat content of a system under given conditions. Enthalpy models are used to calculate the heat balance in CHEMCAD simulations.

If you have a K-value or enthalpy method that you'd like to use, you can write C++ code to introduce your model into the CHEMCAD system. A detailed description of how to create custom K-values and enthalpy models is included in the *User-added Modules Guide*, which is available on the Chemstations website.

When you've successfully added a custom K-value method, you can select it on the K-value Models tab of the Thermodynamic Settings dialog box, by using the Global K-value Option setting called **ADDK**.

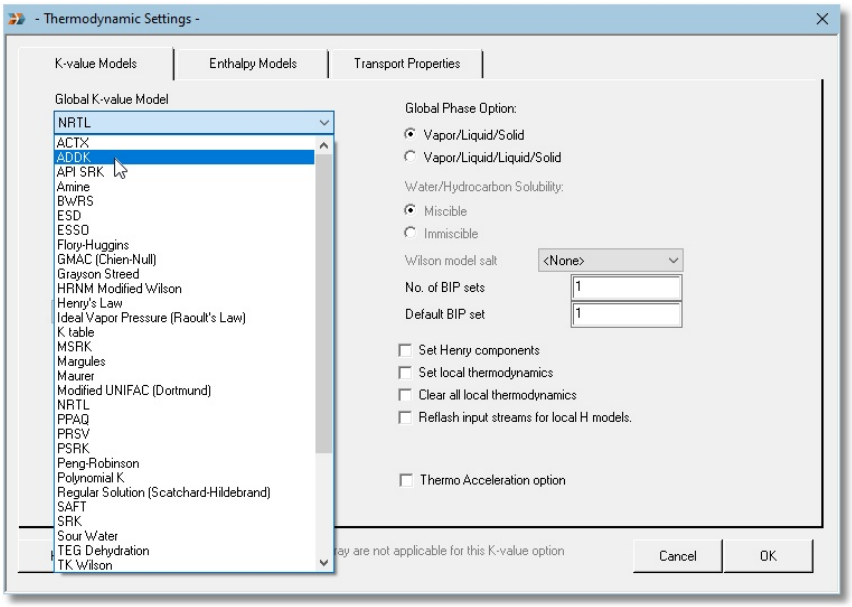

Figure 9-06: Selecting the ADDK K-value option

After adding a custom enthalpy model, you can select it on the Enthalpy Models tab of the Thermodynamic Settings dialog box, by using the Global Enthalpy Option setting called **ADDH**.

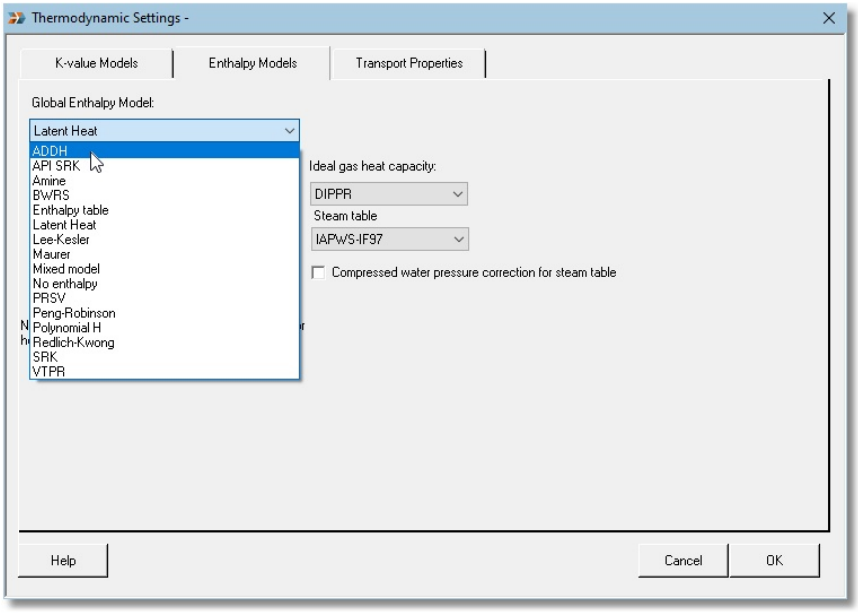

Figure 9-07: Selecting the ADDH enthalpy model

Creating a Custom Mixing Rule

A mixing rule determines how CHEMCAD calculates the properties of a mixer, based on the properties of its pure components. You can create custom mixing rules for any of the selections listed on the Transport Properties tab, either using VBA as described in the following section or using C++.

Visual Basic Applications (VBA)

You can customize CHEMCAD using Visual Basic Applications, or VBA. The Explorer pane's Visual Basic tab provides access to the following types of customizable items:

- Reactions
- Properties
- UnitOps

If you have written code in VBA that you would like to make available in CHEMCAD, you can insert that code into one of the templates that CHEMCAD provides, or use any of these templates as a starting point and launch a VBA editor from within CHEMCAD.

Defining a Reaction, Mixing Rule, or UnitOp

To define a custom reaction, mixing rule, or UnitOp using VBA, follow these steps:

1. Click the **Visual Basic** tab in the Explorer pane and expand the relevant item: **Reactions**, **Properties**, or **UnitOps**.
2. Double-click the relevant template item to open the VBA editor.

3. Copy the existing subroutine and paste the code below the example in the code window. Rename the new subroutine copy.
4. Edit the new subroutine as needed to achieve the result that you want.
5. Return to CHEMCAD by either of two methods:
   - Use **[ALT-TAB]** or the Windows taskbar, leaving the VBA editor window open.
   - Click the **View CHEMCAD** button at the far left end of the VBA editor's toolbar to close the editor window.

Note: You can also use the **[ALT–F11]** key combination to toggle between CHEMCAD and the VBA editor.

6. Save the current CHEMCAD simulation, then expand the relevant Explorer item again to see your newly defined item in the list.

Using a VBA-defined Reaction

Once you have defined a new reaction, you can use it for a kinetic or batch reactor:

1. Find the **Vessel Reactor** or **Kinetic Reactor** symbol on the palette, and drag a copy onto the flowsheet. Add and specify streams for this UnitOp as appropriate.
2. Double-click the icon to define reactor specifications. Make the following selection to use your VBA-defined reaction.
   - **Vessel reactor:** After specifying the reactor's initial charge, you'll see the Vessel Reactor General Information dialog box. On the **General** tab, select the kinetic rate expression option called **Define each reaction**.
   - **Kinetic reactor:** On the **General Specifications** tab of the Kinetic Reactor dialog box, select the kinetic rate expression option called **Define each reaction**.
3. For each reaction that you define, you'll enter data into a Kinetic Data dialog box. Choose the Kinetic Rate Expression option called **User - VBA**. This brings up a drop-down list to the right of the Kinetic Rate Expression field, where you can choose a user-defined reaction. Select the appropriate option for each reaction that you define for this UnitOp, and then click **OK** to continue to the next reaction.

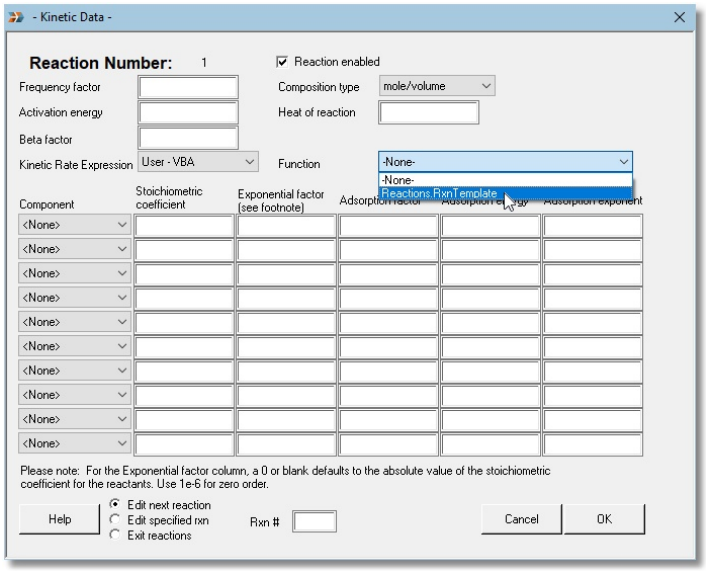

Figure 9-08: Selecting a VBA-defined reaction in the Kinetic Data dialog box

4. When you have defined the last reaction, click **OK** to return to the main CHEMCAD window.

Using a VBA-defined Mixing Rule

Once you have defined a new mixing rule, you can include it in your CHEMCAD simulations:

1. On the **Home** tab, in the **Setup** group, click **Thermodynamic Settings**.
2. In the Thermodynamic Settings dialog box, drop down the list of options for the mixing rule that you used as a template for your new rule. Select your rule from the list.
3. Click **OK** to return to the main CHEMCAD window.

Using a VBA-defined UnitOp

Once you have defined a new VBA UnitOp, you can include it in your CHEMCAD simulations:

1. Find the **VBA UnitOp** symbol on the palette, and drag a copy onto the flowsheet. Add streams into and out of the UnitOp as you normally would.
2. Double-click the icon to define the UnitOp's specifications.
3. In the Visual Basic UnitOp dialog box, drop down the **Function** list to see the available VBA UnitOps. Select the one you want to use and click **OK**.

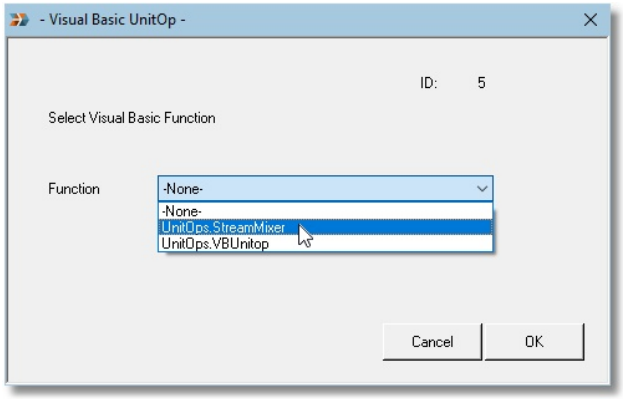

Figure 9-09: Selecting a VBA UnitOp

Customizing UnitOp Palettes

The introductory discussion of the CHEMCAD interface described how to use the UnitOp palette and make simple changes to its appearance. More advanced palette customization enables you to do the following:

- Create a custom palette with the UnitOp symbols of your choice
- Copy an existing palette and customize its contents
- Rename a palette
- Use a custom color scheme to change UnitOp symbol colors
- Reset palettes to their default configuration

Creating a Custom Palette

To create a new palette with custom-selected UnitOps, right-click the title bar of any existing palette and select **New**. This creates a palette heading called *New*, and an empty palette.

To give the palette a distinctive name, you can now right-click the palette heading and select **Rename**. Then type the name you want and click **OK**. Before proceeding, ensure that the **Lock Palette** feature is turned off. This will enable you to copy and paste items from existing palettes.

Now find a symbol that you want to copy into your new palette, and hold down **[CTRL]** while you right-click the symbol. Select **Copy** from the resulting menu, then open your new palette. With your cursor anywhere in the palette space, hold down **[CTRL]** and right-click the mouse. Select **Paste** from the pop-up menu to place a copy of the symbol in the new palette.

Copying an Existing Palette

To copy any palette (whether built-in or user-added), first open the palette in question. Then simply right-click the palette heading and select **Copy**. Type a name for the new palette and click **OK**.

Renaming a Palette

To change the name of any palette, first open the palette in question. Then right-click the palette heading and select **Rename**. In the Rename Palette box, type the name you want to use for the palette and click **OK**. The palette will now display the new name.

Note: The **Rename** command is very useful when you have just created a new custom palette, as the initial name for all new palettes is *New*.

Using a Custom Color Scheme to Change UnitOp Symbol Colors

In addition to the three built-in color schemes (Grayscale, System Color, Wireframe), you can create your own custom color schemes, which can be applied to either built-in or user-created palettes. Using a custom color scheme enables you to assign new colors to the standard UnitOp symbols.

To do this, first select or create a palette where you want to change some UnitOp symbol colors. Right-click the palette heading and select **Apply Color Scheme** > **New Color Scheme**. Type a name for your new color scheme and click **OK**. The new color scheme name will now appear in the selected palette header.

The default appearance of any new color scheme is identical to the Grayscale scheme. Now that a custom color scheme is enabled, however, you can begin to assign new colors to any item on the current palette.

Hold down **[CTRL]** while you right-click a UnitOp symbol, then select **Edit Color Scheme**. This brings up the Edit Color Scheme dialog, where you can select new primary and secondary colors for the symbol.

Note: Using two colors gives the symbol a three-dimensional appearance; to create a flat look, choose the same color for the primary and secondary options.

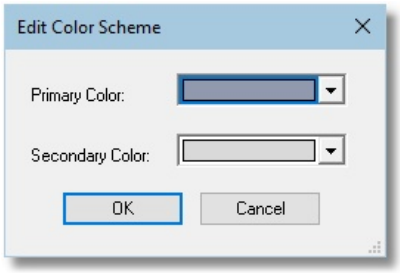

Figure 9-10: Default Grayscale colors in the Edit Color Scheme dialog

Choose new colors and then click **OK**. The symbol appears with the colors you selected on the current palette.

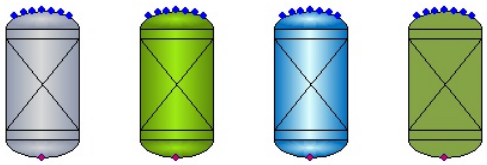

Figure 9-11: The standard Equilibrium Reactor symbol with (from left) Grayscale, System Color, two-tone custom, and single custom coloring

Repeat this process for any other UnitOp symbols for which you want to create custom colors. The changes you make in a custom color scheme will affect *only* those palettes to which you assign the scheme.

You can remove a custom color scheme simply by right-clicking any palette heading and selecting **Delete Color Scheme** > **[scheme name]**. Before you do this, be sure the scheme you are deleting is not currently in use by any palettes.

Resetting Palettes to Default Configuration

As you experiment with palette customization, remember that you can return all the built-in UnitOp palettes to their default settings by right-clicking any palette heading and selecting **Reset All Palettes**.

Note that when you use this command, any user-added palettes will close, but you can open them again at any time. To open a palette that is not currently displayed, right-click any palette heading and select **Open**, then double-click the desired **.trs** format file.

Creating Custom UnitOp Symbols

The Palette pane displays the default symbol for every UnitOp type available in CHEMCAD. Right-clicking the default symbol for any UnitOp opens a sub-palette that offers alternative symbols. Some symbols are different only in their appearance, while others provide a different inlet/outlet configuration from the default symbol. Some UnitOps have a large number of alternative symbols, while others have only one or two.

If none of the available symbols meets your needs, you can create a custom UnitOp symbol for use in CHEMCAD. You determine the symbol's appearance, assign it a UnitOp type, and set the number and location of its inlet and outlet ports. The completed custom symbol becomes part of the sub-palette for its UnitOp type, and is available for use in all simulations that you create or edit with this installation of CHEMCAD.

Users who program custom UnitOps can also create their own symbols for use with those UnitOps. The tool within CHEMCAD that is used to create all custom symbols is called the *UnitOp Designer*.

The main steps for adding a custom UnitOp symbol are as follows:

1. Open a UnitOp Designer tab in the CHEMCAD workspace.

2. Draw and size the symbol.
3. Save the symbol as a .sid drawing file.
4. Add and specify the desired inlet and outlet ports for the UnitOp.
5. Publish the symbol with a name and UnitOp type.

Once you are comfortable working with the UnitOp Designer tool, you can use cloning and other helpful shortcuts to add other symbols you may need. These time-saving techniques are discussed later in this section.

Starting the UnitOp Designer

To begin designing your custom UnitOp symbol, click the **Tools** tab, then in the **Flowsheet** group, click **UnitOp Designer**. This brings up a separate *UnitOp Designer* tab in the CHEMCAD workspace, and displays *UnitOp Designer* in the title bar where the simulation name is usually found.

Whenever a UnitOp Designer workspace tab is selected, the command ribbon displays the UnitOp Designer tools that enable you to create and work with custom UnitOp symbols. If you have other workspace tabs open, such as a simulation flowsheet or charts, you can switch to them at any time; when you switch back to the UnitOp Designer tab, the appropriate tools will display again.

Drawing and Sizing the Symbol

The first step in creating a custom UnitOp is to draw the symbol that will represent it on the UnitOp palette.

The UnitOp Designer tab offers the following tools for creating your new symbol:

- The full Objects gallery for drawing shapes, including Line, Arrow Line, Polygon, Ellipse, Circle, Rectangle, Square, and Rounded Rectangle
- The full Arrange gallery, which includes tools for ordering, grouping, aligning, and rotating drawn objects
- The Text Box tool, for adding text to your UnitOp symbol
- The Image tool, for importing an image file from your computer or network

Use these tools to create the symbol you want to represent your new UnitOp. Note that in some cases, the drawing tools remain active until you either right-click on the workspace or select a different tool. If you create a shape unintentionally and want to remove it, simply click the shape to highlight it, then right-click and select **Delete**.

To ensure that your new symbol is similar in size to other items on the UnitOp palette, you can "borrow" an existing symbol to get a sense of its scale:

1. Click the simulation tab at the bottom of the workspace.

2. Drag a symbol of the desired size from the palette to the workspace.
3. Right-click the symbol on the flowsheet and select **Copy**.
4. Click back to the UnitOp Designer tab.
5. Right-click any blank area and select **Paste**.

You can now draw your new symbol to a scale that matches this symbol. Be sure to delete the borrowed symbol, along with any drawing objects that you do not want to include, before continuing.

Saving the Symbol Drawing

When you have created your new UnitOp symbol, you will save it as a composite shape before continuing to the next step.

In the **Commands** group, click **Add Ports**. This brings up the Save File Before Adding Ports dialog box, which prompts you to name the file with a .sid extension. The default location for storing composite shapes used in custom UnitOps is **My Simulations\Symbols**. Name the file and then click **Save** to continue.

Adding and Locating Ports

Now that you have created a composite shape to represent your new UnitOp, you need to place and specify the desired number of inlet and outlet ports.

Before you begin, be sure that you know how many inlet and outlet ports the desired UnitOp type is set up to use. The number of ports you add will need to be compatible with the UnitOp's configuration.

To start adding ports, click **Add Inlets** in the **Objects** group, then click on the outside edge of your composite shape where you want to place an inlet. A small blue dot will appear to mark the port's location. Continue in this way until you have the desired number of inlet ports for your UnitOp.

Repeat this process with the **Add Outlets** command, placing the desired number of outlets on your UnitOp.

To adjust the position of a port, simply click the port dot to highlight it and then drag it to its new location.

> **Note:** Placing ports precisely on a symbol outline can be challenging when done with a mouse. Alternatively, you can use your keyboard's arrow keys to fine-tune the position of a selected port.

Specifying Ports

Once the ports are all in the correct locations, you can specify them as desired. There are two specifications available for UnitOp ports: *Index* and *Link Direction*.

The Index setting determines the order in which the ports will be calculated within the UnitOp. By default, the first inlet port that you add is assigned index 1,

the second is assigned index 2, and so forth; outlet ports are also numbered in this way.

The Link Direction setting is optional. When specified, it determines the orientation of the stream segment entering or exiting a particular port. Link orientations are given as cardinal directions. For example, you may want all the inlet ports on the left side of a column to enter horizontally from the left, or the outlet port on the bottom of a vessel to exit downward, regardless of where connecting UnitOps are located.

To change the assigned order of a port or specify its link direction, right-click the port and select **Port Identification**.

The Select New Port Index dialog suggests a new Index value, which you can keep or change. To specify the direction of stream entry or exit from the port, select the desired direction from the Link Direction drop-down list. When you have finished specifying the port, click **OK** to close the dialog box.

Once you have viewed or changed the settings for a particular port and then closed the dialog box, the port number displays next to the inlet or outlet dot. It is recommended that you specify (or at least verify) the index setting for each inlet and outlet port before continuing.

Publishing the UnitOp Symbol

The final step in creating a custom UnitOp symbol is publishing the symbol to the appropriate UnitOp sub-palette. To begin this step, click **Publish UnitOp Symbol**. This brings up the UnitOp Symbol Properties dialog.

At the top of the dialog, type a name for the new UnitOp symbol. You can use a standard UnitOp name, such as *Compressor* or *Flash*, or provide a unique name. To ensure that the name displays properly in the palette, it's recommended that you keep the name brief.

Next, make a selection from the UnitOp Type drop-down list, to determine how CHEMCAD will categorize your new symbol. In the space below, type a short description of the UnitOp.

When you have finished specifying the symbol's properties, click **OK**. In the Messages pane, the Notifications tab will display a message: *The symbol '[name]' has been published successfully*. You can now go to the Palette pane, right-click the UnitOp type you assigned, and see your new symbol displayed on the UnitOp sub-palette.

To close the UnitOp Designer tool, click the **X** on its tab at the bottom of the CHEMCAD workspace. You will be asked if you want to save changes to your document; if you have finished working on custom UnitOps for the time being, click **No**.

Time-saving Strategies for Creating Multiple Custom Symbols

In some situations, you may want to create two or more custom symbols that are similar. You might need two symbols that look nearly the same, or perhaps you want to create two identical symbol drawings with different port configurations. Instead of starting over for each symbol, you can use existing .sid files to save time and effort.

Use an Existing Drawing as a Starting Point for another UnitOp

If you need two or more custom UnitOps that are similar in appearance, but not quite the same, you can clone one custom symbol and make the needed changes for other symbols.

To do this, first open the UnitOp Designer (**Tools** tab, **Flowsheet** group, **UnitOp Designer**) and create your first custom UnitOp, as described above. When you have completed the publishing step, close the UnitOp Designer tab, then launch the UnitOp Designer tool again.

On the **UnitOp Designer** tab, in the **Commands** group, select **Open UnitOp Drawing**. This should bring up the directory where you stored your .sid file after the initial drawing step of your custom UnitOp creation. Select the desired .sid file and click **Open**.

The drawing file opens in the UnitOp Designer tab. You can now make any needed changes to the drawing: add or delete items, resize an item, change text, and so forth.

When you have finished making changes, click **Add Ports**, then give this drawing a unique .sid filename and proceed as before. To return to the same starting place again, simply open the original drawing and repeat the process.

Clone a Custom UnitOp Symbol and Change Port Configuration

If you have just created a custom UnitOp symbol, and want to create an identical symbol with a different port configuration, you can do this quickly and easily.

As soon as your first symbol is published, simply use the port buttons to place any additional inlets and outlets, or move the ports to different locations, as required. Be sure to right-click and select **Port Identification** for each new port, and number your inlets and outlets in the order they are to be calculated.

When your port configuration is set, continue by clicking **Publish UnitOp Symbol**. After you specify the symbol's name, type, and description, click **OK** to publish the symbol.

To see the two symbols side by side, click back into the main simulation tab. Right-click the relevant UnitOp type to open the sub-palette, and try placing your new symbols on the flowsheet. You will see that the port configuration is the only visible difference between the two symbols.

Saving a Published UnitOp for Later Port Reconfiguration

In some cases, you can anticipate the need to re-use a custom UnitOp symbol, with a different port configuration, at a later date. You can save a published symbol, complete with its port information, to use as a starting point for future custom UnitOps:

1. After publishing a custom UnitOp, close the UnitOp Designer tab. When asked "Save changes to UnitOp DesignerX?" click **Yes**.
2. Give this .sid file a unique name that you will remember next time—e.g., "Vacuum Column Template" or "Atmospheric Column with Ports"—and click **Save**.
3. When you need another version of this UnitOp with a different port configuration, launch CHEMCAD and open the UnitOp Designer tool (**Tools** tab, **Flowsheet** group).
4. In the **UnitOp Designer Tools** tab, in the **Commands** group, click **Open UnitOp Drawing**. In the Open dialog box, choose the "template" .sid that you saved before, and click **Open**. The .sid file will open, displaying its ports and their configuration.
5. Click **Add Ports**. Give your new version of this symbol a unique .sid name, then click **Save**.
6. Add, move, delete, or reconfigure ports as needed, then publish as before.
7. If you want to keep this new version as a template for future changes, be sure to save when CHEMCAD prompts you as you close the UnitOp Designer tab.

Cloning from the Flowsheet with Publish to Palette

In some cases, you may want to capture the appearance of a UnitOp icon on your CHEMCAD workspace and place it in a palette for future use. For example, you may have flipped a pump icon to place the outlet on the left side, or rotated a vessel icon 90 degrees to give it a horizontal appearance.

Whenever you want a new custom UnitOp that looks different from an existing one (either built-in or user-created), but has the same port configuration, use the **Publish to Palette** command:

1. Make sure the UnitOp icon you want to put on a palette is visible in the main CHEMCAD workspace. This may require opening a simulation in which you changed the icon's appearance, or dragging a built-in or custom UnitOp icon from a palette onto the workspace.
2. If desired, change the UnitOp's appearance according to your needs. You can use the drawing tools to embellish the UnitOp symbol; right-click the UnitOp and use the **Flip**, **Rotate**, **Line**, or **Fill** commands; or click and drag to change the icon's size or shape.

3. Click and drag to select the UnitOp icon and any drawn additions, then right-click and select **Publish to Palette**.
4. On the UnitOp Symbol Properties dialog, specify the symbol's name, type, and description. When you click **OK**, the new UnitOp symbol is published to the specified UnitOp subpalette.

Creating Custom UnitOps

If you need a UnitOp that falls outside the range of options offered by CHEMCAD, you can create a custom UnitOp. The goal of creating a custom UnitOp is to have a unit where you can enter your own equations to calculate heat and mass balances. Over the years, CHEMCAD users have created custom UnitOps for purposes as diverse as membrane separation units, fuel cells, specialized solids handling units, and crystallizers for the separation of xylenes.

Four items on the All UnitOps palette are dedicated to user-defined UnitOps. You can create a custom UnitOp using any of the following:

- **Excel UnitOp:** Created through a combination of the COM interface and the Data Map interface
- **Calculator:** Created using an inline C program
- **User-added module:** Created using Visual Studio or another C++ compiler
- **VBA UnitOp:** Created through the VBA Editor, which is part of CHEMCAD

The basic procedures for creating custom Excel UnitOps are covered in Chapter 10, *Data Interfaces*. Calculator UnitOps are defined by a programming language called Parser, the syntax for which is documented in the *CHEMCAD Calculator/Parser Module* guide, available on the Chemstations website.

C++ user-added modules are developed using Microsoft's Visual C++ development tool, the same tools that were used in the creation of CHEMCAD's own UnitOps. The procedures for creating C++ user-added modules for use with CHEMCAD are detailed in the *User-added Modules Guide*, which is also available on the Chemstations website.

VBA UnitOps are defined by VBA subroutines, and are described later in this chapter.

The method you choose is an important first step toward creating a UnitOp, but the choice is almost entirely up to you. Calculator UnitOps can be quick and easy to set up, but they can't do everything the other methods can. The Excel/Visual Basic approach is very powerful and uses the familiar Visual Basic language for development. A drawback to this method is that calculation can sometimes be slow due to the use of Microsoft Excel to perform the calculations. The most powerful and fastest calculating method is the C++ user-added module method, but if you are new to C++, it may be challenging to use. VBA UnitOps are as powerful as those created using C++, and are much easier to build.

Whichever method you use to program the calculations of your UnitOp, you will likely need to create a dialog box to provide a user interface. A dialog box enables users to send information into your UnitOp, for example the number of stages for a distillation UnitOp. No matter what method you use to program your UnitOp, you will use the Dialog Editor program to create the user interface.

Creating a Custom UnitOp Dialog Box

CHEMCAD uses dialog boxes to set variables for all types of UnitOps. Using the Dialog Editor program, you can create a custom dialog box for use with any type of user-added unit.

You can also edit an existing UnitOp's specification dialog box—for example to add text notes, to translate from English to another language, or to limit the UnitOp's functionality—although this is not commonly done.

The Dialog Editor program enables you to create and modify dialog boxes, which are controlled by files with the .my extension. These files, along with .map files and .lab files, define dialog boxes for use in CHEMCAD.

To use the Dialog Editor program, you'll need a good understanding of Windows, along with a basic knowledge of Visual Programming concepts such as objects and properties. You should also have a firm understanding of simulation in CHEMCAD before venturing into Dialog Editor.

The Dialog Editor program is separate from CHEMCAD. To launch it, open the full list of available programs from your Windows **Start** menu and select **Chemstations** > **Dialog Editor**.

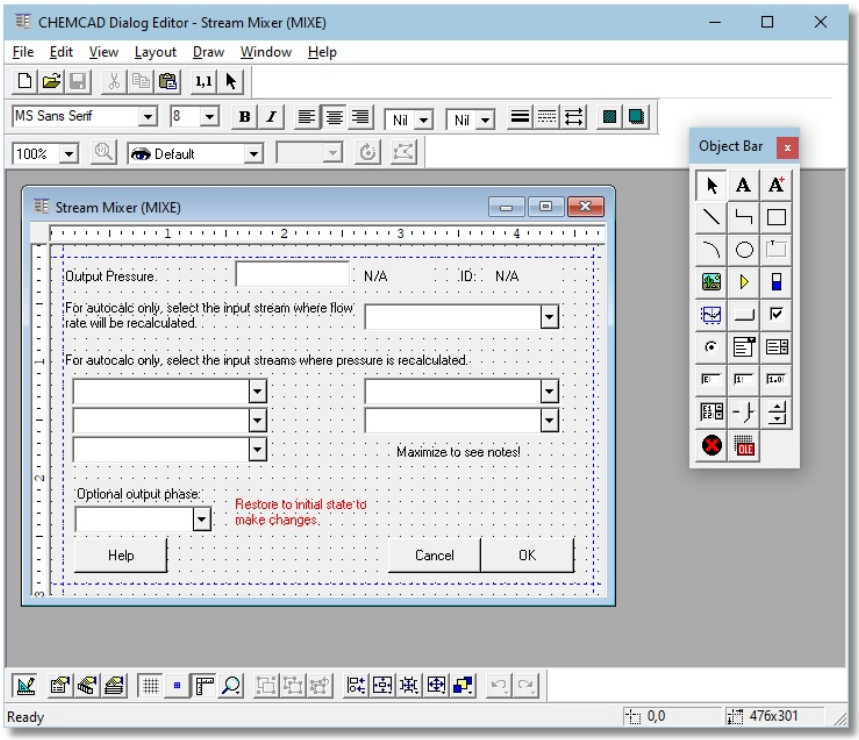

Figure 9-12: The Dialog Editor window showing an open dialog

A detailed description of how to use the Dialog Editor is available on the Chemstations website.

Customized Costing Calculations

CHEMCAD includes some very basic costing routines to help determine the capital cost of equipment. Using a simplified form of C known as the Parser language, you can modify these routines to better suit your needs. Details of this procedure are found in the *CHEMCAD Calculator/Parser Module* guide, available on the Chemstations website.


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Chapter 10

Data Interfaces

CHEMCAD enables you to exchange data with other programs through a variety of methods. This saves time, effort, and the potential for keystroke error and data omissions. In some cases, these data interfaces can enable CHEMCAD to link directly into your plant information systems to run simulations without human intervention.

The data interfaces that CHEMCAD uses are as follows:

- The Excel Data Map interface, which can link any value in a CHEMCAD simulation to any cell in an Excel worksheet, or vice versa (note that running CHEMCAD simulations from Excel requires a COM interface, described below)
- The Visual Basic Application interface, which enables you to build custom reactions, mixing rules, and UnitOps
- The OPC interface, which permits any OPC Client application to access values in a CHEMCAD simulation
- COM interfaces, which allow any COM-enabled program (such as MATLAB) to access and control a CHEMCAD simulation

Excel Data Mapping

The Excel Data Mapping feature allows you to link, retrieve, and insert data from an Excel spreadsheet into a CHEMCAD simulation. It also lets you insert data from a CHEMCAD simulation into an Excel spreadsheet with just a few clicks. The integration of CHEMCAD and Excel is a powerful and easy-to-use tool that saves you time and work.

With Excel Data Mapping, you can quickly and easily get the most of CHEMCAD/Excel integration, even if you have no experience with Visual Basic or Excel programming. In fact, you can use and benefit from this feature even with very little knowledge of the Excel program.

To use Excel Data Mapping, you must first create one or more Data Maps, and then set up rules for the execution of each Data Map in use.

Creating an Excel Data Map

The tool used to create and edit Data Maps in CHEMCAD is the Excel Data Map Editor. This tool displays within the CHEMCAD workspace, and resembles an Excel spreadsheet. It has all you need to link stream and UnitOp parameters to one or more Excel spreadsheets. On each Excel Data Map, you can link up to 500 parameters in a single spreadsheet, and you can have up to ten Data Maps per simulation.

To link your simulation to an Excel spreadsheet, first create the target Excel workbook, making a note of the file's name, its location, and the name of the specific worksheet to which you want to link. Then follow these steps to create a new Data Map:

1. Click the **Tools** tab, then in the **Data Map** group, click **New**. A spreadsheet will open within the CHEMCAD workspace.

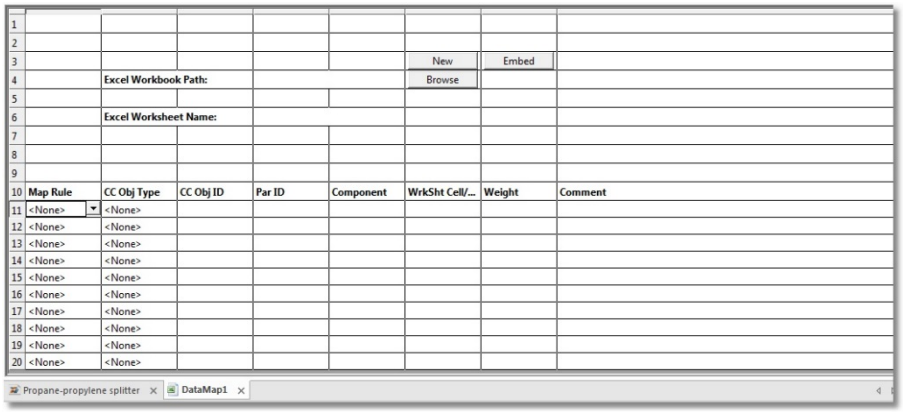

Figure 10-01: The Excel Data Map Editor

2. Click the **Browse** button and locate the target workbook. Select the workbook file and click **Open**.
3. In the cell next to **Excel Worksheet Name**, type the name of the worksheet to which you want to link your simulation.

Note: If you need to verify the name of the worksheet, you can click the **Open** button to launch Excel and view the workbook.

4. Double-click the cell below **Map Rule** to see a drop-down list of mapping options:
   - **To Worksheet Only** enables you to send data from streams or UnitOps in CHEMCAD to the selected worksheet.
   - **To CC Only** enables you to send data from any cell on the worksheet to the selected stream or UnitOp parameter in your simulation.
   - **For data reconciliation** enables you to manipulate the data using CHEMCAD's Data Reconciliation feature.

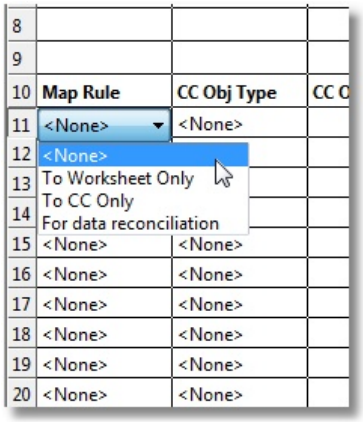

Figure 10-02: Selecting a Map Rule option in the Excel Data Map Editor

5. Double-click the cell below **CC Obj Type** to see a drop-down list of mapping options:
   - **Stream** enables you to link an Excel cell or cell range to a stream on the flowsheet.
   - **UnitOp** enables you to link an Excel cell or cell range to a UnitOp on the flowsheet.
   - **Misc** enables you to change dynamic flowsheet settings.
6. Click the cell below **CC Obj ID**. Type the ID number of the stream or UnitOp to which you want to link.
7. Double-click the cell below **Par ID** to see a drop-down list of parameters for the selected UnitOp or stream. Scroll down and select an option from the list.

Note: When you are importing cell data into CHEMCAD, the list of parameter options is limited, as many values in a CHEMCAD simulation are calculated based on other values.

8. If you chose a parameter that is related to a specific component (e.g., *Comp Mole fraction*), you will need to specify the component. Double-click the cell below **Component** to see a drop-down list of available components. Select a component from the list.

9. Click the cell below **WrkSht Cell/Range**. Type the cell address or cell range to which you want to link. Cell addresses should be formatted with the column letter and row number, e.g., **A1** or **D17**. Cell ranges should be formatted as two such addresses (representing the range's first and last values) separated by a colon, e.g., **A1:A12** or **B5:E20**.
10. If you are performing a data reconciliation, you can use the **Weight** column to give certain items in the reconciliation more importance than others.
11. Repeat the procedure until you have specified all the cells or cell ranges that will link to your simulation.
12. When you are ready to save the Data Map, first make sure the **Tools** tab is selected. Then in the **Data Map** group at the left end of the ribbon, click **Save Data Map As**. Type a name for your Data Map and then click **OK**. The newly created Data Map now appears in the **View/Edit** drop-down list in the **Data Map** group.

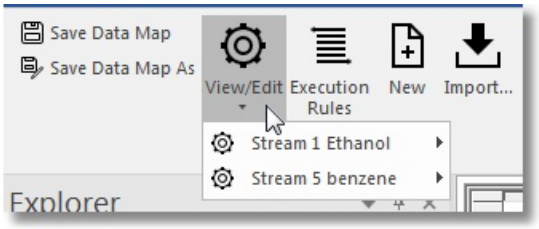

Figure 10-03: List of available Data Maps in the simulation

13. To leave the Data Map open and return to your simulation, use the tabs at the bottom of the main CHEMCAD workspace. To close the Data Map, click the red **X** button on its tab at the bottom of the workspace.

Data Map Execution Rules

After configuring one or more Excel Data Maps for a simulation, you must set up execution rules to use them. You can configure up to 10 Data Map files per simulation.

To set up Data Map execution rules, follow these steps:

1. On the **Tools** tab, in the **Data Map** group, click **Execution Rules**. The Data Map Execution Rule dialog box appears.

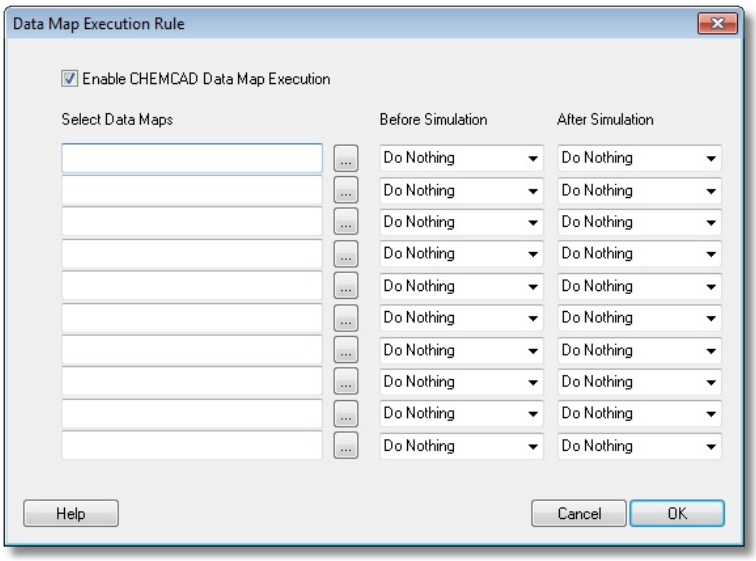

Figure 10-04: The dialog box for configuring execution rules

2. Click the square button next to the first field in the *Select Data Maps* column to bring up the Select Data Map dialog box.

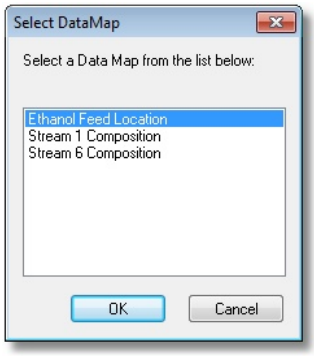

Figure 10-05: Selecting a Data Map from the list

3. Select the name of the Data Map for which you want to set rules, then click **OK** to return to the Data Map Execution Rule dialog box. Repeat this step for all other Data Maps whose rules you want to set up at this time.

4. In the Before Simulation Runs field next to each selected Data Map, click the drop-down list to choose an action for that Data Map to perform before calculations begin:
   - **Do Nothing** performs no action before the simulation is run. You might use this option to disable a Data Map temporarily.
   - **To Workbook** sends the requested data to Excel before running the simulation. You might use this option when you want to pull data from inlet streams or UnitOp specifications.
   - **To CHEMCAD** sends the requested data in Excel to CHEMCAD before running the simulation. You might use this option when you want to feed data to inlet streams or UnitOps with data from the Excel worksheet.
5. In the After Simulation Runs field next to each selected Data Map, click the drop-down list to choose an action for that Data Map to perform after calculations are complete:
   - **Do Nothing** performs no action after your simulation has run. You might use this option to disable a Data Map temporarily.
   - **To Workbook** sends the requested data to Excel after running the simulation. You might use this option when you want to send data from streams or calculated parameters of UnitOps to the workbook in Excel.

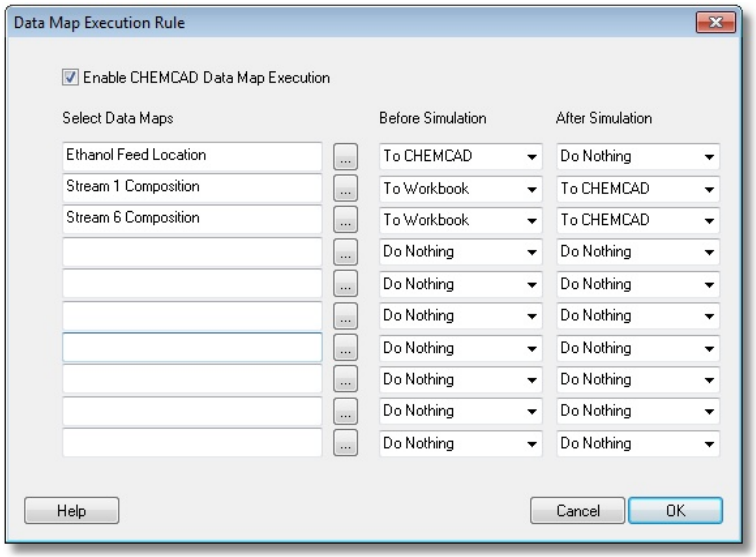

Figure 10-06: Three different Data Maps with rules set up

6. When you have configured all the Data Maps that you want to use, click **OK** to save your rules and close the Data Map Execution Rule dialog box.

You can now run the simulation. If you open the Excel files that are linked to the simulation, you will be able to see the parameters of streams and UnitOps related to the Excel Data Map. You can also perform your own calculations in the workbook based on the data linked to CHEMCAD.

Creating Excel UnitOps

You can build an Excel spreadsheet that functions as a UnitOp within CHEMCAD. This is useful for extremely simple UnitOps such as mixers and dividers, or for simple separations.

1. Start by creating a custom dialog box for your new UnitOp, as described in Chapter 9, *Customizing CHEMCAD*.
2. Next, create an Excel workbook containing your desired calculations for the new UnitOp.
3. Open a simulation and find the **Excel** UnitOp symbol on the Palette. Drag this UnitOp symbol onto the workspace.
4. Draw the appropriate streams into and out of the Excel UnitOp.
5. Double-click the Excel UnitOp symbol to open the Excel WorkBook Unit dialog box.
6. On the File Paths tab, use the top **Browse** button to specify the location and file name of the custom dialog box that you created. Use the second **Browse** button to specify the location and file name of the Excel workbook that contains the calculations for this UnitOp.
7. Now you need to specify how this spreadsheet will link to CHEMCAD. Click the **Data Maps** tab to link the spreadsheet using one or more Data Maps, or click the **Excel Macros** tab to link the spreadsheet using the COM interface.
   - On the **Data Maps** tab, specify the execution rules as described earlier in this chapter.
   - On the **Excel Macros** tab, specify the names of the Excel macros that you have programmed to use the COM interface, in the order that you want them to be calculated.
8. Click **OK** to return to the main CHEMCAD window.

Specification Sheets

Using the interface with Microsoft Excel, CHEMCAD allows you to output simulation data to an Excel spreadsheet resembling a vendor specification sheet, as discussed in Chapter 8, *Output and Reports*. Customizing these spec sheets saves you time by outputting data in the format required by your company or vendor.

To customize the spec sheet for a specific UnitOp type, edit the corresponding Excel spreadsheet in the CHEMCAD templates directory. A typical pathname for this directory is:

C:\Program Files\Chemstations\CHEMCAD NXT\templates

If the UnitOp type you want is not represented by the Excel files in this directory, you can copy the generic **specsheet.xls** file and use it as a template for a new UnitOp spreadsheet.

Place the copy in the same directory, and make its file name the standard four-character abbreviation for the UnitOp type in question. For example, to create a spec sheet template for the Flash UnitOp, you would need to name the file copy **flas.xls**. See the CHEMCAD Help information about your specific UnitOp if you need to look up this abbreviation.

Before you continue, you will need to turn off the Read-only attribute for the new spreadsheet file. The quickest way to do this is to right-click the file within the Windows Explorer, select **Properties**, and then clear the **Read-only** check box in the Properties dialog box.

Once the copy is renamed and the Read-only attribute is turned off, you can open the spreadsheet and edit it as needed.

Using CHEMCAD as an OPC Server

CHEMCAD is capable of setting up an OPC server which allows direct data transfer between any CHEMCAD simulation and any OPC client application.

OPC stands for *OLE for Process Control*. OPC provides a standard method for different devices and applications to share data. Using OPC, you can share data between CHEMCAD simulations and SCADA systems, data historians, distributed control systems (DCS), and human-machine interfaces (HMIs).

In fact, the acronym *OPC* is now considered by many to mean *Openness, Productivity, Connectivity*, because this technology forms the basis for sharing and manipulating plant data.

OPC-enabled systems are classified as either *OPC servers* or *OPC clients*. OPC servers are either applications or devices that provide data. OPC clients are interfaces that use and manipulate this data. OPC clients can connect to multiple OPC servers at any time and read and write data to all of them.

OPC Applications

OPC can be applied as follows:

- **Inferential sensors:** Sometimes called *soft sensors*, inferential sensors use one or more measured variables to estimate another variable. Using CHEMCAD simulations and data from your plant's DCS, you can embed simulations to provide data such as concentrations, heat duty, and fouling factor, which would not normally be available.
- **Operator training:** You can couple an operator HMI to a dynamic simulation to create a training simulator that can help train operators in a safe and effective way.

OPC Compliance

Chemstations is a Member of the OPC Foundation, an organization devoted to maintaining the OPC standards. CHEMCAD has been certified for, and interop tested for, OPC DA standard 2.05a.

Enabling CHEMCAD as an OPC Server

To enable OPC within CHEMCAD, start by clicking the **File** tab and then selecting **Preferences**. On the left side of the Preferences dialog box, click **Connections**, then **OPC**. Check the **Enable OPC Server** box and click **OK**. When you do this, CHEMCAD registers an OPC server named **CHEMCAD.SimulationServer.1** on your machine.

Once you load a simulation, all of that simulation's stream properties and UnitOp settings and variables are automatically published as tags to the OPC server's namespace.

Every value tag has a units tag associated with it, which shows the engineering units used to report the value. To change the engineering units, click **Engineering Units** (**Home** tab, **Setup** group) within a CHEMCAD simulation.

When the OPC server feature is enabled, CHEMCAD automatically registers itself as an OPC server. If you want to unregister CHEMCAD and remove it from the list of OPC servers, you can open a Windows command prompt and type the following command:

```
{program directory}\CCNXT.Exe –unregister
```

For example, if your program directory were **C:\Program Files\Chemstations\CHEMCAD NXT\Program**, you would type the following:

```
C:\Program Files\Chemstations\CHEMCAD NXT\Program\CCNXT.exe -unregister
```

Reading and Writing Values to CHEMCAD Using OPC

You can use OPC to have values read from or written to a simulation, and to run the simulation. Both steady-state and dynamic simulations can be run in this way.

Values are updated to the OPC server whenever CHEMCAD completes a steady-state run or a dynamic time step. Values can also be read; in the case of a dynamic simulation, reading values between time steps will cause the program to extrapolate from the last converged results.

Values can be written at any time. If CHEMCAD is in the process of executing a time step or a steady-state simulation, the values are held in a buffer until the simulation is converged, at which time the values are written to CHEMCAD.

When values are written to a CHEMCAD stream, the stream is immediately reflashed, and all OPC tags for that stream are updated.

OPC Server Operations

In addition to reading and writing process data to CHEMCAD, it is useful to be able to send commands to CHEMCAD, for example to tell CHEMCAD to start or stop running a simulation.

This is done with a series of flags in the CHEMCAD group of the OPC server. To use any of these flags, write a 1 to flag. CHEMCAD will execute the desired command and return a value indicating success or failure. A return of 0 indicates that the command has completed successfully, while a negative return indicates a problem of some kind.

The available commands are as follows:

- **Refresh Server** tells CHEMCAD to refresh all data sent to the OPC server.
- **Run Steady State** runs a steady-state simulation. When the simulation finishes, the flag will be reset either to 0 (run converged) or to a negative number indicating the number of errors that occurred during the run. To view the error message text, you must open the CHEMCAD interface directly.
- **Restore to initial state** returns a dynamic simulation to time zero. A return of 0 indicates success; a value of -1 indicates failure.
- **Run Dynamic** starts a dynamic simulation. A return of 0 indicates success; a value of -1 indicates failure.
- **Run Dynamic One Step** runs a single time step of a dynamic simulation. A return of 0 indicates success; a value of -1 indicates failure.
- **Set Initial State** sets the current process conditions as the time-zero conditions, overwriting the previous time-zero conditions. A return of 0 indicates success; a value of -1 indicates failure.
- **Stop Simulation** stops a dynamic simulation. A return of 0 indicates success; a value of -1 indicates failure.

CHEMCAD OPC Namespace

An OPC namespace defines and organizes all the available commands and data. OPC namespaces are divided into groups, each of which contains items. Items are sometimes referred to as *tags*.

Note: Most of the data items in a simulation have engineering units associated with them. In these cases, we usually define two separate tags, one containing the data value and the other containing the units string. All units strings are read only from OPC. The units strings are governed by the settings inside the simulation.

The groups in CHEMCAD's OPC namespace are organized as follows:

- **CHEMCAD.SimulationServer:** This is the OPC server name. By convention, this name is followed by a version number, e.g., **CHEMCAD.SimulationServer.1**, to indicate the OPC Server version. This is the server name to which OPC clients will connect.
- **CHEMCAD Group:** This group contains any information that is not dependent on a stream or UnitOp, and all commands used to run CHEMCAD.
- **Streams Group:** This group contains a series of subgroups, one for each stream on the flowsheet numbered by stream ID number.
- **UnitOperations Group:** This group contains a series of subgroups, one for each unit operation on the flowsheet, numbered by UnitOp ID number.

COM Interfaces

Component Object Model (COM) is a Microsoft-standard platform that enables programs to share content such as data and calculation routines. This interface makes it possible for other programs to control a CHEMCAD simulation.

CHEMCAD acts as a COM server, so any program that can act as a COM client can be made to interface with CHEMCAD in this way. If you aren't certain whether your application can act as a COM client, check with the software vendor.

Note: Using the COM interface to CHEMCAD is a complicated procedure that requires some experience in programming. If your organization lacks in-house expertise in programming, consider bringing in a third-party resource to assist you with the procedure.

The following section is a brief walk-through of a simple COM interface between Excel and CHEMCAD.

Connecting Excel and CHEMCAD: A Simple COM Interface

While you can export or import data values using Excel Data Map, more complicated interactions—such as running a simulation from another program—require the extra control afforded by the COM interface.

The following is a simplified description of the procedure for connecting these two programs and enabling Excel to load a simulation, change a value, run the simulation again, read the same value, and then close the simulation.

In this procedure, you'll use Excel to do the following:

- Open CHEMCAD
- Read in values from CHEMCAD into an Excel workbook
- Change a value in the simulation

- Run the simulation
- Read the revised values back into Excel

Normally, using COM interfaces involves some programming. We have created an example called VBCLient.xls to help you overcome that hurdle; you don't need to write any code at all to use this tool. Even if you need to write your own program, the code in the macros of VBClient will come in handy as a guide.

Using the VBClient Example

Follow these steps to use the VBClient example:

1. Open Excel and load the workbook called **VBClient.xls**. This workbook has three worksheets:
   - **Commands** contains buttons for controlling a CHEMCAD simulation.
   - **Streams** displays all stream data in the simulation. This sheet can be used for both input and output of stream variables to the CHEMCAD simulation.
   - **UnitOps** displays all UnitOp-related data for the simulation. This sheet can be used for both input and output of UnitOp variables to the CHEMCAD simulation.
2. On the Commands sheet, you will see a series of buttons used to load CHEMCAD, load a simulation, read data from the simulation, write data back to the simulation, and run the simulation. Click **Load CHEMCAD** to load CHEMCAD into memory. When a number appears next to *CHEMCAD Version*, the program is loaded.
3. Click **Load Simulation** to browse for and load a simulation into CHEMCAD. When a file path and name appear next to *Simulation*, the simulation is loaded.
4. Now make a change to the data shown on the Streams and UnitOps sheets.

   Note: Some values are read-only. For example, VBClient does not allow you to change a stream's total flow rate directly; you must instead change the component flow rates to make a change to the total flow rate.

5. Click **Send Changes** to push your changes to the CHEMCAD simulation.
6. Click **Run All** to run the simulation.
7. Note the changes to the data on the Streams and UnitOps sheets.

A Peek under the Hood

Right-click **Load CHEMCAD**, select **Assign Macro**, and then click **Edit**. The Visual Basic editor in Excel opens to display the code behind the button:

```
Sub LoadCHEMCAD()

   ' initialize global variables

   strJobName = ""
   selUpdateStrUopData = True

   selOK = False

   Set objCHEMCAD = Nothing

   ' load CHEMCAD
   Set objCHEMCAD = CreateObject("CHEMCAD.VBServer")

   If objCHEMCAD Is Nothing Then
      Dim msg As String
      msg = "Can not load CHEMCAD"
      MsgBox msg

   End If

   Call UpdateVersion

End Sub
```

The most important line in that whole subroutine is:

```
Set objCHEMCAD = CreateObject("CHEMCAD.VBServer")
```

In that single line, Excel loads CHEMCAD into memory.

Loading a simulation is accomplished with this simple line from the subroutine called LoadJob:

```
retval = objCHEMCAD.LoadSim(strJobName, 0)
```

Running a simulation can be as simple as this line from the RunJob subroutine:

```
retflag = objCHEMCAD.RunJob
```

The **COM Interface Reference** section of the CHEMCAD Help file (listed under the heading **Customization**) provides a full reference of the commands available through COM.


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