

P & I Design Ltd

Process Instrumentation Consultancy & Design

2 Reed Street, Gladstone Industrial Estate,
Thornaby, TS17 7AF, United Kingdom.
Tel. +44 (0) 1642 617444 Fax. +44 (0) 1642 616447
Web Site: www.pidesign.co.uk

CHEMCAD 6.0
PROCESS FUNDAMENTALS
AND BASIC NAVIGATION

by John E. Edwards
jee@pidesign.co.uk



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1.0 Stream Condition Definition

When defining a stream condition the Gibbs phase rule applies. The variables that define a process condition are in two categories:-

Extensive variables	Mol, Mass, Volume
Intensive variables	Temperature, Pressure, Density, Specific Volume, Mass and Mol Fraction of Components i .

The number of intensive variables that can be independently specified for a system at equilibrium is called the number of degrees of freedom F and is defined by the **Gibbs Phase Rule**. In a system involving no reactions this is given by:

$$F = 2 + m - p$$

Where m = no of chemical species i p = number of system phases

Where r we have independent reactions at equilibrium

$$F = 2 + m - r - p$$

Considering a single component liquid in equilibrium with its vapour and an inert gives:-

$$m = p = F = 2$$

Two variables P and T or Vapour Fraction with T or P will define the stream.

For a binary liquid system one degree of freedom is consumed by the composition leaving either P or T to be specified. In a VLE system it is preferable to specify P which then allows system analysis using Txy plots.

When setting up the Flash UnitOp applying the phase rule will ensure that the relevant flash conditions are being set.

Setting any two parameters from the variables temperature, pressure, enthalpy or V/F will define the flash condition.

The stream flash calculation can be used to determine the boiling point and dew point of mixtures with and without inerts present. The bubble point of a liquid at the given pressure is determined by a flash calculation at a vapour fraction of 0. The dew point of a vapour at the given pressure is determined by a flash calculation at a vapour fraction of 1. For a pure component the bubble point and the dew point are identical so a flash calculation at a vapour fraction of 0 or 1 will yield the same result.

The Txy diagram for Benzene/Toluene, a near ideal mixture, is shown later. The bubble point for a given composition is read directly from the liquid curve and the dew point is read directly from the vapour curve.



Table Presenting Molar and Mass Relationships for Mixture with "i" Species								
Component	MW	% v/v	Volume in	Mass in	% w/w	Mass Flow	Molar Flow	% mol
	kg/kmol		1 m ³ m ³ /m ³	1 m ³ kg/m ³		kg/h	kmol/h	
A	M _A	P _A	$V_A = \frac{P_A}{100}$	$\frac{P_A M_A}{2240}$	$\frac{100 P_A M_A}{\sum P_i M_i}$	$\frac{W P_A M_A}{\sum P_i M_i}$	$\frac{W P_A}{\sum P_i M_i}$	P _A
B	M _B	P _B	$V_B = \frac{P_B}{100}$	$\frac{P_B M_B}{2240}$	$\frac{100 P_B M_B}{\sum P_i M_i}$	$\frac{W P_B M_B}{\sum P_i M_i}$	$\frac{W P_B}{\sum P_i M_i}$	P _B
C	M _C	P _C	$V_C = \frac{P_C}{100}$	$\frac{P_C M_C}{2240}$	$\frac{100 P_C M_C}{\sum P_i M_i}$	$\frac{W P_C M_C}{\sum P_i M_i}$	$\frac{W P_C}{\sum P_i M_i}$	P _C
Total		100	1	$\frac{\sum P_i M_i}{2240}$	100	W	$\frac{100 W}{\sum P_i M_i}$	100

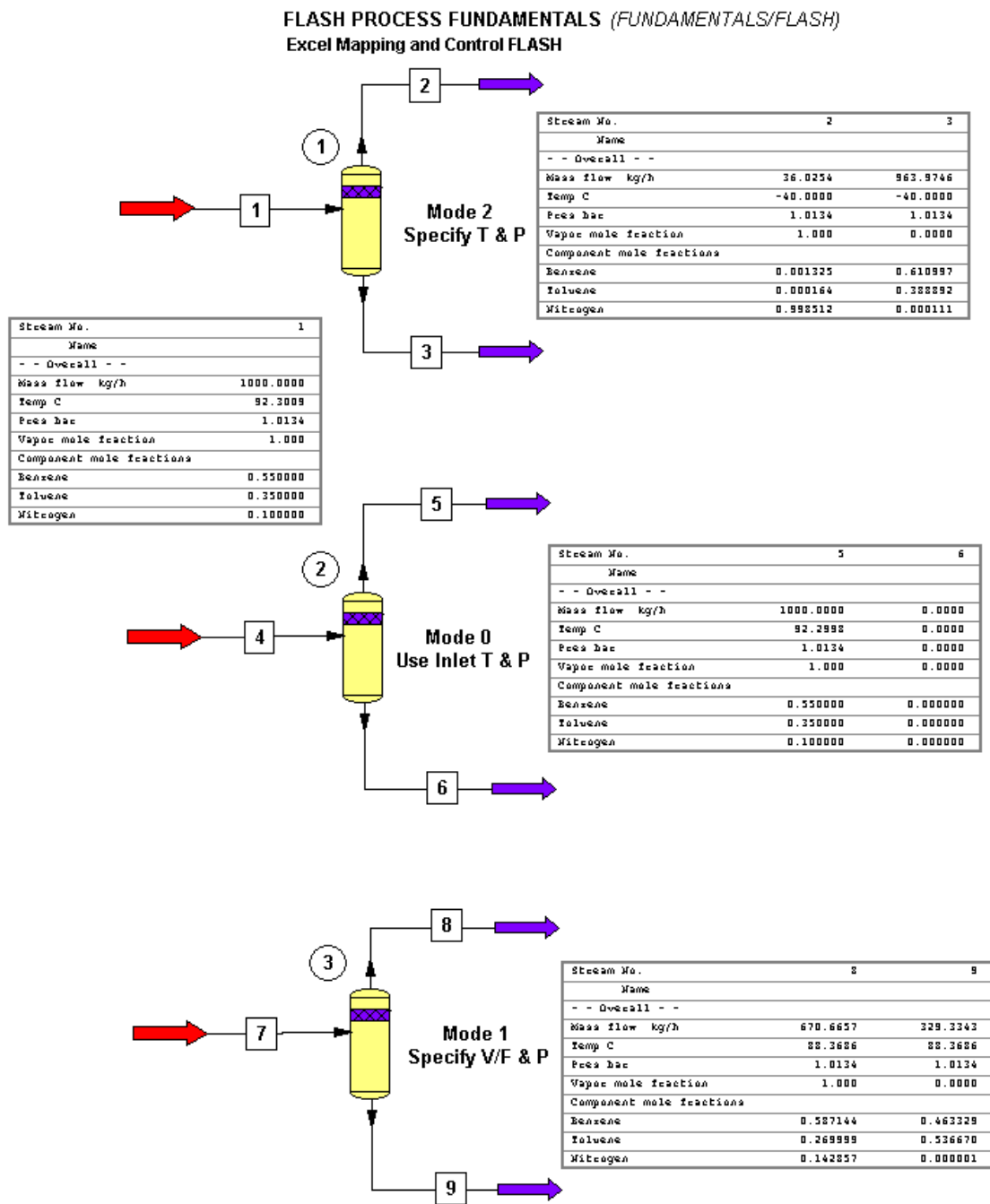
Acknowledgements to the late Doug Lindsley for this format.

We have the following definitions, noting that each mol occupies the same volume ie mol% = vol %

$$\begin{aligned} \text{Total Flow (kg/h)} \quad W & & \text{Density of mixture (kg/m}^3\text{)} \quad G_O = \frac{\bar{M}}{2240} \\ \text{Total Flow (Nm}^3\text{/h)} \quad Q = \frac{W}{G_O} = \frac{2240 W}{\sum P_i M_i} & & \text{Average MW (kg/kmol)} \quad \bar{M} = \frac{\sum P_i M_i}{100} \end{aligned}$$



2.0 Flash Process Fundamentals

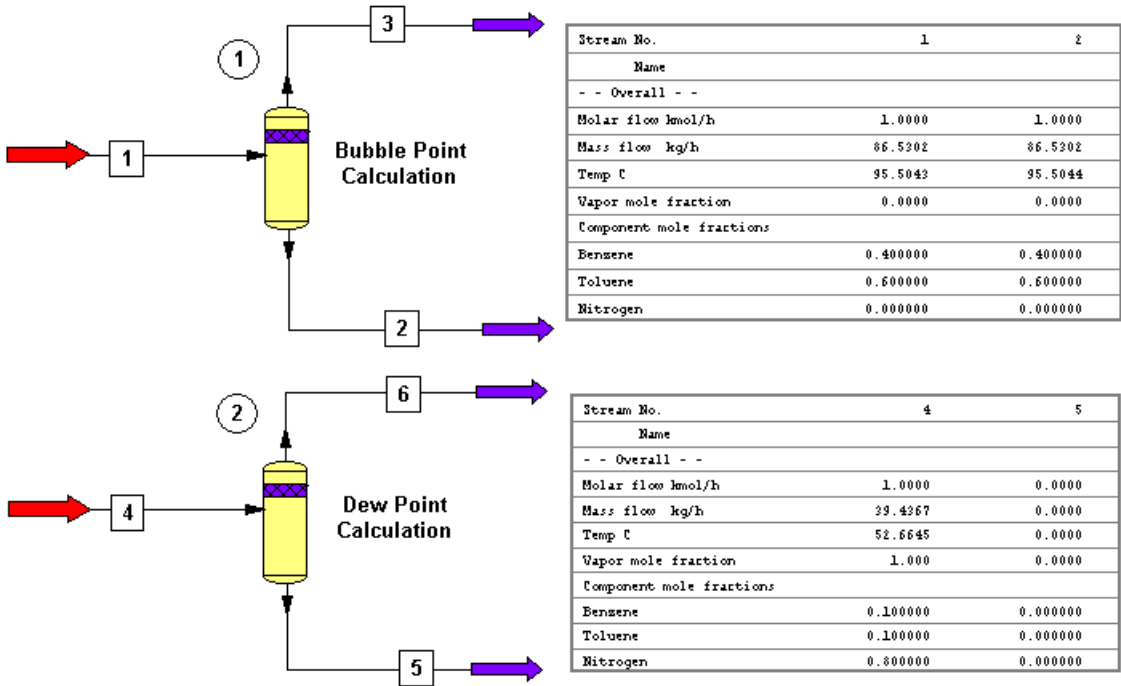


FLASH UNITOP FUNDAMENTALS				
System Total Pressure	1.00	atm	1.0134	bar
Flash UnitOp Basis Condensation Mode				
Condenser Exit Conditions	-40	deg C	V/F Mass	0.036
Flash Mode	Heat		Process Specification	
	MJ/h		Para 1	Para 2
Specify T & P, Calculate V/F & Heat	2	-593.44	-40.000	1.0134
Flash UnitOp Basis Inlet Condition Mode				
Flash Mode	Heat		Process Specification	
	MJ/h		Para 1	Para 2
Use Inlet T & P, Calculate V/F & Heat	0	0.00	Inlet T	Inlet P
Flash UnitOp Basis Vapour Split Mode				
Vapour Split	0.700	mole frac	Process Requirement	
Flash Mode	Heat		Process Specification	
	MJ/h		Para 1	Para 2
Specify V/F & P, Calculate T & Heat	1	-130.47	0.700	1.0134
Temperature	88.37	degC		
Inlet Stream Condition				
Set Vapor Fraction	1.00	Dew Pt = 1, Bubble Pt =0		
Component Liquid Mixture	Composition		Temperature	
	mol %	mol frac	degC	
Benzene	55	0.55	92.30	
Toluene	35	0.35		
Nitrogen	10	0.1		
Total Flow	1000	kg/h		
Data Input	Flash Modes Available			
Data to CHEMCAD	0	Use Inlet T & P, Calculate V/F & Heat		
Data from CHEMCAD	1	Specify V/F & P, Calculate T & Heat		
Excel Calculated Data	2	Specify Inlet T & P, Calculate V/F & Heat		
By: J.E.Edwards	3	Specify T & H, Calculate V/F & P		
File Reference FLASH	4	Specify V/F & T, Calculate P & Heat		
Copyright P&I Design Ltd	5	Specify P & H, Calculate V/F & T		

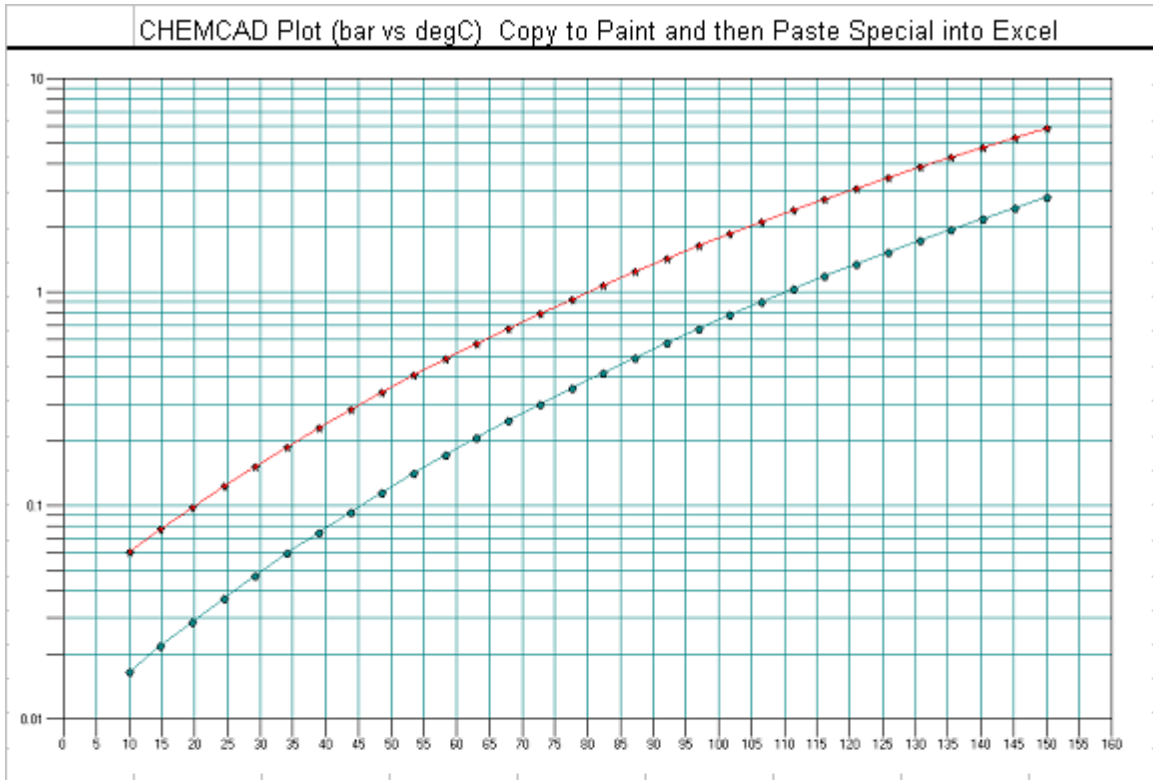


3.0 Bubble and Dew Point Process Fundamentals

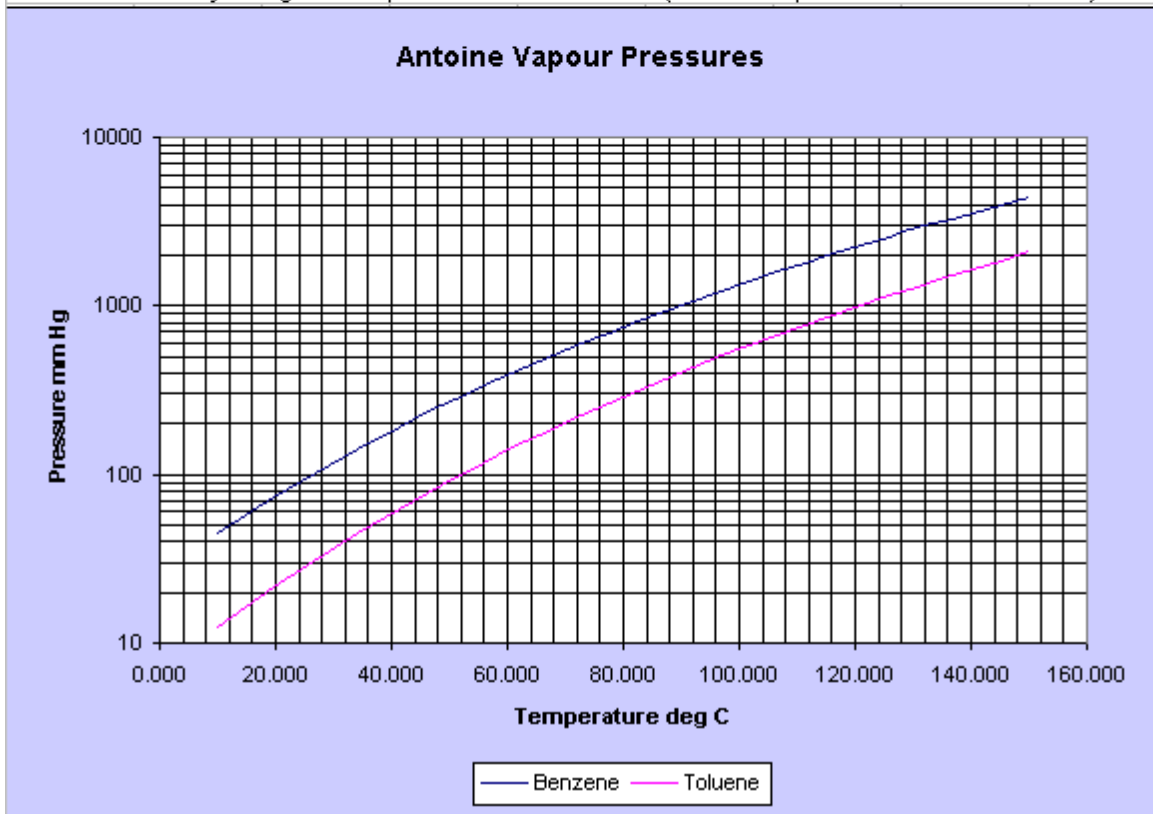
BUBBLE POINT & DEW POINT FUNDAMENTALS (FUNDAMENTALS/STREAM DEFINITION)
Excel Mapping and Control BP(T)DP(T)



3.0 Bubble and Dew Point Process Fundamentals (Cont.)



Excel Plot Facility using data exported from CHEMCAD (In Plot Graph Data to Excel CSV file)

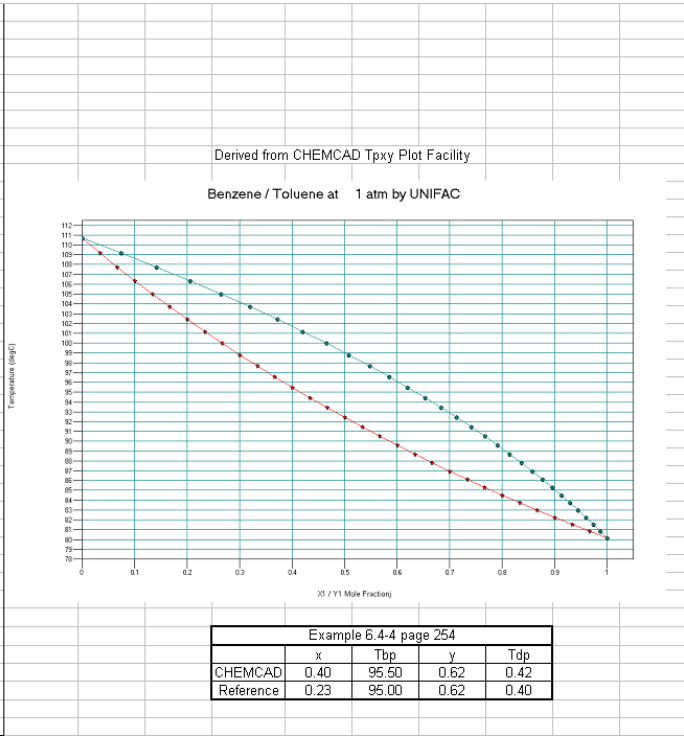


3.0 Bubble and Dew Point Process Fundamentals (Cont.)

CHEMCAD 5.3.7 Page 1
 Copied from CHEMCAD as a WordPad document
 Job Name: STREAM DEFINITION Date: 04/11/2004 Time: 08:48:11

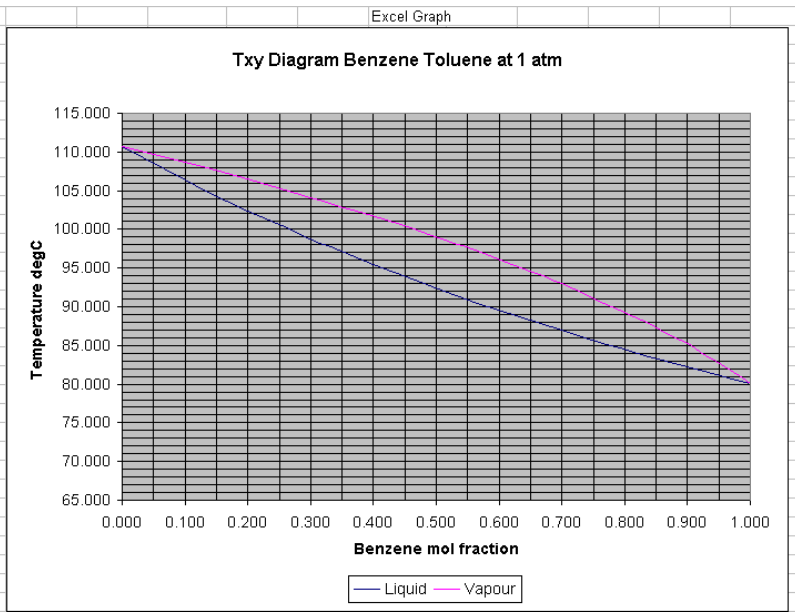
XY data for Benzene / Toluene
 K value model: UNIF

Mole Fractions						
T Deg C	P bar	X1	Y1	Gamma1	Gamma2	Phi1 Phi2
110.680	1.013	0.00000	0.00000	0.972	1.000	1.000 1.000
109.198	1.013	0.03333	0.07342	0.974	1.000	1.000 1.000
107.762	1.013	0.06667	0.14173	0.975	1.000	1.000 1.000
106.369	1.013	0.10000	0.20534	0.977	1.000	1.000 1.000
105.017	1.013	0.13333	0.26465	0.978	1.000	1.000 1.000
103.705	1.013	0.16667	0.32001	0.979	0.999	1.000 1.000
102.431	1.013	0.20000	0.37173	0.981	0.999	1.000 1.000
101.194	1.013	0.23333	0.42010	0.982	0.999	1.000 1.000
99.991	1.013	0.26667	0.46539	0.983	0.998	1.000 1.000
98.821	1.013	0.30000	0.50783	0.985	0.998	1.000 1.000
97.684	1.013	0.33333	0.54763	0.986	0.997	1.000 1.000
96.578	1.013	0.36667	0.58499	0.987	0.996	1.000 1.000
95.501	1.013	0.40000	0.62010	0.988	0.995	1.000 1.000
94.452	1.013	0.43333	0.65310	0.989	0.995	1.000 1.000
93.431	1.013	0.46667	0.68416	0.990	0.994	1.000 1.000
92.436	1.013	0.50000	0.71341	0.991	0.993	1.000 1.000
91.466	1.013	0.53333	0.74097	0.992	0.991	1.000 1.000
90.521	1.013	0.56667	0.76696	0.993	0.990	1.000 1.000
89.599	1.013	0.60000	0.79149	0.994	0.989	1.000 1.000
88.701	1.013	0.63333	0.81464	0.995	0.988	1.000 1.000
87.824	1.013	0.66667	0.83651	0.996	0.986	1.000 1.000
86.969	1.013	0.70000	0.85719	0.997	0.984	1.000 1.000
86.134	1.013	0.73333	0.87673	0.997	0.983	1.000 1.000
85.319	1.013	0.76667	0.89523	0.998	0.981	1.000 1.000
84.524	1.013	0.80000	0.91273	0.998	0.979	1.000 1.000
83.747	1.013	0.83333	0.92930	0.999	0.977	1.000 1.000
82.989	1.013	0.86667	0.94500	0.999	0.974	1.000 1.000
82.248	1.013	0.90000	0.95987	1.000	0.972	1.000 1.000
81.525	1.013	0.93333	0.97397	1.000	0.969	1.000 1.000
80.819	1.013	0.96667	0.98733	1.000	0.967	1.000 1.000
80.129	1.013	1.00000	1.00000	1.000	0.964	1.000 1.000



Data manually entered into Excel

110.680	0.000	0.000
109.198	0.033	0.070
107.762	0.067	0.142
106.369	0.100	0.205
105.000	0.133	0.265
103.700	0.167	0.320
102.400	0.200	0.372
101.200	0.233	0.420
100.000	0.266	0.465
98.800	0.299	0.508
97.700	0.333	0.548
96.600	0.366	0.585
95.500	0.399	0.620
94.500	0.433	0.653
93.400	0.466	0.684
92.400	0.499	0.713
91.500	0.532	0.741
90.500	0.566	0.767
89.600	0.599	0.791
88.700	0.632	0.815
87.800	0.666	0.837
87.000	0.699	0.857
86.100	0.732	0.877
85.300	0.766	0.900
84.500	0.799	0.913
83.700	0.832	0.929
83.000	0.865	0.945
82.200	0.899	0.960
81.500	0.932	0.973
80.800	0.965	0.987
80.100	0.999	1.000



APPENDIX I

CHEMCAD 6.0 BASICS

NAVIGATING

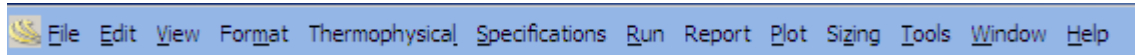
FILE HANDLING

USER COMPONENT DEFINITION

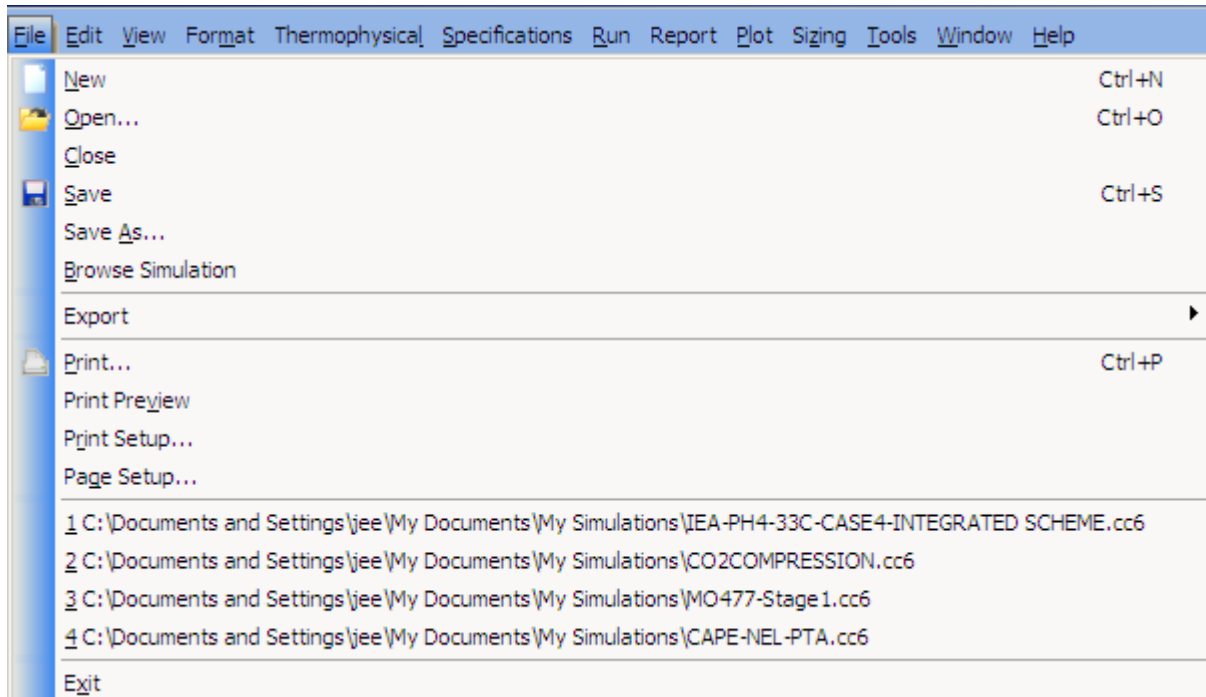


MENU BAR COMMANDS

The main menu bar gives access to all the commands required to drive CHEMCAD.
The main menu bar is as shown below:



Commands available on the File menu are

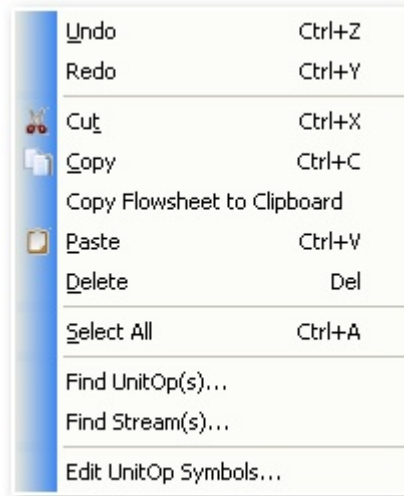


A useful feature worth noting is that any of the recent simulations listed above Exit can be opened directly from here which is very useful if working between several simulations.

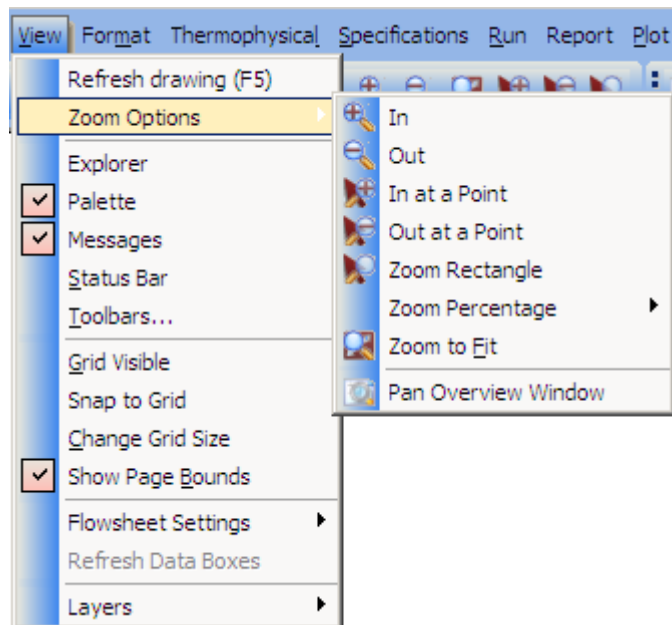


MENU BAR COMMANDS

Commands available on the Edit menu are



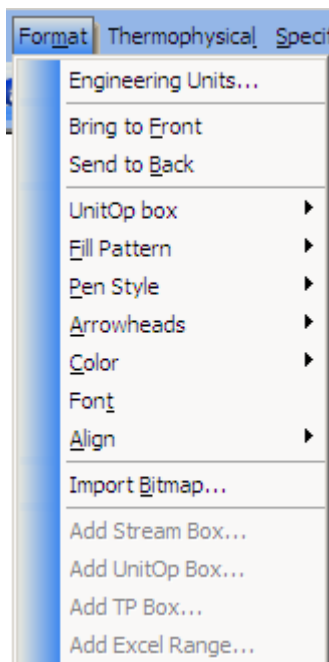
Commands available on the View menu are



The Refresh Data Boxes command updates the contents of all data boxes in the simulation. Select this command after running the simulation to ensure that the data boxes display the current results.

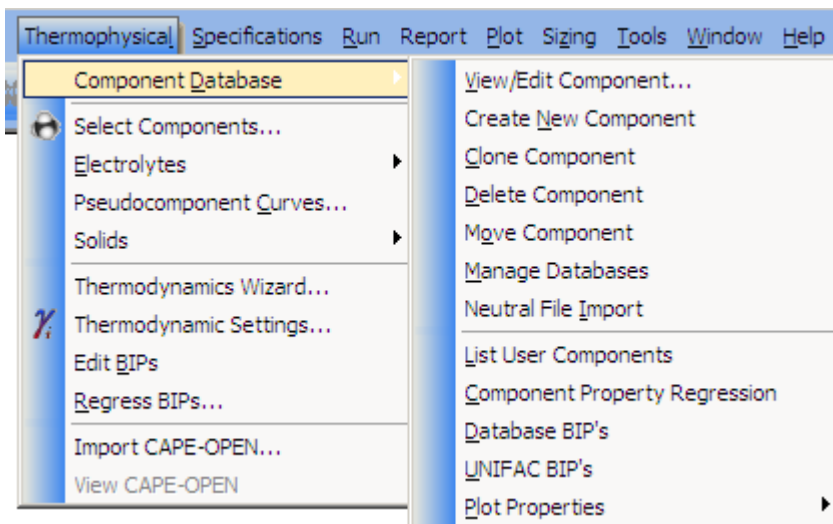
MENU BAR COMMANDS

Commands available on the Format menu are



This is where you set up the engineering units for the simulation. You can also customise the look of the text, lines, and shapes that you use on the flowsheet. The Import Bitmap command enables you to add a logo or other image to your flowsheet, and the bottom section of this menu includes commands for adding various types of data boxes.

Commands available on the Thermophysical menu are

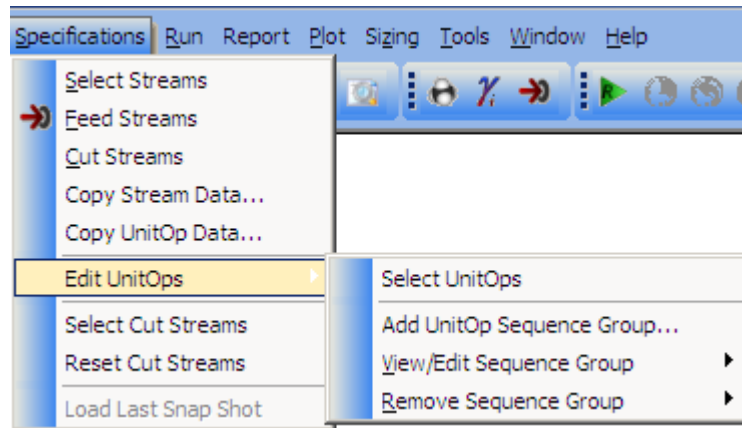


Refer to User Added Components later for more on this menu.

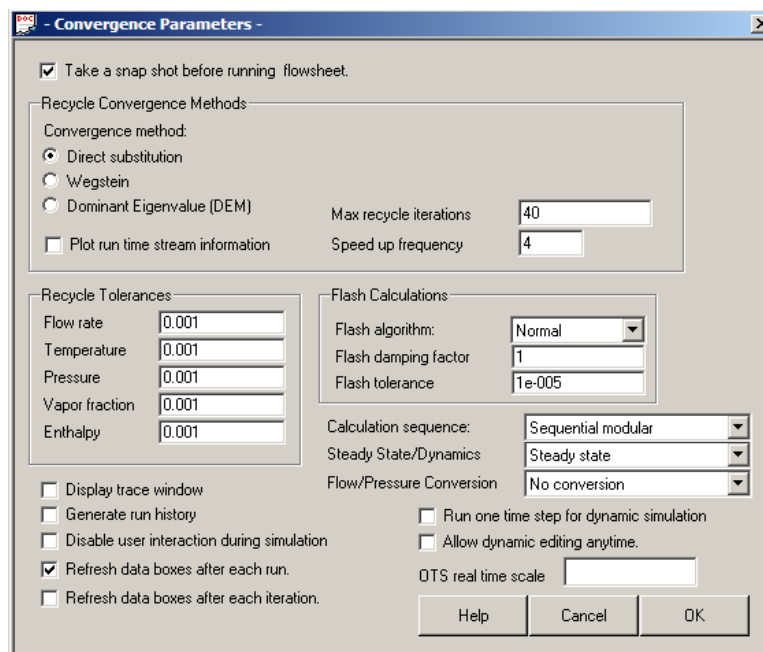
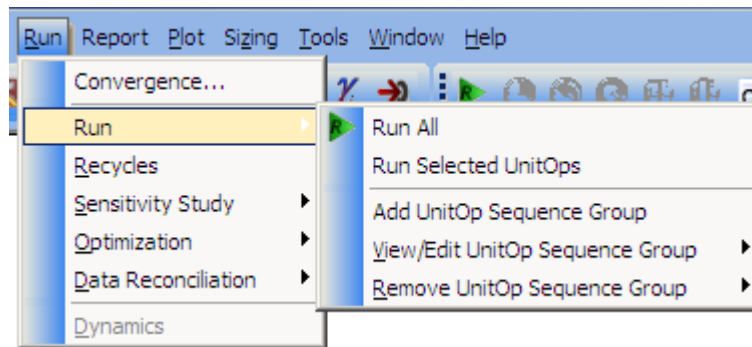


MENU BAR COMMANDS

Commands available on the Specifications menu are



Commands available on the Run menu are

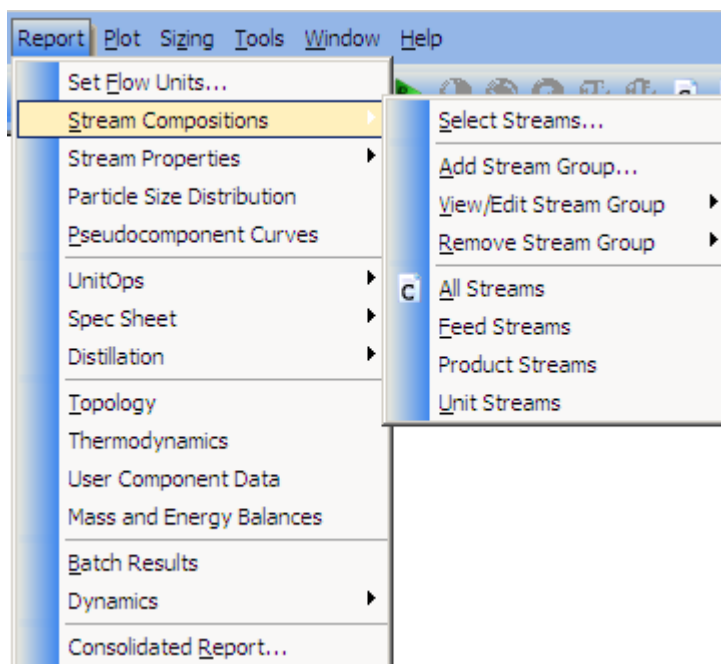


The simulation conditions are set here. This covers calculation sequence methods, steady state or dynamic convergence method, and recycle tolerances.

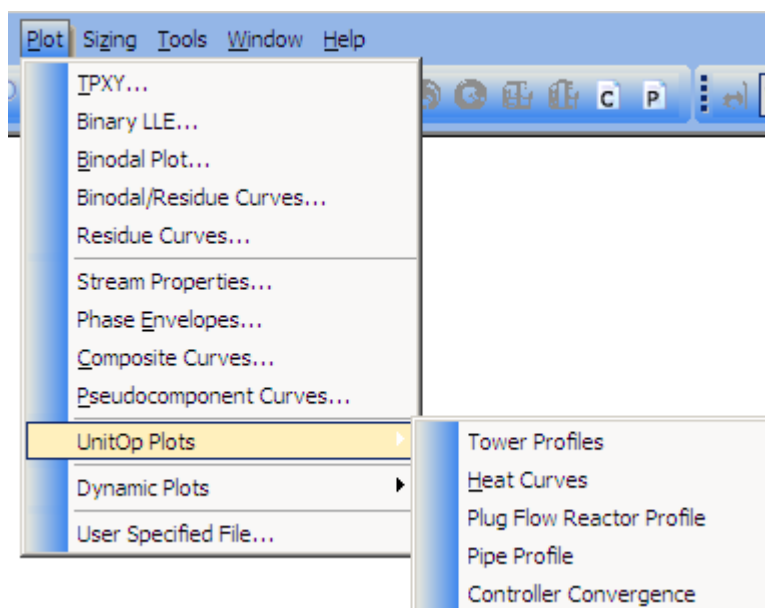


MENU BAR COMMANDS

Commands available on the Report menu are



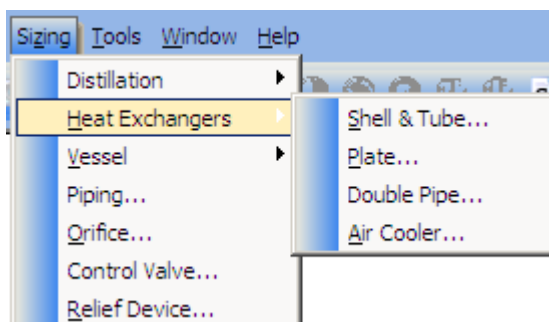
Commands available on the Plot menu are



Each plot that you create resides in a tabbed window that you can leave open until you close the simulation. You can customise each open plot and transfer plot data directly to Excel. The menu shown here is for a simulation running in dynamic mode, as the Dynamic Plots menu item is not shadowed.

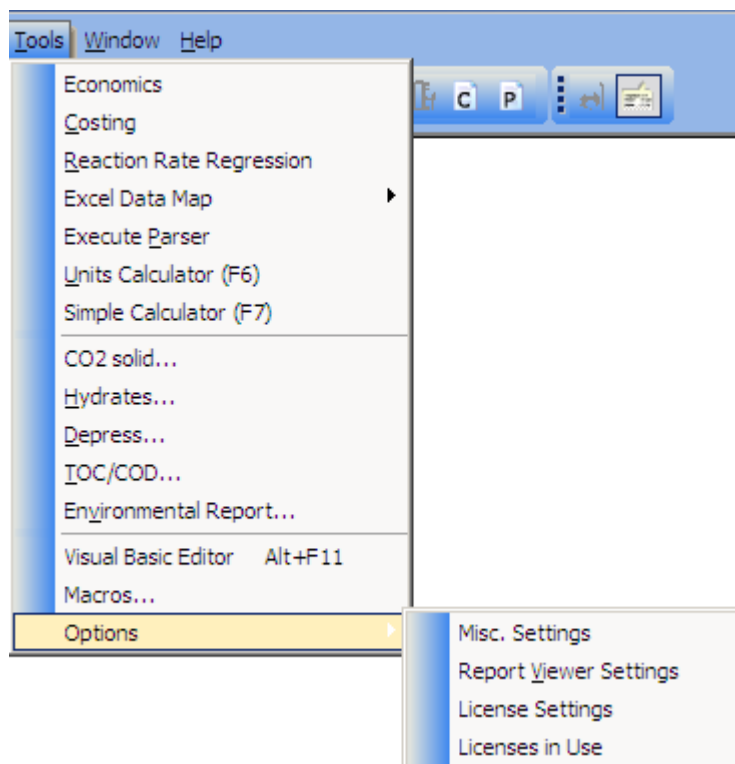
MENU BAR COMMANDS

Commands available on the Sizing menu are



The sizing facility allows you to size flowsheet pipes, valves, and orifice plates using the model stream data for the stream selected. Relief devices are sized using stream data, but caution must be used to ensure conditions are applicable to the relief condition being studied.

Commands available on the Tools menu are



Units Calculator is available using function key F6.

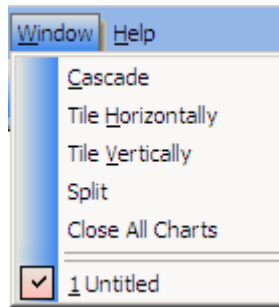
Excel Data Mapping provides a powerful feature for transferring data between the CHEMCAD model and Excel. This feature can be used for customising reports or enhancing modelling capabilities.

The Options menu gives access to the license parameters.

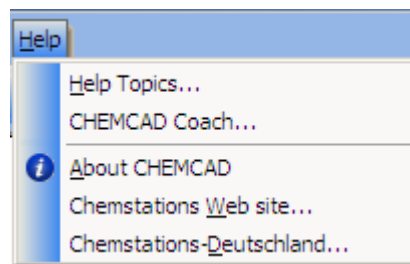


MENU BAR COMMANDS

Commands available on the Window menu are



Commands available on the Help menu are



Coach provides the new user with a simple to follow introduction to CHEMCAD.

FUNCTION KEYS

- F1 Opens CHEMCAD Help
- F6 Opens units calculator; if in a data entry field with specified units, opens at applicable units calculator
- F7 Opens simple calculator



USING THE TOOLBAR BUTTONS

The toolbar shortcut buttons are shown below with a brief description.



File control buttons



- | | | |
|---|--------|---|
| 1 | New: | Opens a window to begin a new simulation |
| 2 | Open: | Opens an existing simulation |
| 3 | Save: | Saves the currently open simulation |
| 4 | Print: | Prints (or plots) the current display or output |
| 5 | About: | Indicates CHEMCAD version |

Editing buttons



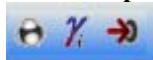
- | | | |
|---|--------|---|
| 6 | Cut: | Removes selected portions of the flowsheet and copies them to clipboard |
| 7 | Copy: | Copies selected portions of the flowsheet to the clipboard |
| 8 | Paste: | Pastes portions of a flowsheet or symbol from the clipboard |

View control buttons



- | | | |
|----|----------------------|---|
| 9 | Zoom percentage: | Selects the percentage to be used when zooming in and out |
| 10 | Zoom in: | Zooms in a specified percentage on the centre of the flowsheet |
| 11 | Zoom out: | Zooms out a specified percentage from the centre of the flowsheet |
| 12 | Zoom to fit: | Zooms to fit flowsheet to screen |
| 13 | Zoom in at a point: | Zooms in a specified percentage on a user-specified point of the flowsheet |
| 14 | Zoom out at a point: | Zooms out a specified percentage on a user-specified point of the flowsheet |
| 15 | Zoom rectangle: | Zooms in on an area of the flowsheet indicated by a user-drawn rectangle |
| 16 | Pan overview: | Opens and closes the Pan Overview window allowing user to pan the flowsheet |

Flowsheet preparation and specification buttons



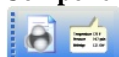
- | | | |
|----|-------------------------|--|
| 17 | Select Components: | Opens component database to allow component selection |
| 18 | Thermodynamic Settings: | Allows selection of K-Value, Enthalpy Value and Transport Properties |
| 19 | Edit Feed Streams: | Allows change of feed stream parameters |

Simulation control buttons



- | | | |
|----|------------------------------|--|
| 20 | Run All: | Runs a steady state simulation |
| 21 | Set Run Time: | Allows selection of "simulated time" and integration time steps for a dynamic simulation |
| 22 | Reset to Initial State: | Resets a dynamic simulation to the initial state (time zero) |
| 23 | Run dynamic simulation: | Starts a dynamic simulation from the initial state (time zero) |
| 24 | Plot Dynamic Streams: | Plots results of a dynamic simulation for specified Streams |
| 25 | Plot Dynamic UnitOps: | Plots results of a dynamic simulation for specified UnitOps |
| 26 | View all stream compositions | |
| 27 | View all stream properties | |

Components and results view buttons



- | | | |
|----|----------------------|---|
| 28 | Component List: | Displays a list of the components currently selected for this flowsheet |
| 29 | Flowsheet Quickview: | Allows streams and UnitOps quick view by pointing with mouse |



FILE TYPES and HANDLING

Types of files:	Simulation files	.CC6
	User component files	.PPDB (for user-added components)
	User symbols (icons)	.SYM
	Export formats	.DXF, .XML

WHERE SIMULATION FILES ARE STORED

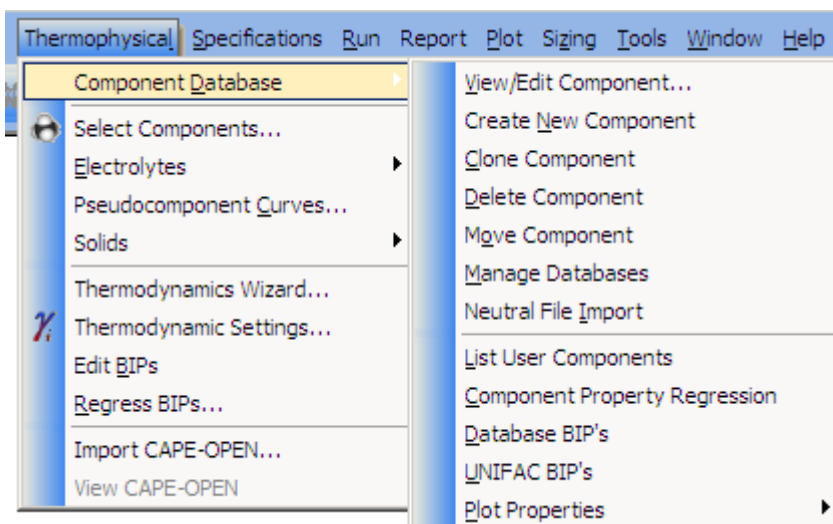
During installation, a directory is created in My Documents called My Simulations. Users can create their own subdirectories within the My Simulations directory.

SAVE AS COMMAND

The Save As command makes a copy of the current simulation and saves it under a new name in a user-specified directory (normally the current directory). The Save As command is located on the File menu.

USER-ADDED COMPONENTS

CHEMCAD allows you to add any number of components to the component database. This permits you to save data for compounds that are not in the database, or to change individual properties for some of the standard components. Additional components can be created in user component databases, which can be shared among multiple CHEMCAD users.



ADDING NEW COMPONENTS

You can define new component properties in one of several ways.

- Estimate from correlations suited for hydrocarbon pseudocomponents
- Estimate using the modified Lydersen method (Joback or UNIFAC)
- Estimate using a combustion solid correlation
- Define an electrolyte

Group Contribution Correlation

The modified Lydersen method estimates the physical properties of individual components from their molecular weight and molecular structure. It may be used to estimate properties for all kinds of compounds, whether they are hydrocarbon, chemical, polar or non-polar. It is necessary that the functional groups in the molecule be in the CHEMCAD database.



The required input is the molecular weight and the compound molecular structure. It is recommended that you input the normal boiling point and specific gravity. This method can estimate these two properties, but other properties generated by the program will be more accurate if you can supply them.

After invoking the Create New Component command, follow this procedure to create a new compound.

Example: Ethyl Alcohol is composed of 1 Methyl group (-CH₃), 1 Methylene (>CH₂) group, and 1 hydroxy group (-OH).

1. Enter a name for the component and any optional entries such as boiling point, specific gravity, and API gravity. For our example, select the correlation method called Group contribution – Joback. Click OK.
2. Fill out the Group Assignments dialog box to include all the functional groups and quantities of each group found in this molecule. Note that there are hydrocarbon groups listed for both ring and straight chain molecules. Click OK.
3. Use the View/Edit Component Data menu to review data generated by the program and to change estimated data with any available experimental values.

Pseudocomponent Correlation

This method is used primarily for hydrocarbons in the form of lumped components. The method is empirical and requires only a minimal amount of information to generate reasonable properties for fractions.

You can use this method for estimating properties for a pure component, or for pseudocomponents that may be constituents of pure hydrocarbon mixtures.

Only the average boiling point and specific gravity of the mixture are required input.

Follow this procedure after selecting Create New Component from the menu.

1. Select Pseudocomponent and click OK.
2. Enter the component name, normal boiling point, and either the specific gravity or API gravity.
3. Choose the correlation for estimating molecular weight. Select from:
 - Chemstations (default)
 - New API
 - Old API
 - Lee Kesler



4. Choose the Critical Properties Method. Select from:
 - Cavett (default)
 - API
 - Lee Kesler
5. Click OK to save data and the program will generate the properties and automatically call up the View/Edit Component Data menu.
6. Use the View/Edit Component Data menu to review data generated by the program and to change estimated data with any available experimental values.

Combustion Solid Correlation

This correlation estimates the physical properties of coal combustion solid components. The required input is the name of the component and the solid element analysis by weight percentage or stoichiometrics. You can optionally provide the net heat value, gross heating value, or solid heat capacity. If you do not provide a heating value, CHEMCAD calculates it based on the component molecular weight.

Electrolyte Correlation

The correlation is meant to be used for the creation of an electrolyte component. It is recommended that you supply the electrolyte state, electrolyte type, molecular weight, electrolyte charge, heat of formation, standard Gibbs of formation, entropy, and heat capacity for the component.

Note: The minimum data required to use a pure component in a simulation includes name, molecular weight, critical temperature, critical pressure, specific gravity, accentric factor, and the coefficients for the ideal gas heat capacity. Some of these values will be estimated by CHEMCAD. Electrolytes and solids have different requirements.

EDITING COMPONENTS

View/Edit Component

Use this command to edit user-added components directly. To edit a standard component, you must first use the Clone Component command to create a user (editable) component.

Clone Component

The Clone Component command calls up the Select Single Component dialog box, where you can choose a component to be copied. The component to be cloned may be either a standard component or one that you defined previously.

Delete Component(s)

This command erases a component from the list of user-defined components. When you select this option, the program will give you a list of the user-added components in the database. It will not present you with ALL the components in the database, as you are not allowed to erase components from the CHEMCAD database.

You can select a component by formula or by typing in its synonym (if available). To select multiple components for deletion at the same time, hold down the [CTRL] key as you click to highlight each component to be deleted. When you have selected the desired component(s), click Delete to remove your selection(s) from the user-added component database.

