

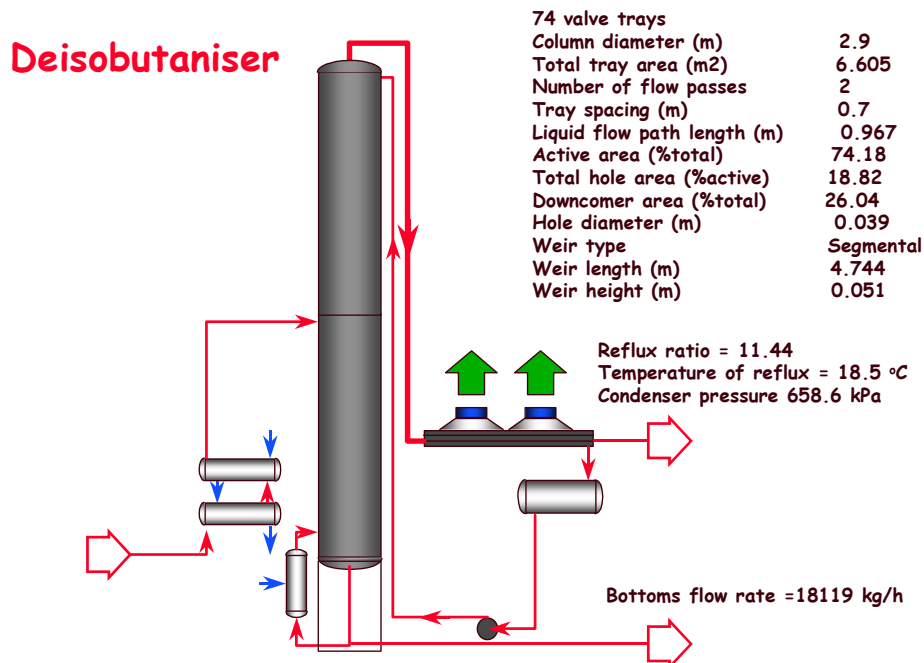
ChemSep 5.0 for Windows!

Harry Kooijman and Ross Taylor

ChemSep is a program for performing multicomponent separation process calculations. *ChemSep* was created specifically for use in courses on thermodynamics and/or separation processes. *ChemSep* integrates flash, the classic equilibrium stage column model and a **nonequilibrium** or **rate-based** column model in one easy to use program.

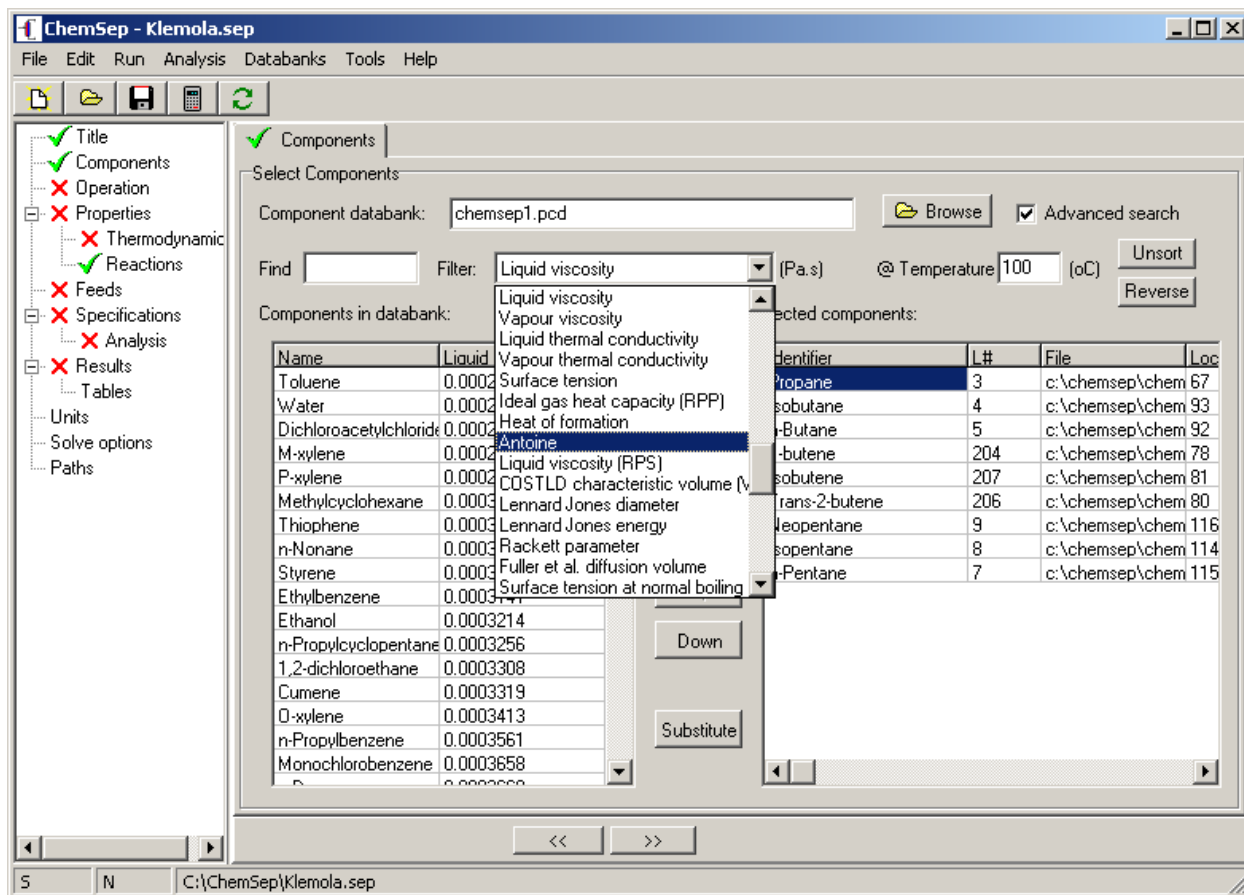
Graphical User Interface: New in Release 5.0 is a graphical user interface for Windows that retains much of the look and feel of the classic *ChemSep* interface. Problem solving is even easier with the new version however; new features make navigation within the interface much faster and the novice is taken through the problem solving process in a natural way. Input may include simple algebraic calculations as well as units. *ChemSep* checks your input, lets you know when each phase of problem setup is complete, and flags potential sources of difficulty before running a simulation.

Nonequilibrium column model: Taking the guesswork out of column simulation, *ChemSep* features a sophisticated nonequilibrium or rate-based model (Krishnamurthy and Taylor, 1985; Taylor and Krishna, 1993). The model in *ChemSep* includes the only available rate-based model for liquid-liquid extraction. The built in *Design Mode* allows the engineer to use proven rate-based technology in preliminary design. *ChemSep* features more column mass transfer coefficient correlations than any other similar model.



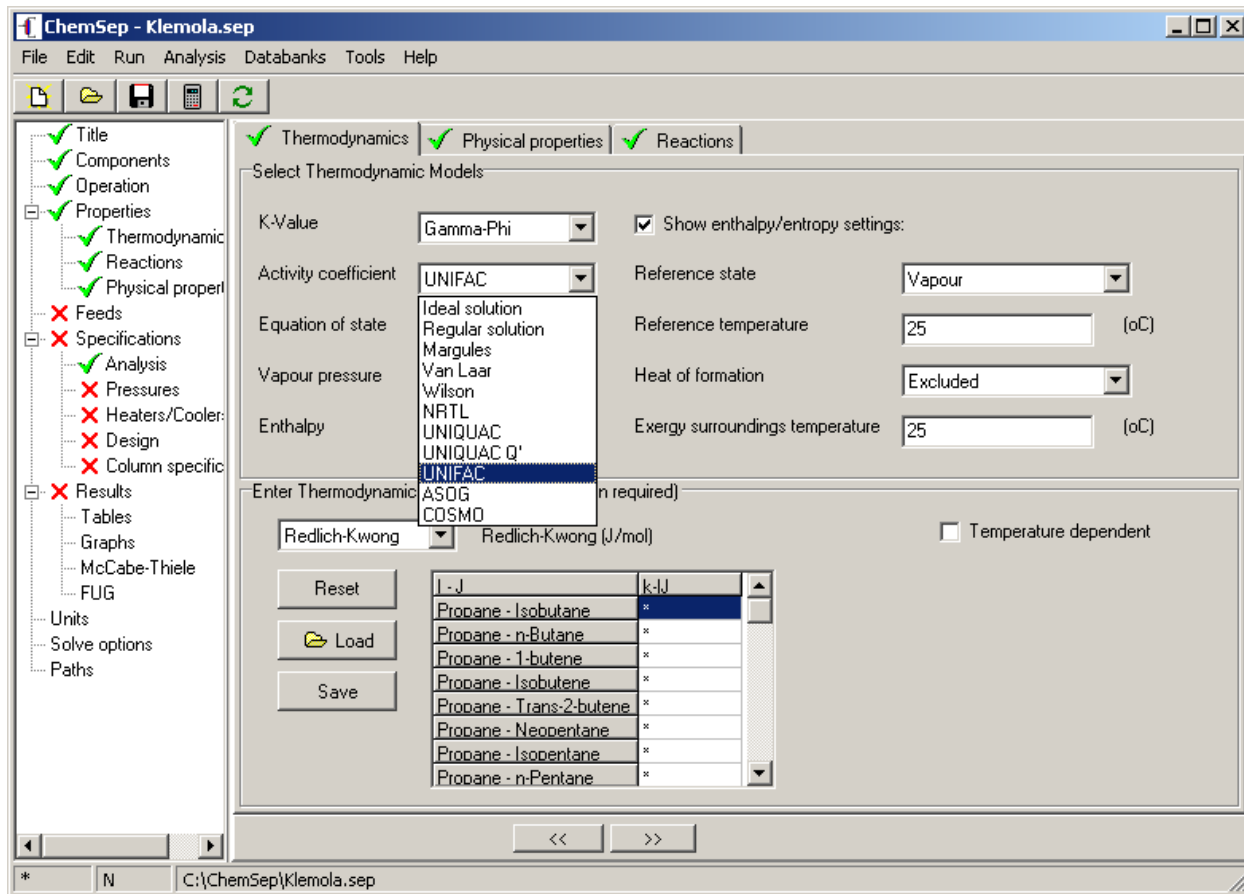
Most of the illustrations that accompany this article are based on our simulation with *ChemSep* of an industrial deisobutanizer described in detail by Klemola and Ilme (1996) and shown schematically above.

Databank: ChemSep comes with a databank of 189 common chemicals. Available at additional cost is a license to the industry standard DIPPR databank of over 1000 chemicals. Users can create their own libraries of physical property data. Selected components appear in the list on the right. The list can be re-ordered and components replaced at a later stage if so desired. If a text string is typed into the *Find* field the list shrinks to include only those components whose names include the text string. Chemical formula, structure, CAS number, or one of 50+ property values including temperature dependant properties can be used to select components. The illustration below shows component selection on the basis of their liquid viscosities at 100 Celcius. The advanced search capability is available only after clicking in the *Advanced Search* checkbox in the top right of the panel.



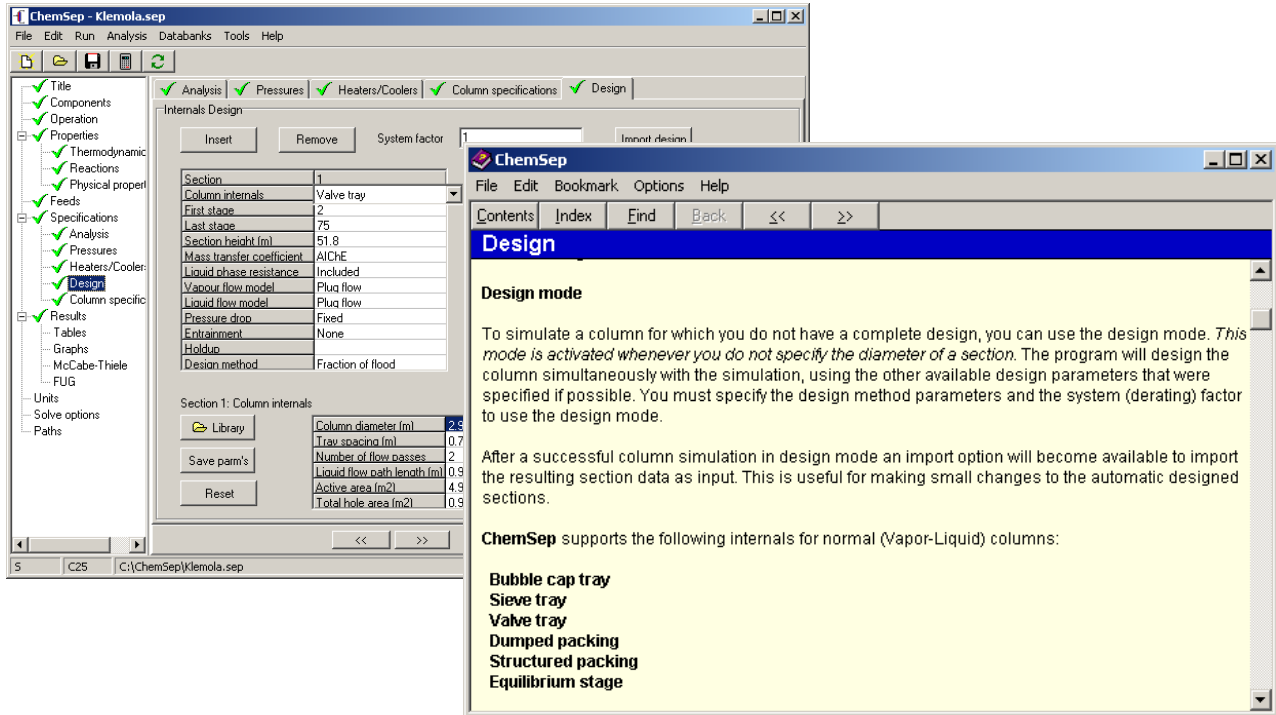
Components can be identified (see the first column of the selected components list on the lower right of the figure above) by their name, formula, or structural formula. It is also possible to simply type any desired text string to be used as the component label within the program.

Thermodynamic and Physical Property Models: ChemSep includes almost all of the most widely used thermodynamic models: 7 K-value models including DECHEMA (modified Raoult's law), Equation of State, and Chao-Seader; 10 Activity coefficient models including UNIFAC; and 8 equations of state including Peng-Robinson and Hayden-O'Connell (with chemical theory). *ChemSep* also includes a large number of physical property models (viscosity, thermal conductivity, surface tension, diffusivity) that are needed in nonequilibrium column modeling.



In this example (and following Klemola and Ilme, 1996) we used the Gamma-Phi approach with the UNIFAC model for liquid phase activity coefficients, the Antoine equation for the vapor pressures and the SRK equation of state for the vapor phase fugacity coefficients. The lower half of the panel remains blank until the user selects a model that requires parameters. Parameters can be typed in by the user or loaded from libraries. The * in the figures indicated that default values are assigned. For the SRK model shown here the default values are zero, for activity coefficient models *ChemSep* will use UNIFAC to estimate any missing parameters. The right hand half of the upper panel is normally blank until the user clicks in the checkbox at the top (as is done here so that the reference state for enthalpy and entropy calculations is displayed so that they can be changed if desired).

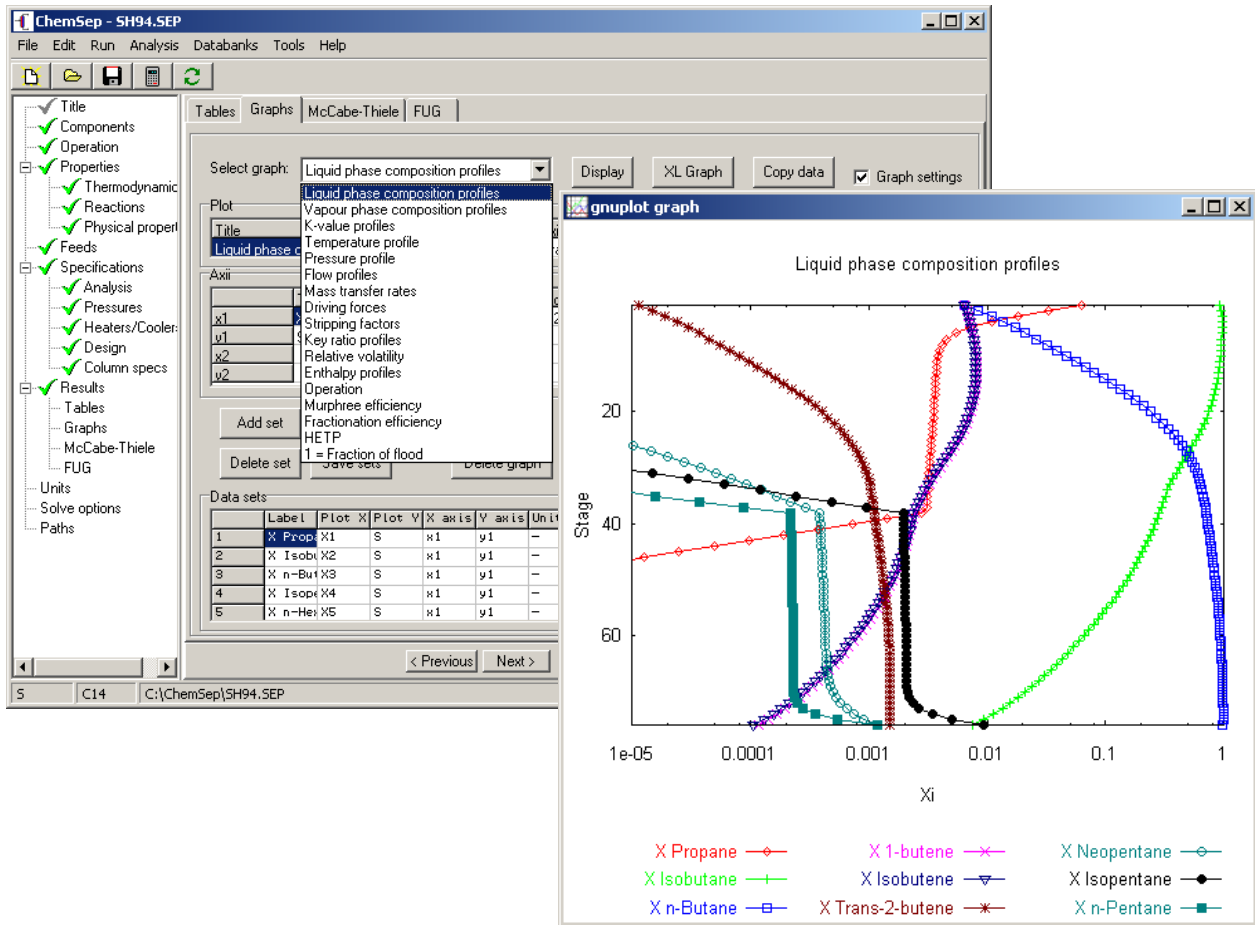
Column Design: For a nonequilibrium simulation we must say something about the type of column. Below is shown the design panel on which the equipment design details for the deisobutanizer are recorded and the help page that proffers advice for the perplexed. Locating the cursor on the field(s) on the top line (Column internals) brings up a pull down list from which the user selects the type of tray or packing (a single column can have many different types of internal; if desired). In addition, a spreadsheet appears at the bottom of the panel in which the design details for that section are recorded. If the diameter is left unspecified (denoted by a *) *ChemSep* enters design mode and the internals are sized during the simulation. *ChemSep* incorporates methods for the simultaneous design of many different kinds of column internal.



ChemSep includes over 40 correlations for mass transfer coefficients in different types of column, as well as 18 different ways to estimate pressure drop and 16 for holdup.

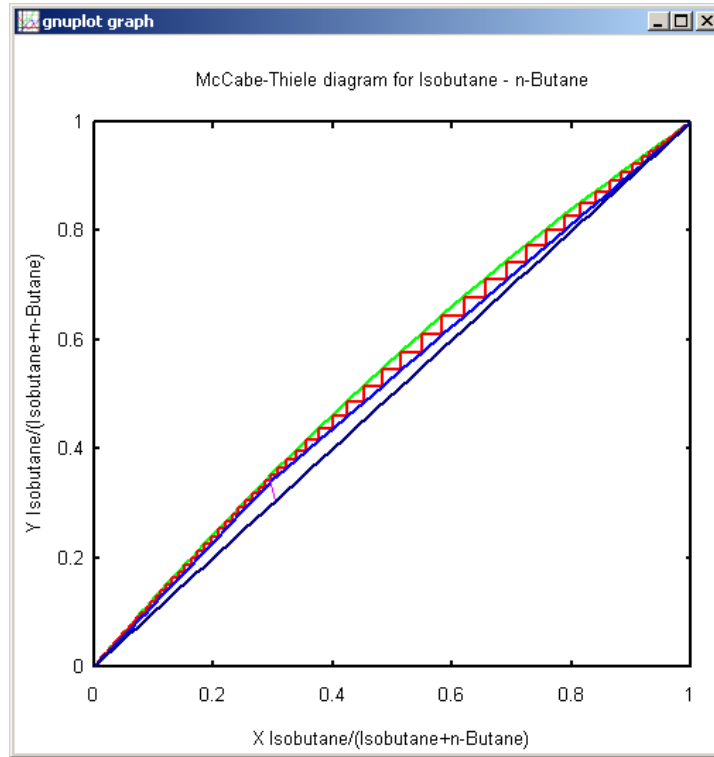
Degrees of Freedom Analysis: *ChemSep* tells you the number of degrees of freedom and identifies how many variables remain to be specified. When all degrees of freedom are satisfied *ChemSep* displays a green checkmark next to all input panels. While any degree of freedom remains to be satisfied *ChemSep* displays a large red X next to the input panels that require attention.

Powerful plotting capabilities: ChemSep has extensive support for plotting almost any kind of column profile including composition, flow, temperature, pressure, K-values, and more (see figure below). The plots are completely configurable. ChemSep uses the Open Source package Gnuplot (for Windows) to display a plot in its own separate window. Except where noted, the plots that appear in this article were created with Gnuplot and pasted directly into the word processor used to create this article. The illustration below shows graph selection in action and the resulting plot. The *Graph settings* checkbox (upper right) allows the user to configure the details of the graph before it is displayed.



Users can design their own plots and include them in the pull-down plot selection list for future use. From the results of a nonequilibrium simulation one can plot profiles of any physical property as well as numerous design-related variables such as froth height in a tray column, approach to flooding, or specific interfacial area (these are just a few of many variables that can be plotted).

McCabe-Thiele Diagrams are a standard feature in *ChemSep* (even for multicomponent systems like the deisobutanizer).

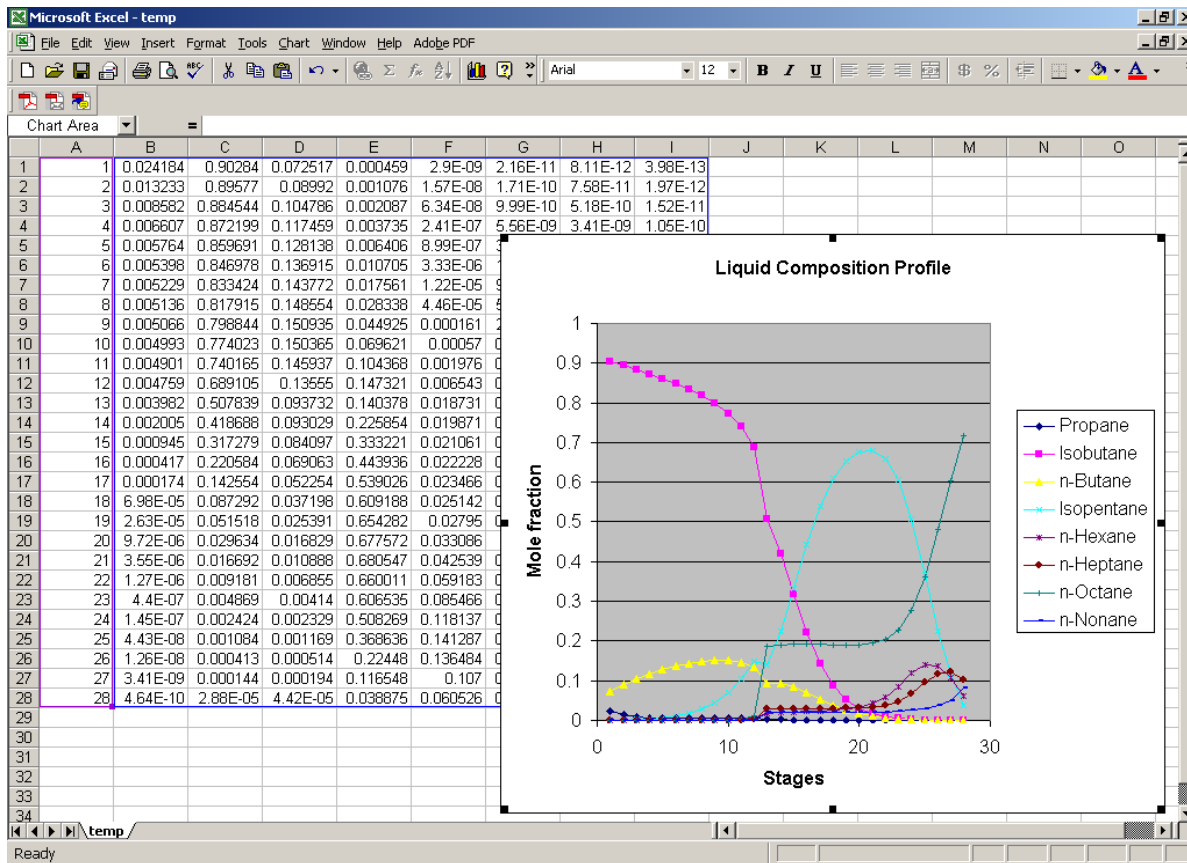


Tabular Output can be viewed in *ChemSep*, or sent directly to text editor such as Notepad or spreadsheet program such as Excel.

The screenshot shows the ChemSep software interface with the 'Tables' window open. The 'Streams' table is selected, showing a list of streams and their properties. The 'Internal design' table is also visible, showing mole fractions for various components.

Stream	Top	Bottom
Stage 1	1	76
Pressure 1	658.6	658.6
Vapour flow 1	0	0
Temperature 1	18.5	60.82
Enthalpy 1	-1.99E+04	-1.481E+04
Entropy 1	2.131E+05	2.519E+05
Mole flow 1	2.476	6.661E-13
Propane Specifications	36.17	0.656
Isobutane Specifications	0.2535	84.54
n-Butane Specifications	0.2495	0.01005
1-butene Specifications	0.2502	0.009261
Isobutene Efficiencies	0.1298	0.0004457
Trans-2-butene	0.1009	9.483E-09
Neopentane	0.8072	1.189E-14
Isopentane	0.1009	7.451E-13
n-Pentane		
Total molar flow	125.8	39.4
Mole fractions (-)		
Propane	0.01969	0.06286
		7.713E-15

Export: Simulation results may be saved in a variety of formats such as text, html and csv. Tables and graphs may be sent directly to Excel (see the buttons *XL Table* and *XL Graph* that sends the data directly to Excel where it can be plotted as shown below for an example from Seader and Henley (1998).



ChemSep-Lite Now Available for Nothing!

A version of *ChemSep* with limited functionality is available for free download from www.chemsep.org/downloads/index.html. That's right, no fee at all, not now, not ever! *ChemSep* Lite is limited to no more than four components, a databank with a limited number of components, no more than 50 stages in a column simulation, and no nonequilibrium model.

Whats Next?

In a subsequent release of *ChemSep* (tentatively scheduled for spring 2005) we plan to build in phase diagrams, property calculations and plots, and residue curve maps. In prior releases of *ChemSep* this functionality was available in the separate program ChemProp.

A CAPE OPEN compliant version will also be available in 2005.

Availability

ChemSep is available for educational use from the CACHE corporation (www.cache.org). For licenses for non-educational use please contact the authors.

Further Information

Additional information about the program can be found at www.chemsep.org. The authors can be contacted at kooijman@chemsep.org and taylor@chemsep.org.

References and Further Reading

The books by Benitez and by Seader and Henley mention *ChemSep* and use it to solve some example problems.

Benitez, J. *Principles and Modern Applications of Mass Transfer*, Wiley, New York, 2002

Klemola, K. and Ilme, J. "Distillation Efficiencies of an Industrial Scale I-Butane/n-Butane Fractionator," *Ind. Eng. Chem. Res.* 35, 4579-4586, 1996

Kooijman, H.A. & Taylor, R. (2001) *The ChemSep Book*, Books on Demand, Norderstedt, Germany (2001) (available from www.cache.org)

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Kooijman, H.A. and Taylor, R. *ChemSep* Release 3.1, CACHE News, 41, 13-19, Fall 1995

Krishnamurthy, R. & Taylor, R. (1985) "A Nonequilibrium stage model of multicomponent separation processes," *American Institute of Chemical Engineers Journal*, 32, 449-465

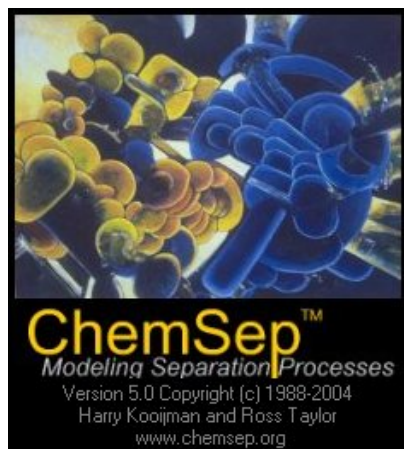
Seader, J.D. and E.J. Henley, *Separation Process Principles*, Wiley, New York, 1998

Taylor, R. and Krishna, R. *Multicomponent Mass Transfer*, Wiley, New York, 1993

Wankat, P.C., *Equilibrium Staged Separations*, Elsevier, New York, 1988.

Final Note

The illustration shown below is the splash screen that is displayed on initial execution of *ChemSep*. The artwork is by Morris Bennett (MA). You can see more of his art at <http://www.chemsep.org/downloads/art/art.html>. Bennett writes:



My paintings are a combination of many different art styles synthesized with directly observed forms in nature. Music and other sounds are also among my influences. I exploit the human tendency to project inner states on outer forms by using my academic training to paint non-representational images.

Guided primarily by intuition, I create my paintings from all four edges, thus most of my work can be rotated to reveal completely different imagery.

My intention is to invite people to explore the worlds I have created and to come away with an increased, though not necessarily definable, understanding of reality.