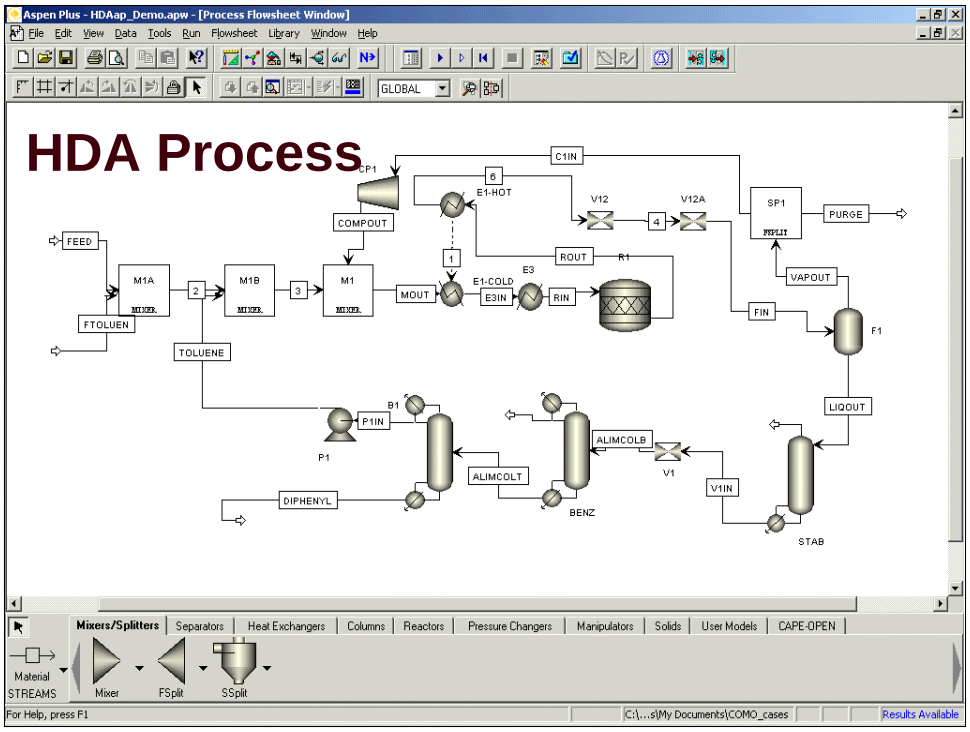
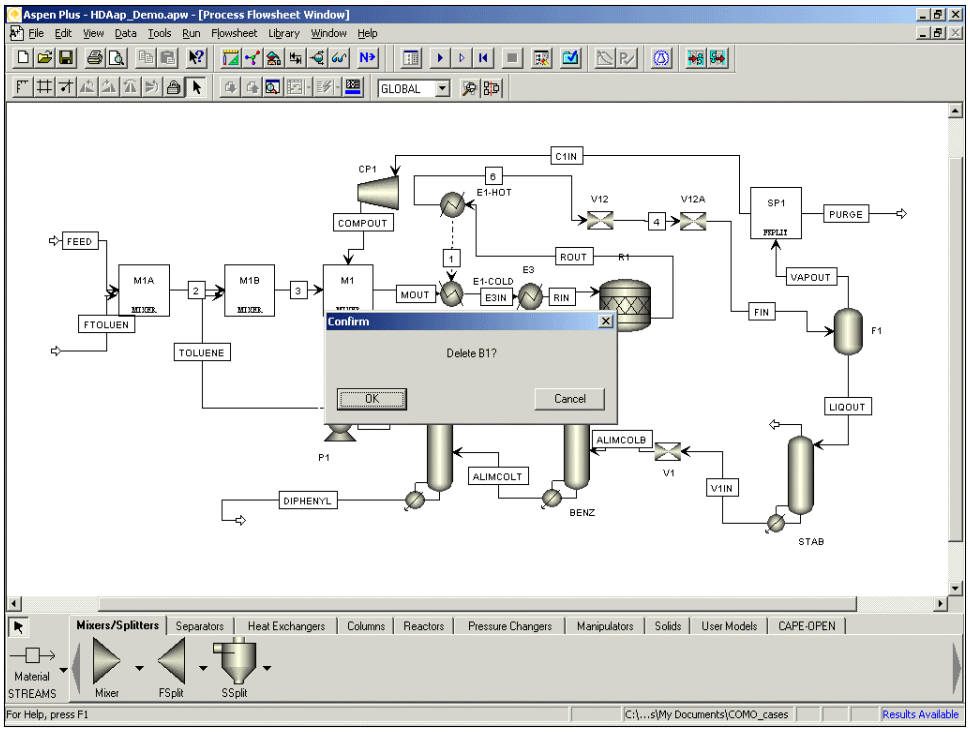
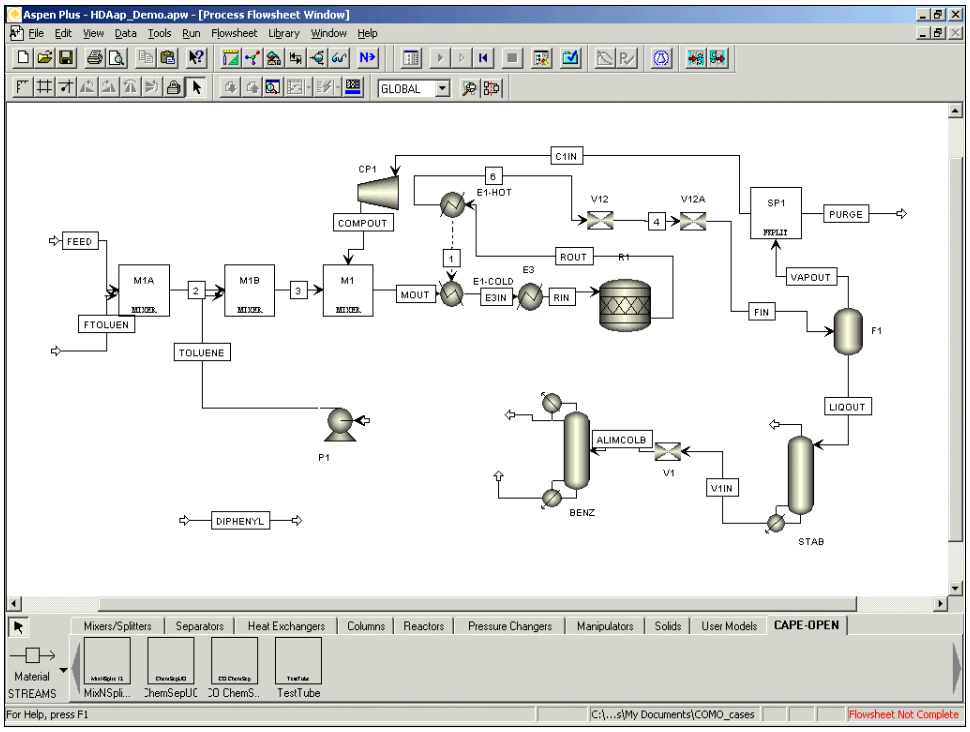


This document shows how it is possible to use **ChemSep** as a unit operation model in a CO compliant flowsheet simulation executive (COSE). In this illustration, we see the well known HDA process as implemented in Aspen Plus.

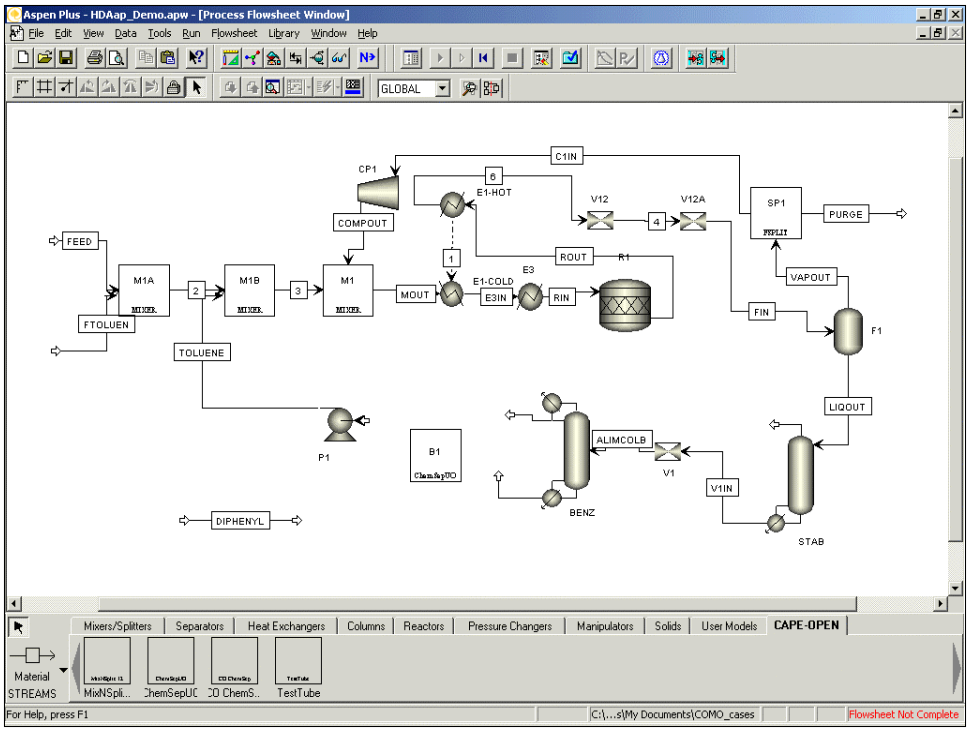
The HDA process contains a number of units that could be modeled using CO **ChemSep**. This includes the flash unit (far right., center), and three distillation columns (lower half). In this illustration we will replace the third distillation column.



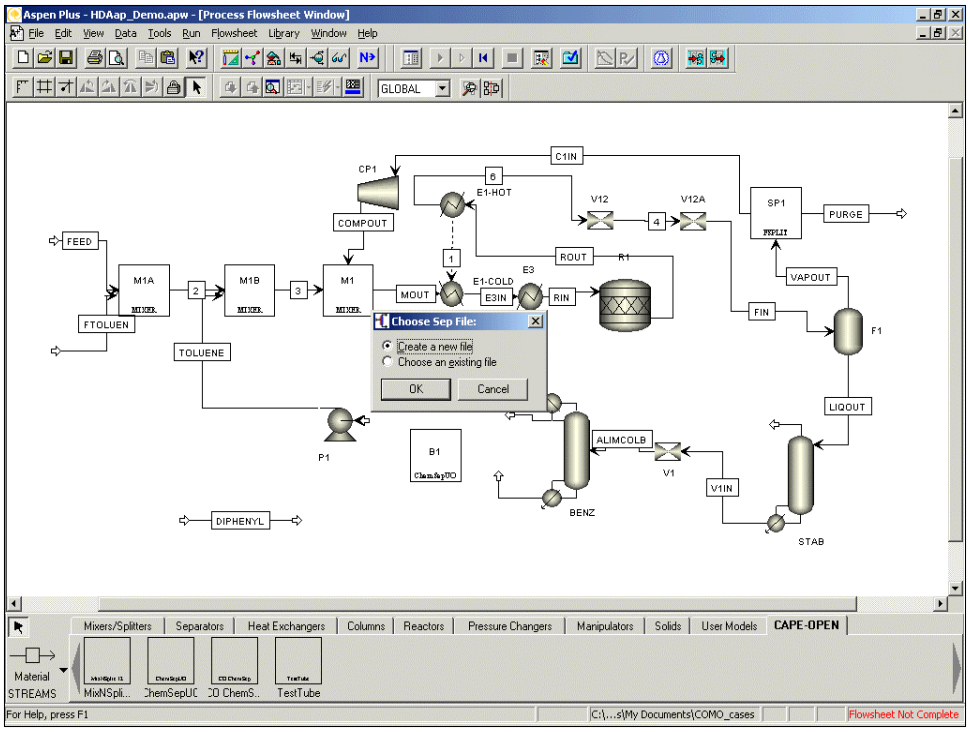
Click on column 3 and press the delete key to remove the Aspen Plus column model.



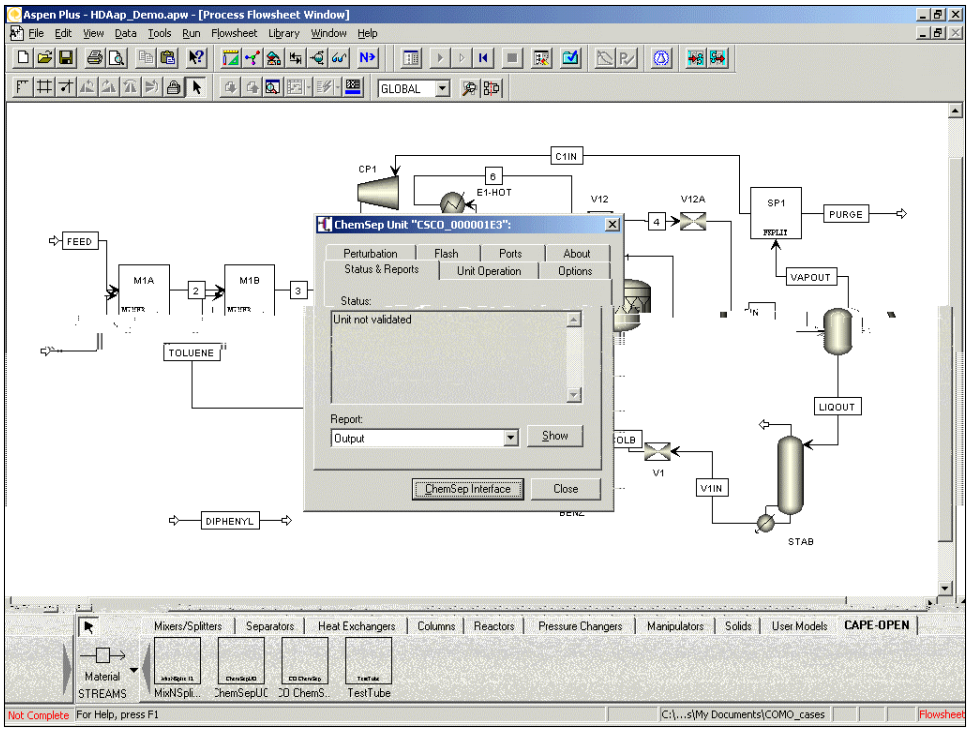
In this illustration we see that Column 3 has vanished from the flowsheet.



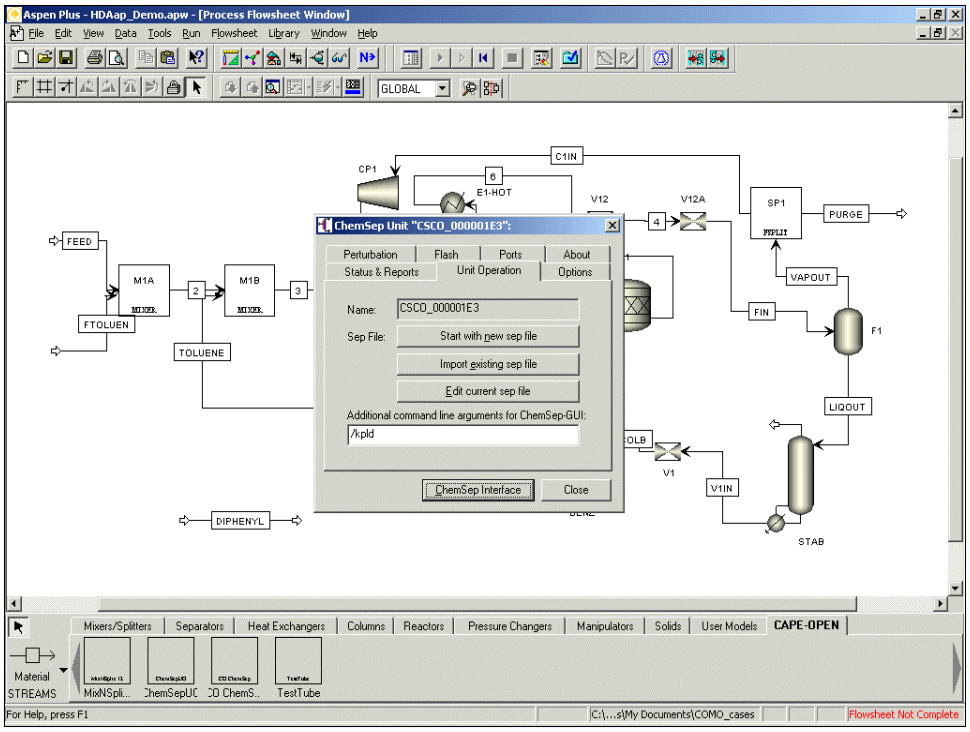
Drag a ChemSep UO from the collection of CAPE OPEN units.



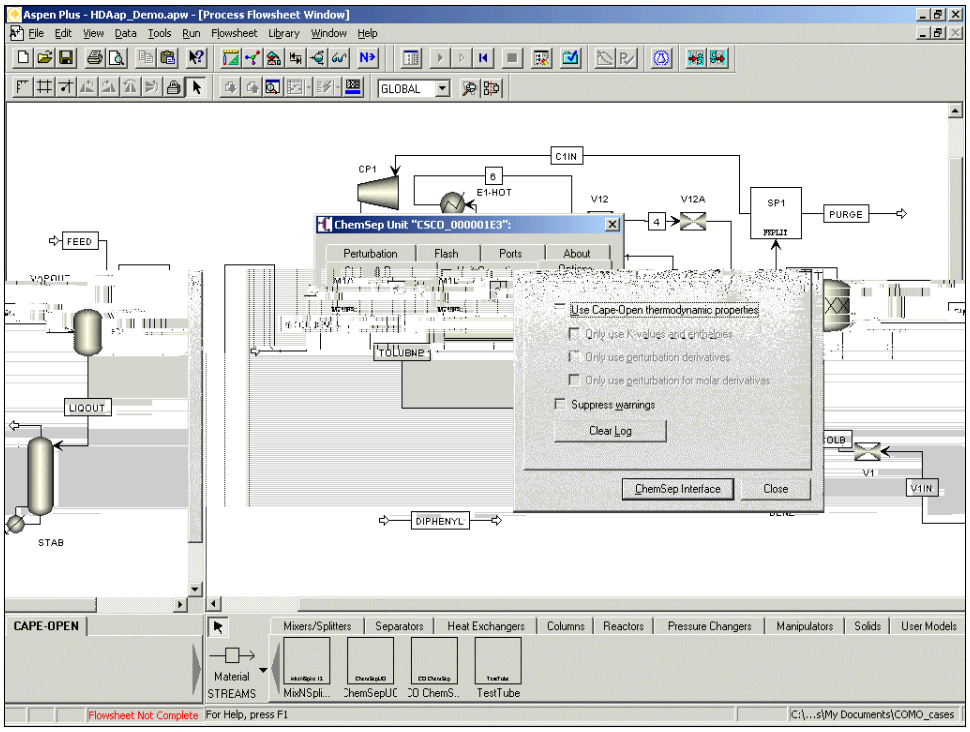
Double click on the **ChemSep** UO and you will be asked if you wish to create a new file or work with an existing model. In this case we select new file.



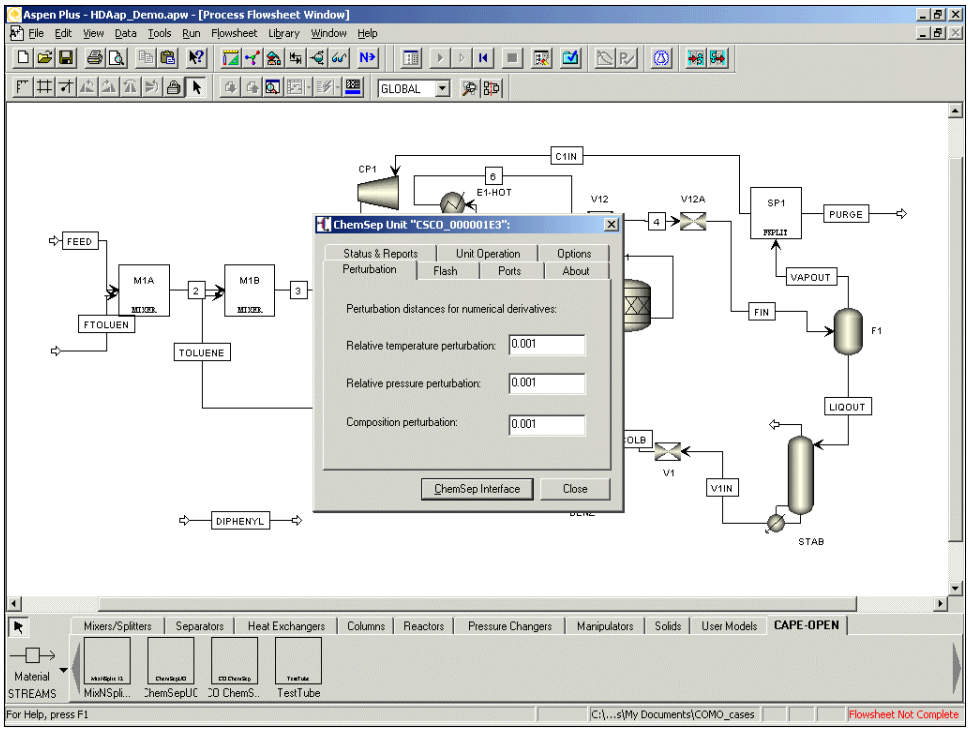
The **CO ChemSep** GUI appears. Note the button to launch the **ChemSep** GUI. But first, just to show off, we will take a look at the various tabs that can be seen on this page beginning with this one; the Status and Report tab that shows that the unit has not been validated.



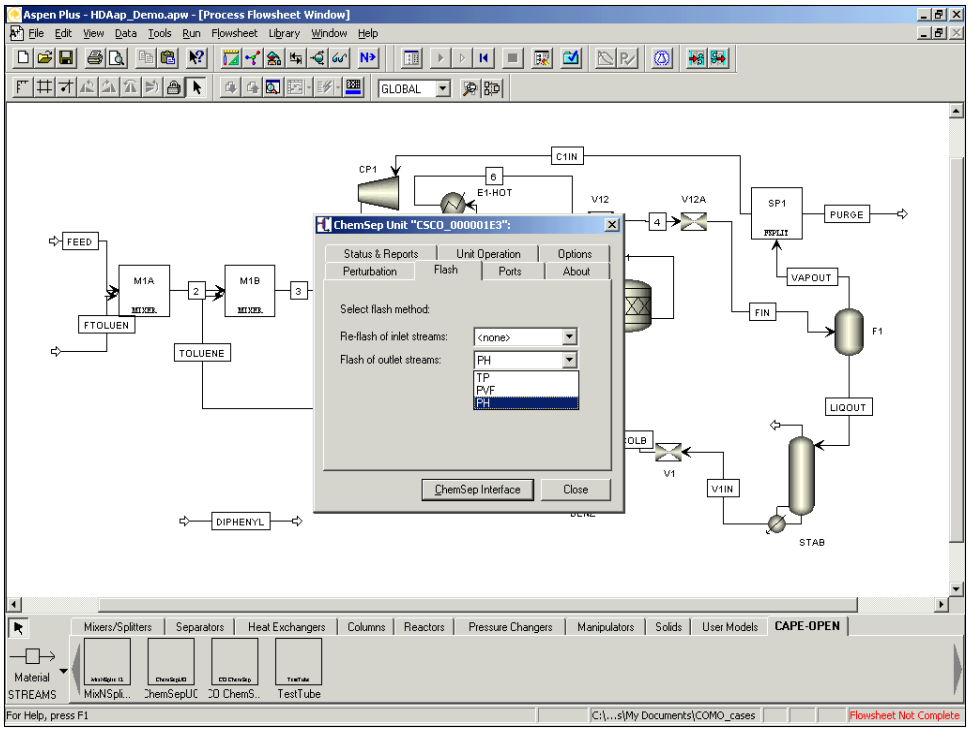
The Unit Operation tab provides buttons that allow you to start a new (Chem)Sep file, import an old one, or edit the current file.



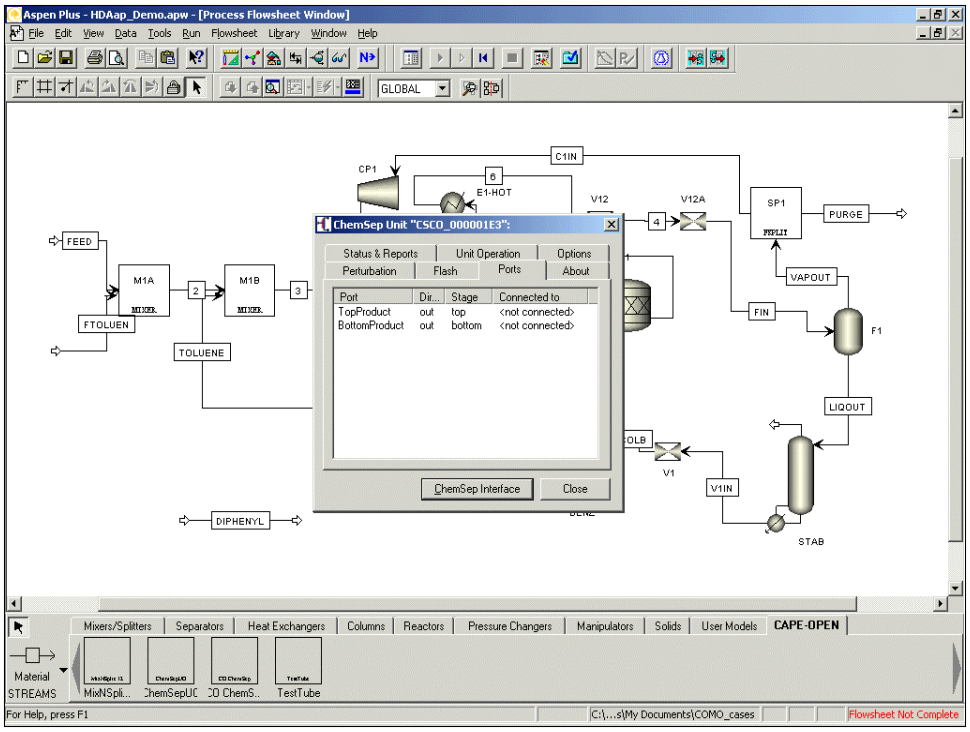
On the Options panel you may choose to use a CAPE OPEN thermodynamic property package or the property calculations that are built into ChemSep. If CO properties are selected you will be given the option for ChemSep to use only CAPE OPEN thermodynamic properties (K-values and enthalpies) – in which case ChemSep uses its own internal methods for estimating other properties. You also will have the option to estimate partial derivatives of thermodynamic properties numerically (in case the COSE does not provide correct derivative information).



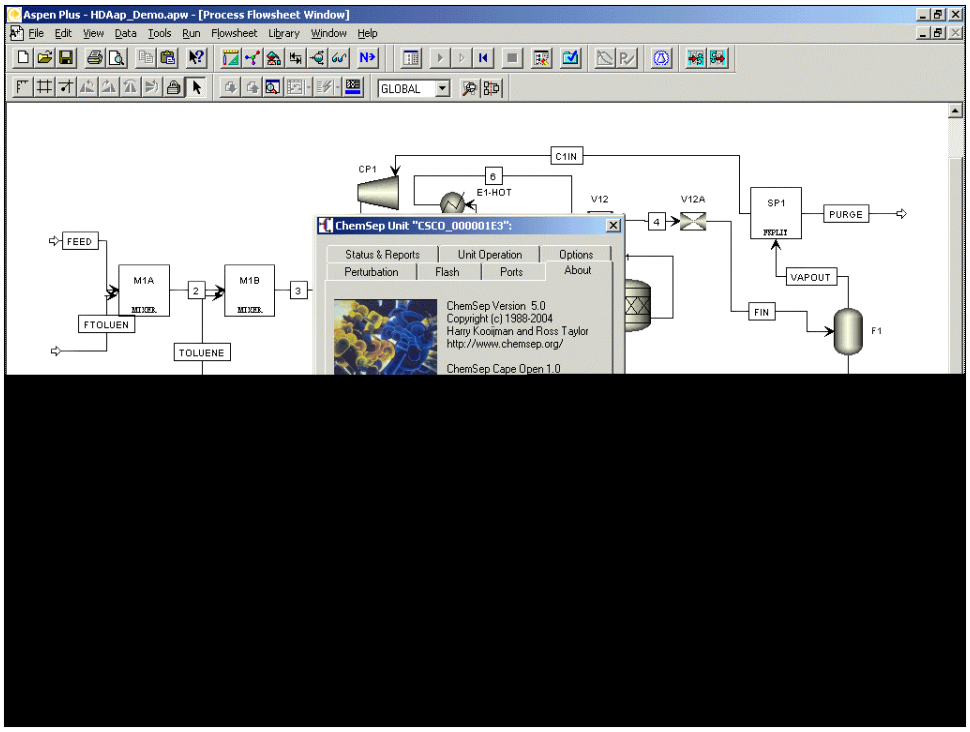
The size of any perturbation to temperature, pressure and composition to use while estimating derivatives may be entered on the Perturbation panel. The default values are 0.001 times the absolute values of the variable.



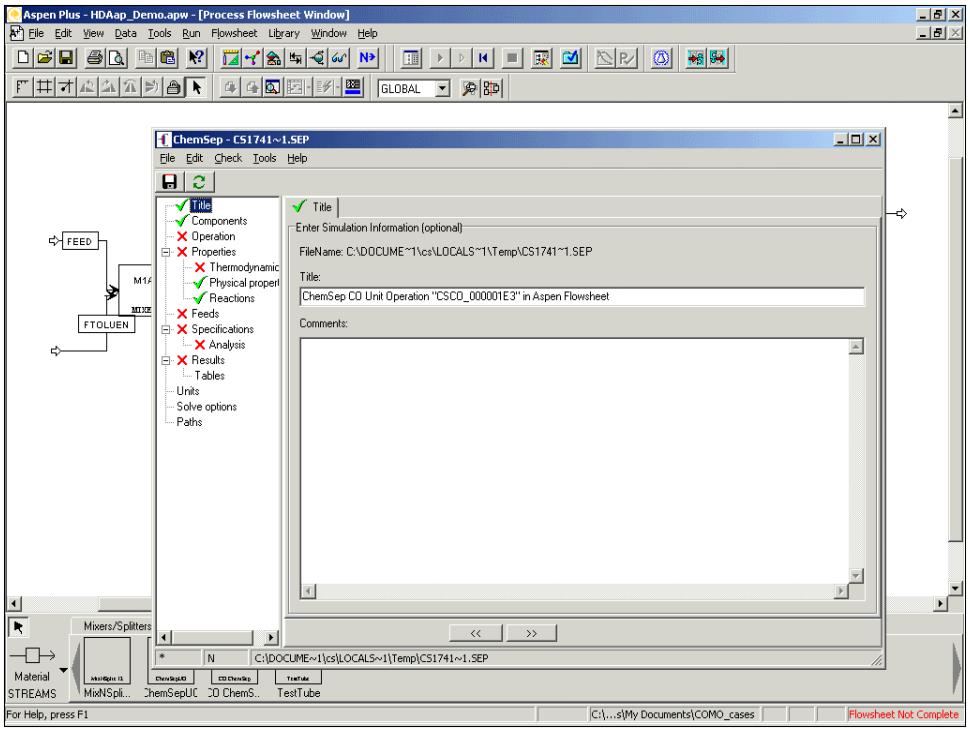
On the Flash panel you may choose to have inlet and exit streams flashed using CO thermodynamics (normally you should do this). The type of flash calculation is specified on this panel.



The Ports panel shows the input and output streams and to which stream on the flowsheet they are connected. At this stage none of the streams are connected.

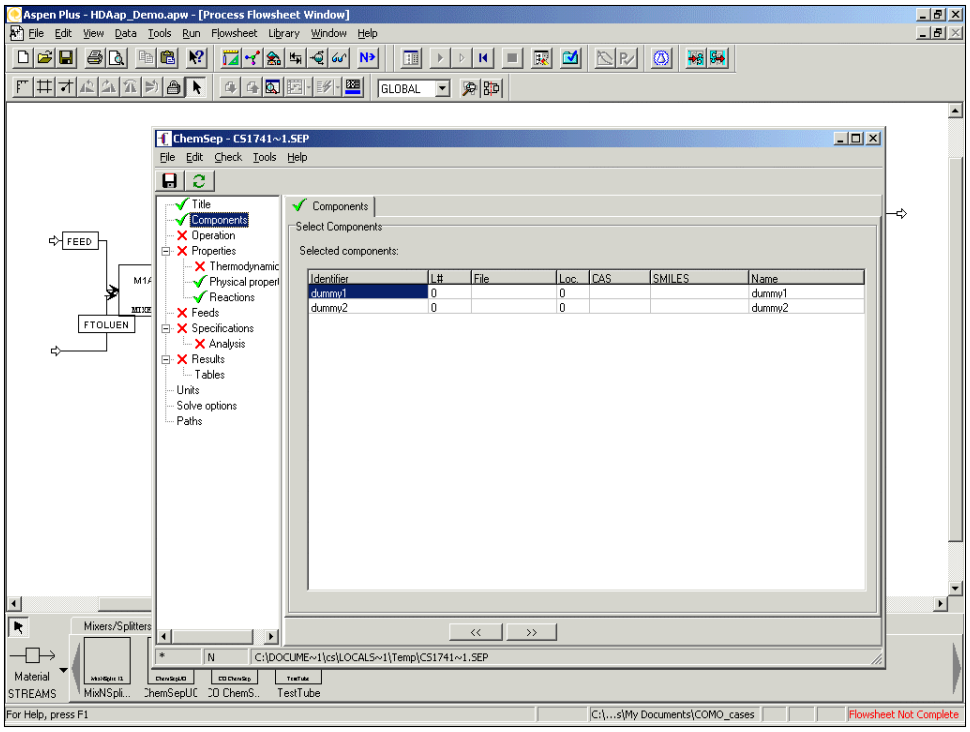


This panel is the equivalent of the “about” panel that accompanies most Windows programs.

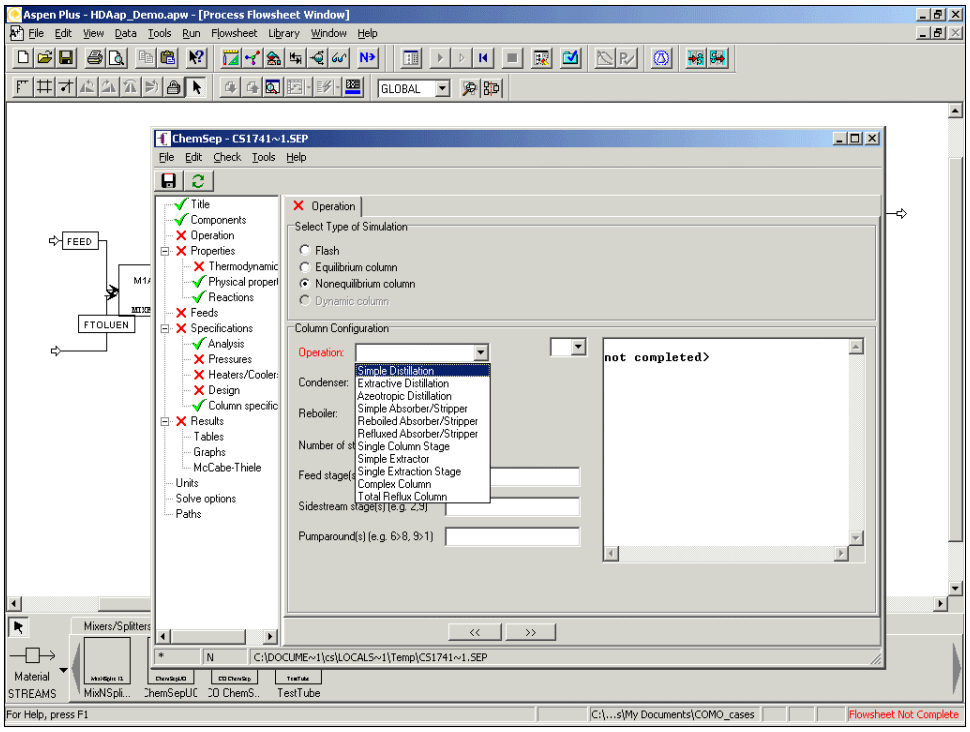


Click on the **ChemSep** Interface button to launch the **ChemSep** GUI.

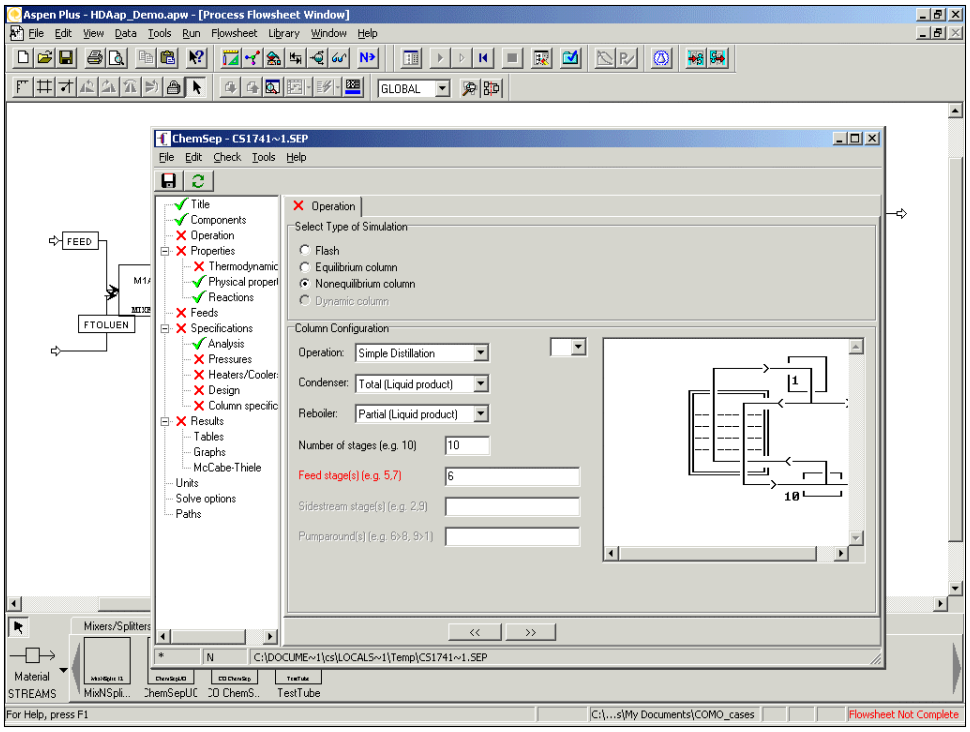
The tree on the left hand side mimics the main level menus of prior versions of **ChemSep**. The red X to the left of most the branches of the tree indicate that input is incomplete and no results are available (in this case that is hardly surprising since we have not done anything yet).



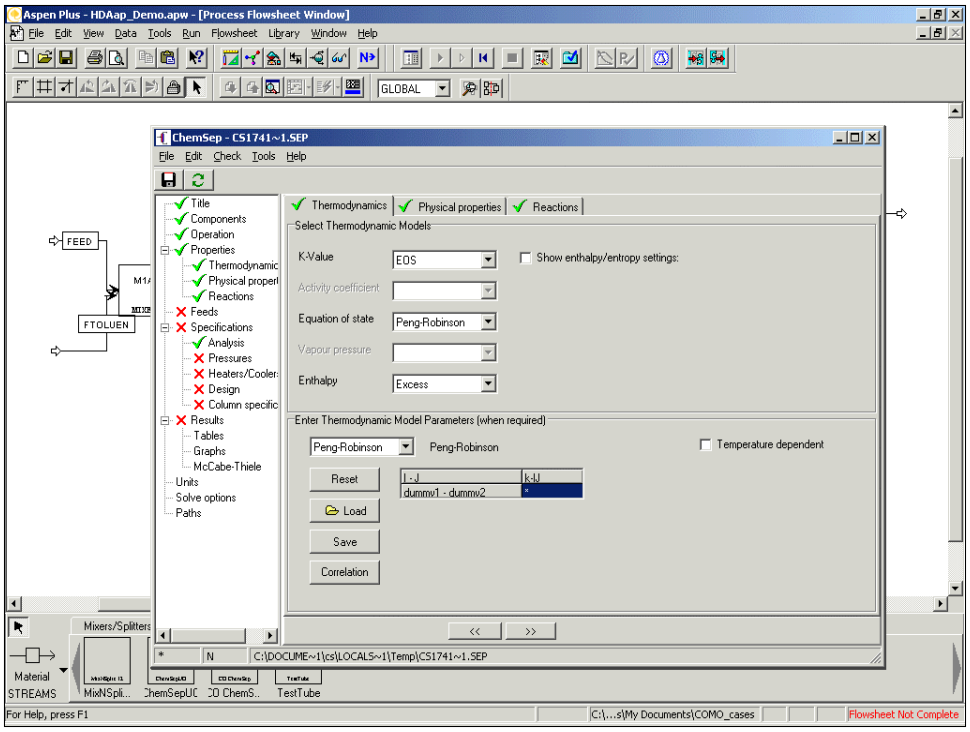
On the components panel we see that no components are available to **ChemSep**. This is because the current version of Aspen Plus does not make component identities available at this stage. A future version of Aspen Plus will make component identities available.



The operation panel shown above is largely blank until the user selects a model from the list shown in the upper one third. **ChemSep** is mainly a single column simulation program with the added capability of modeling single equilibrium flashes.

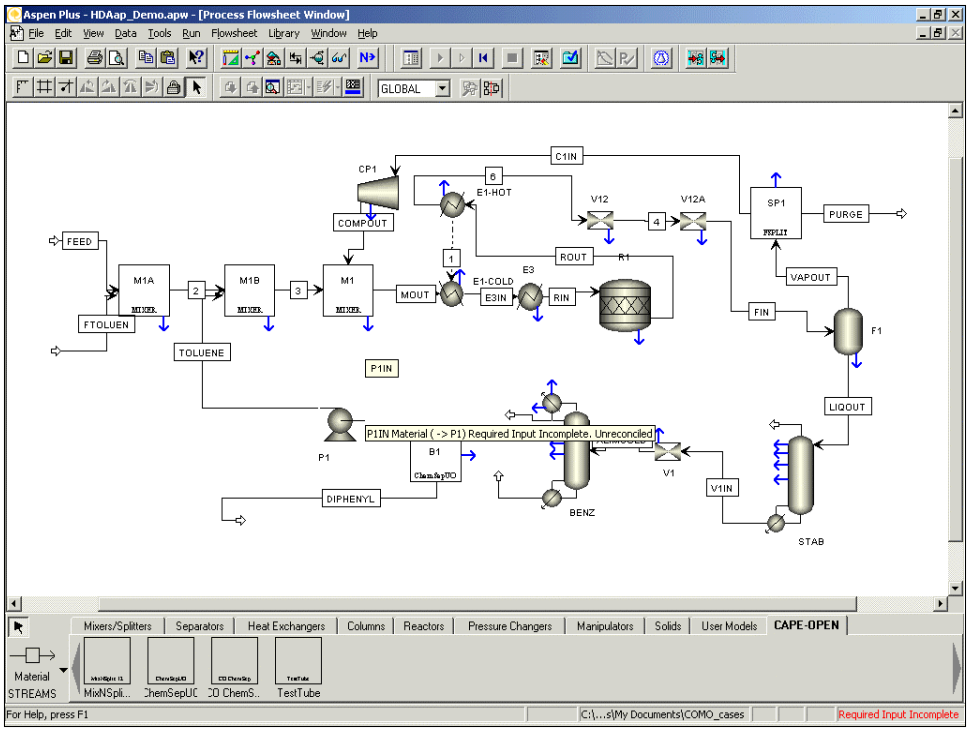


If a column (equilibrium or nonequilibrium) is to be modeled the user must provide some details of the column configuration: what kind (if any) of condenser and reboiler is present, how many stages are to be modeled and the stage location of any feeds, sidestreams and pumparounds. A schematic diagram of the column appears in the window on the right. The feed stage has not yet been set which is why that item appears in red.

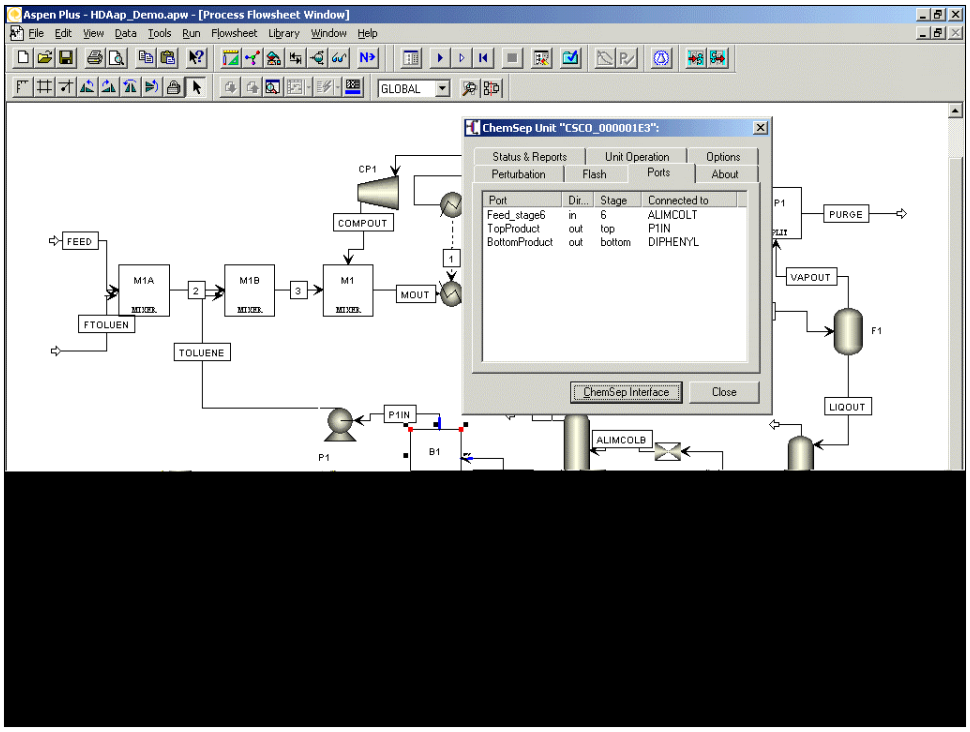


We may use ChemSep's own thermodynamic property routines if we wish. In this case the property models must be selected.

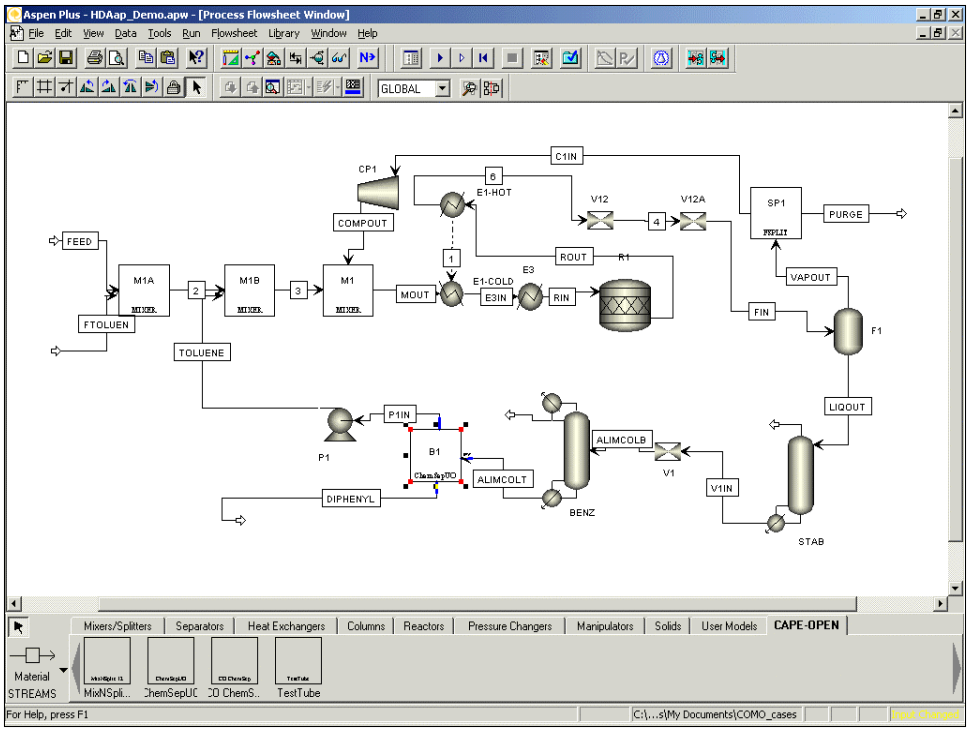
The lower half of the panel remains blank until the user selects a model that requires parameters. Parameters can be typed in by the user or loaded from libraries. The * in the figures indicated that default values are assigned. For the PR model shown here the default values are zero, for activity coefficient 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).



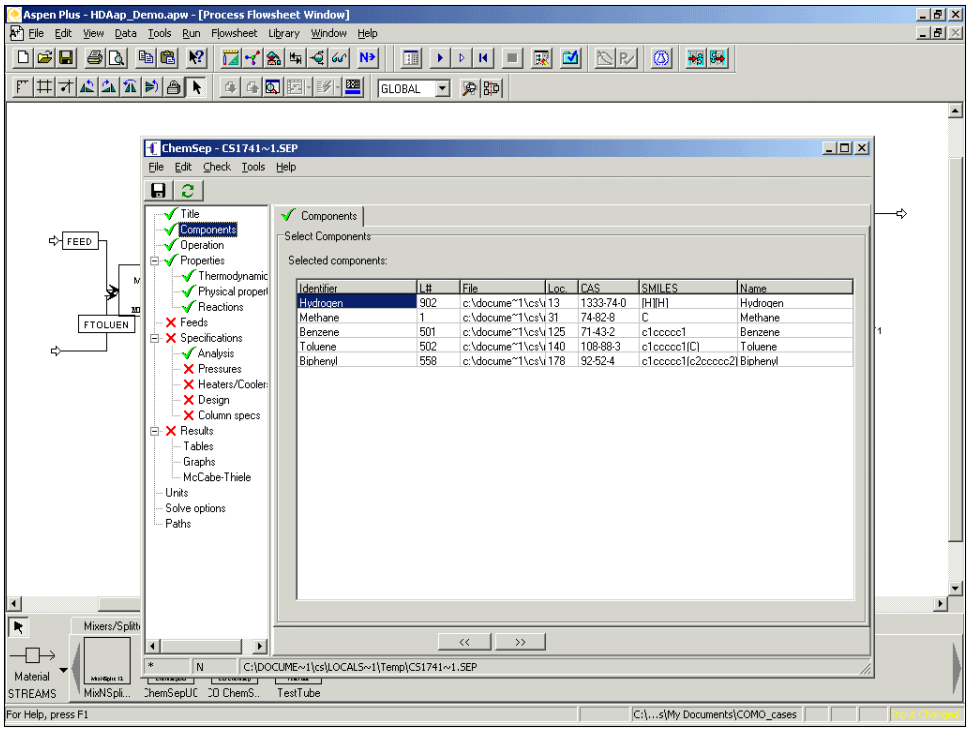
At this point we close the ChemSep interface so that we can complete connecting the CO ChemSep UO to the plant flowsheet. In the normal way connect the inlet and outlet streams to the ChemSep UO block.



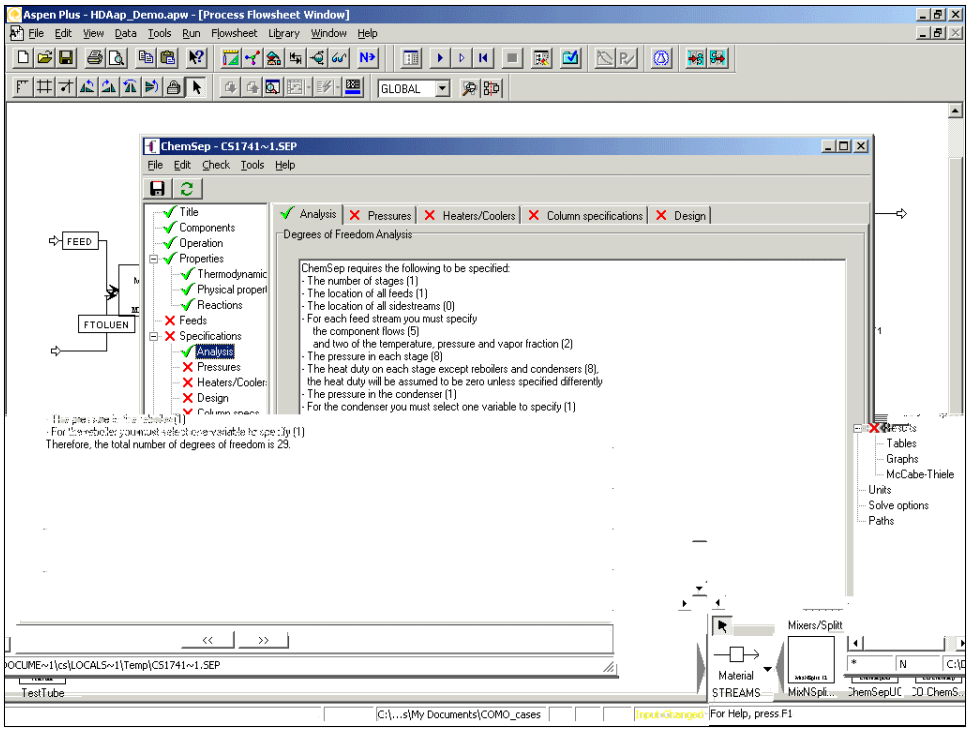
Now click on the ChemSep UO block again to bring up the UO interface once more. Go to the ports panel to verify that all streams are connected as they should be.



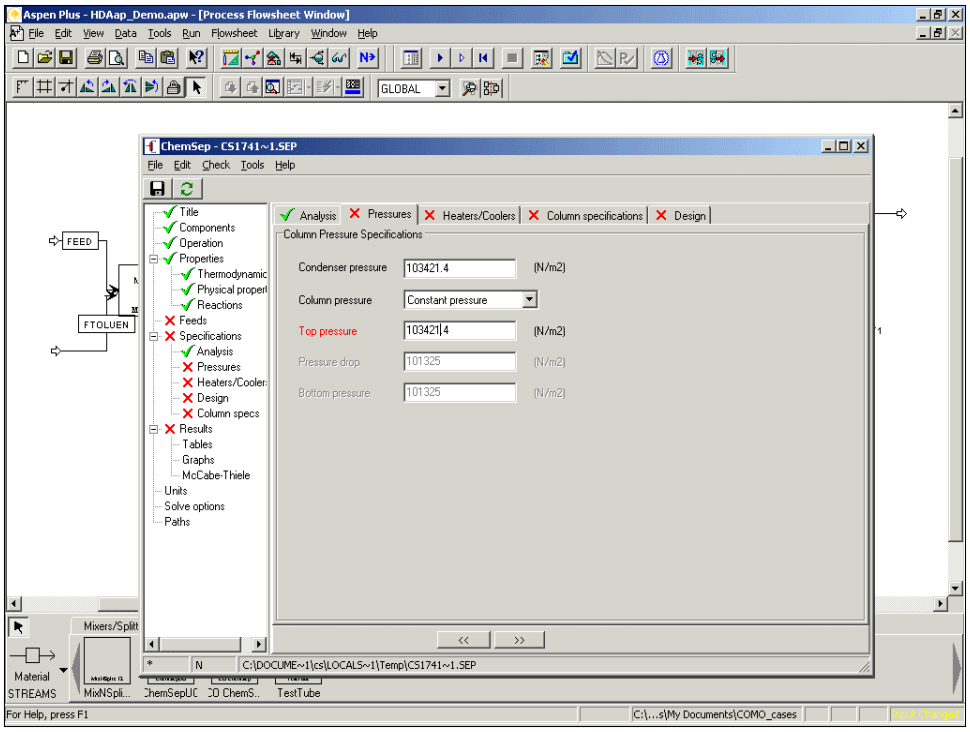
We close the ChemSep GUI once more and return to Aspen Plus.



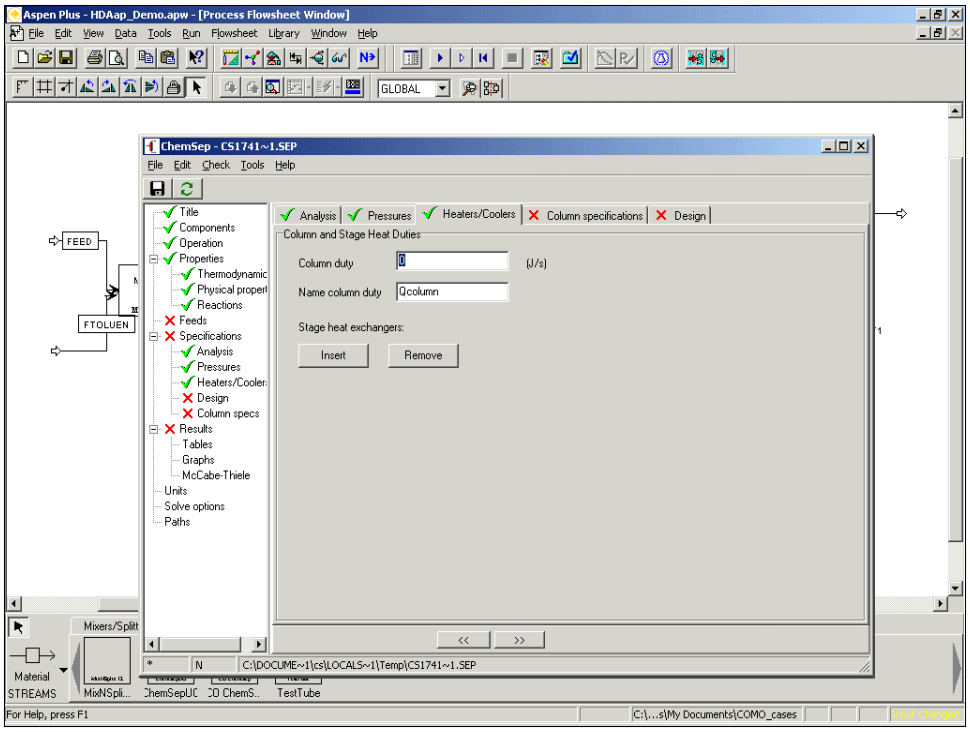
Launch the ChemSep GUI and we will now see a complete list of components.



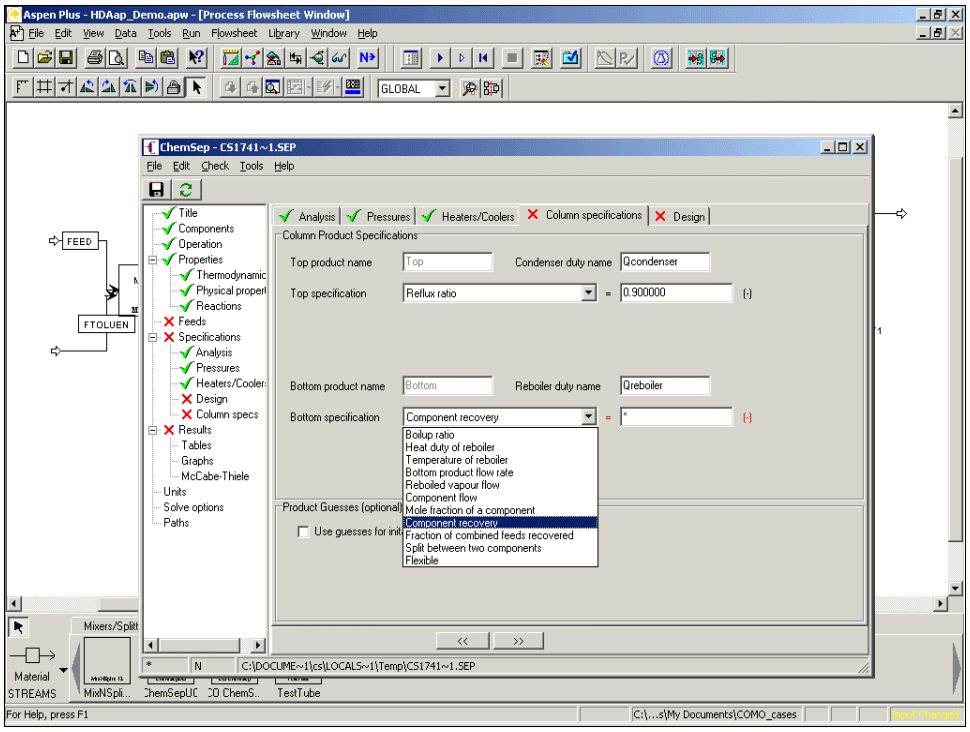
Complete the column specifications. This panel shows a degrees of freedom analysis.



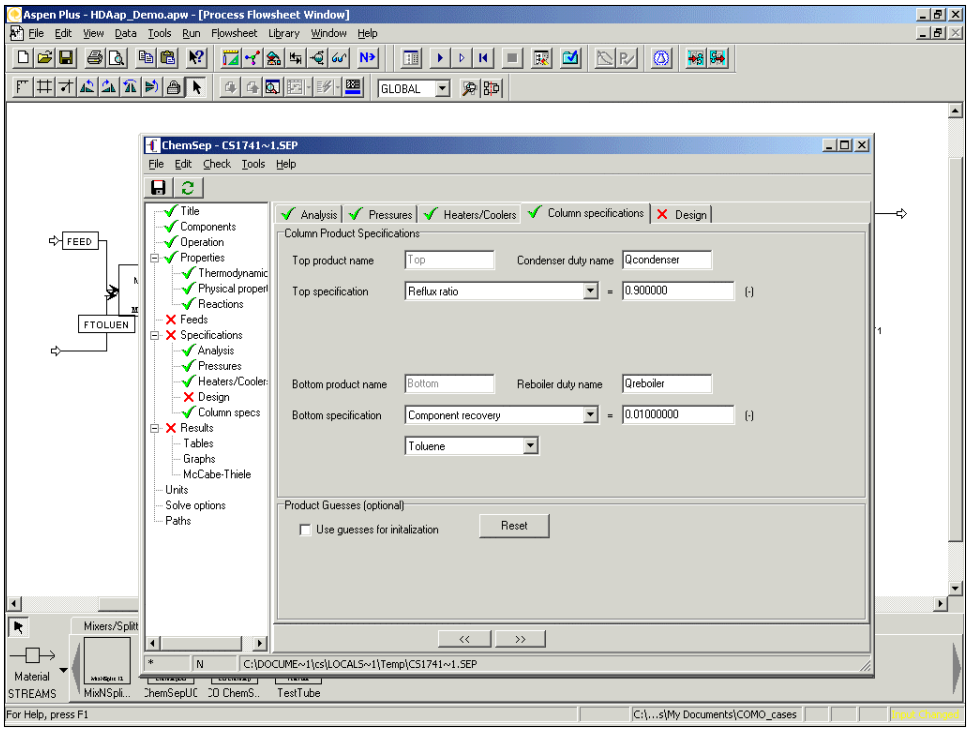
Column pressures and heat duties are specified on their own specification panels (the heat losses panel is shown below).

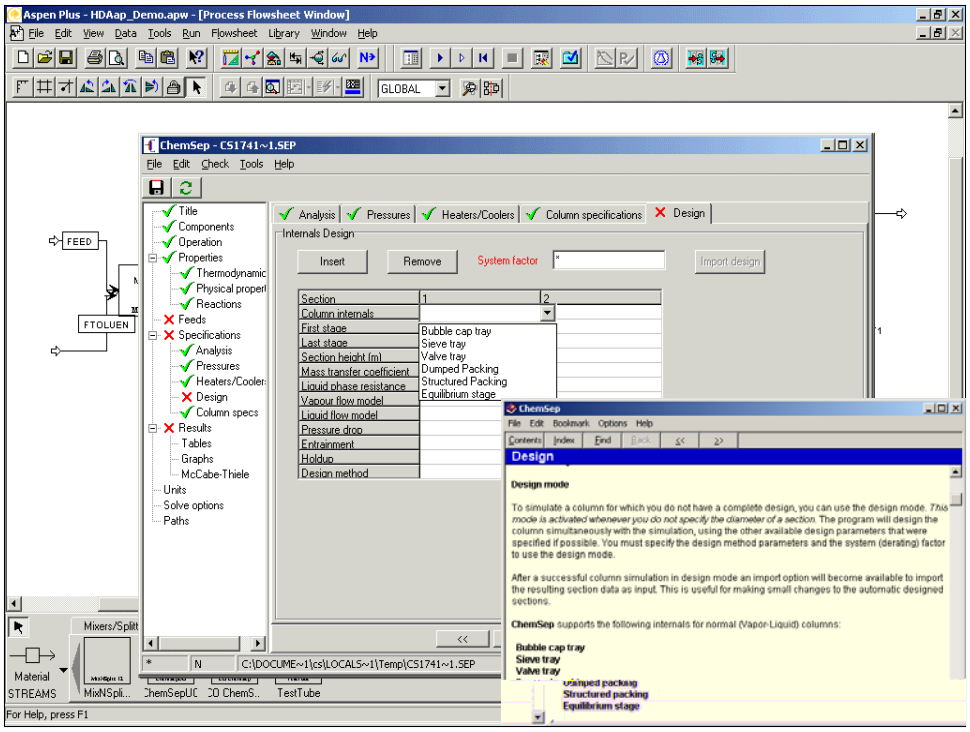


The heat losses from the column (normally assumed to be zero) are recorded on the panel shown above.

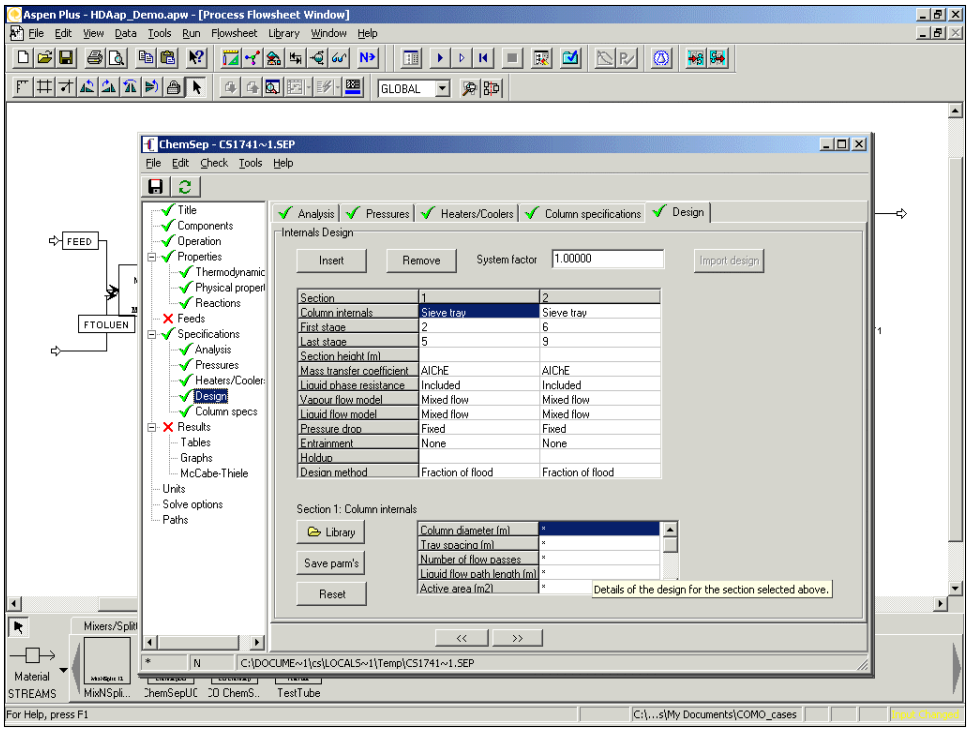


To complete the problem specification we provide the final column specifications. **ChemSep** allows the specification of any column variable as well as all of the usual top and bottom product specifications. In this example we specify the reflux ratio and the mass flow rate of the bottoms product. The latter is a non-standard specification that is made by picking Flexible from the drop down list of bottom specifications.


Aspen Plus - HDAap_Demo.apw - [Process Flowsheet Window]
File Edit View Data Tools Run Flowsheet Library Window Help
GLOBAL
FEED
FTOLUEN
ChemSep - CS1741~1.SEP
File Edit Check Tools Help
Title
Components
Operation
Properties
Thermodynamic
Physical propert
Reactions
Feeds
Specifications
Analysis
Pressures
Heaters/Cooler
Design
Column specs
Results
Tables
Graphs
McCabe-Thiele
Units
Solve options
Paths
Analysis
Pressures
Heaters/Coolers
Column specifications
Design
Column Product Specifications
Top product name
Top
Condenser duty name
Qcondenser
Top specification
Reflux ratio
=
0.900000
(-)
Bottom product name
Bottom
Reboiler duty name
Qreboiler
Bottom specification
Component recovery
=
0.01000000
(-)
Toluene
Product Guesses (optional)
Use guesses for initialization
Reset
<<
>>
C:\DOCUME~1\cs\LOCALS~1\Temp\CS1741~1.SEP
Mixers/Splitt
Material
STREAMS
MixNSpli...
ChemSepUC
CO ChemS..
TestTube
For Help, press F1
C:\...s\My Documents\COMO_cases

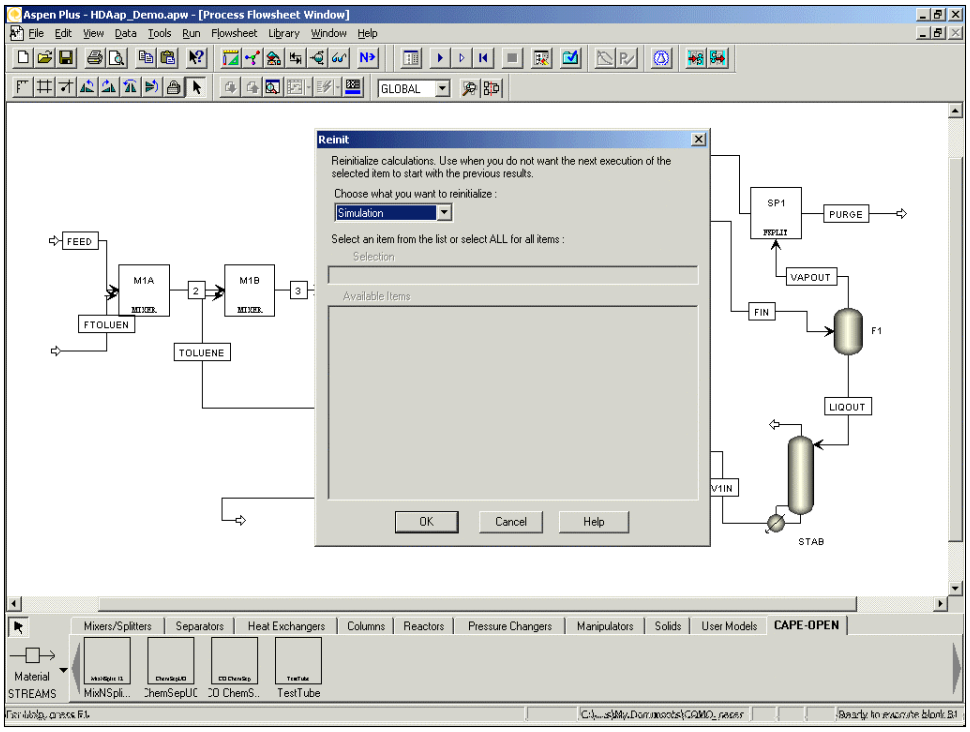


For a nonequilibrium simulation we must say something about the type of column. Here we see the design panel on which the equipment design details for the column are recorded. Technical help is available for the the perplexed (the panel in the lower right hand corner). Locating the cursor on the field(s) 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.

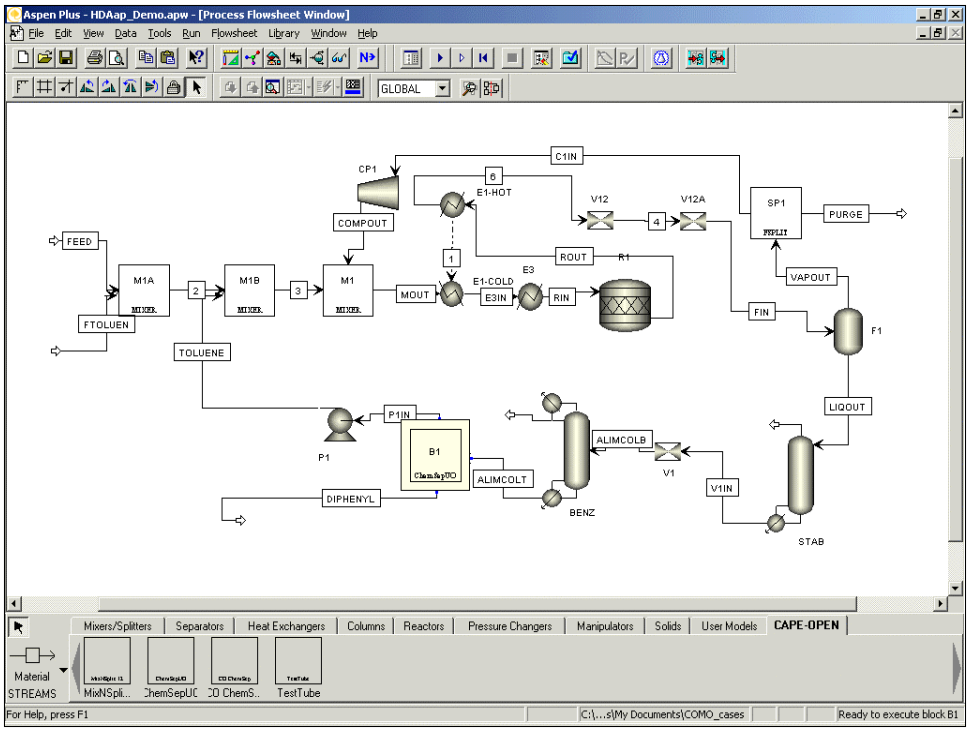


In this case we have chosen a sieve tray. The column is automatically divided into a number of sections according to how many feed and product streams there are. The panel above shows default settings for most things.

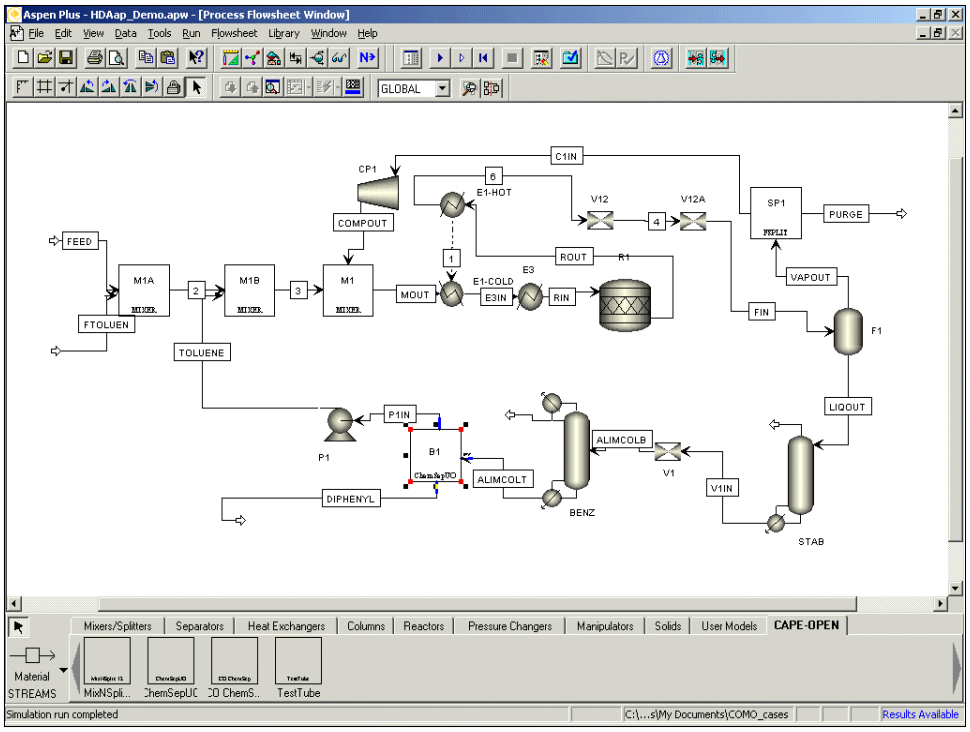
ChemSep includes over 40 correlations for mass transfer coefficients in different types of column, as well as 18 different ways to estimate pressure drop and 16 for holdup.



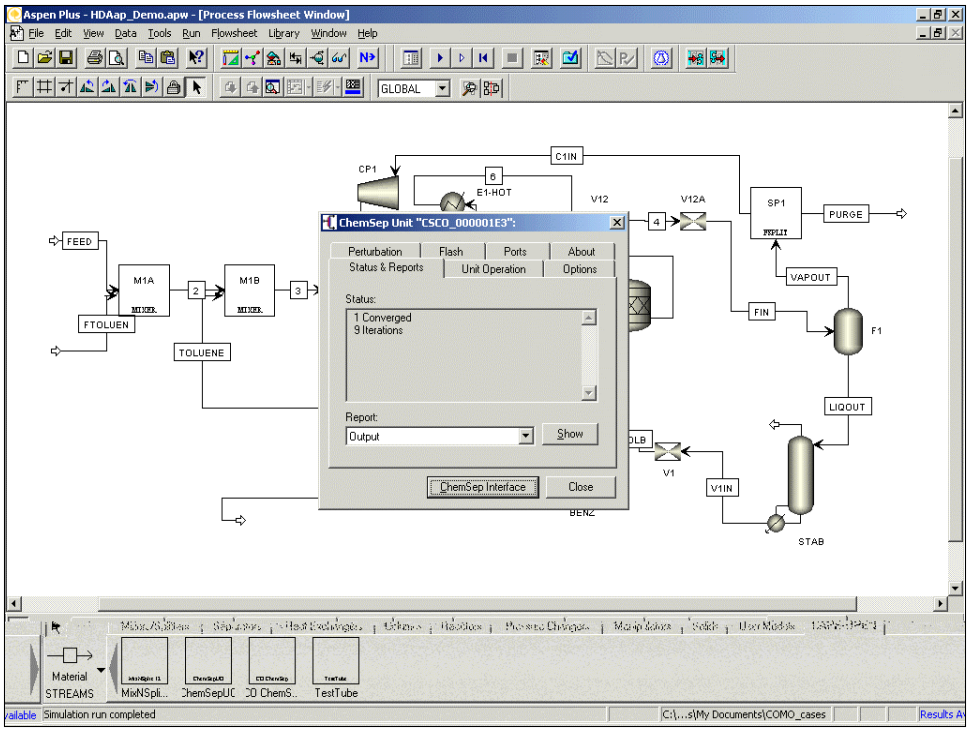
This panel appears when Aspen Plus is asked to reinitialize variables.



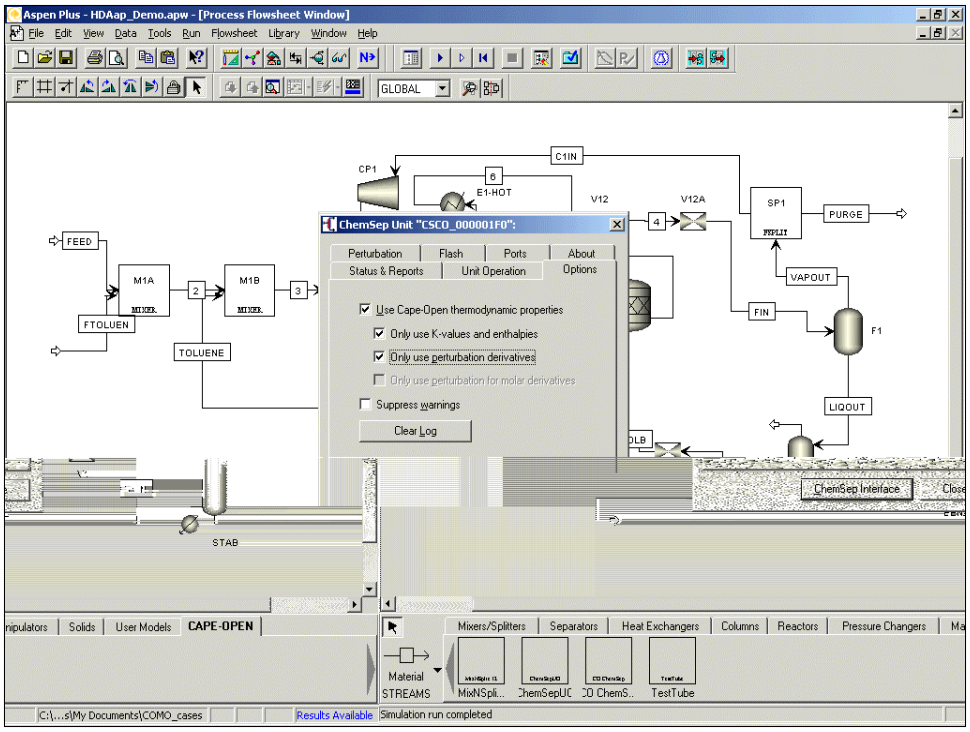
It isn't obvious from the illustration but when this screen image was recorded the flowsheet calculations were taking place.



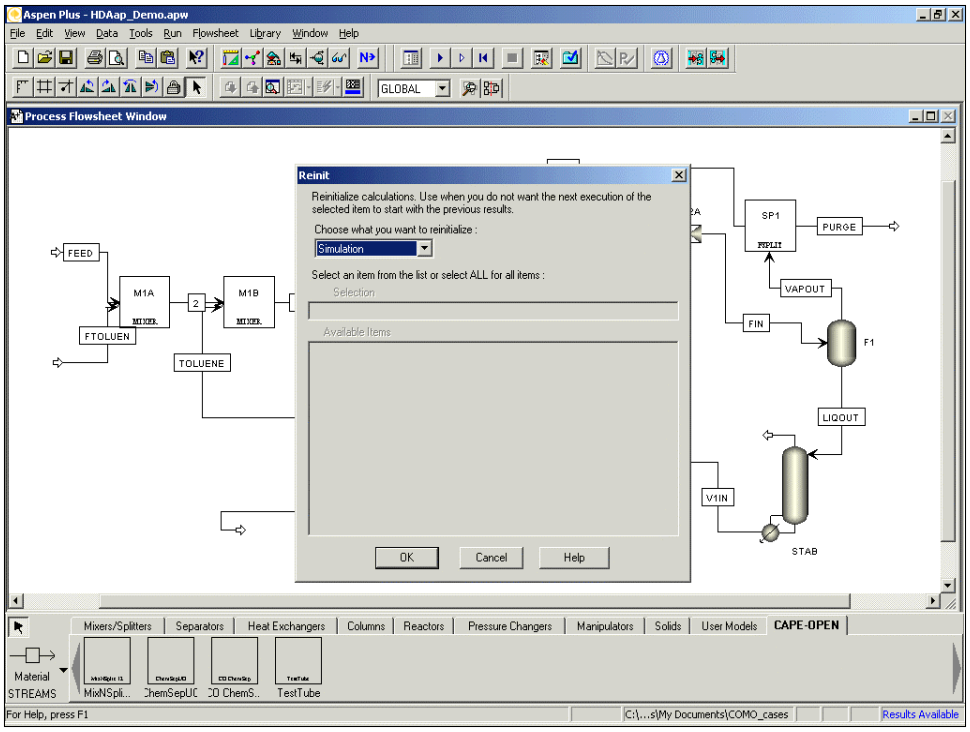
The flowsheet has converged. Click on the **ChemSep** UO symbol.



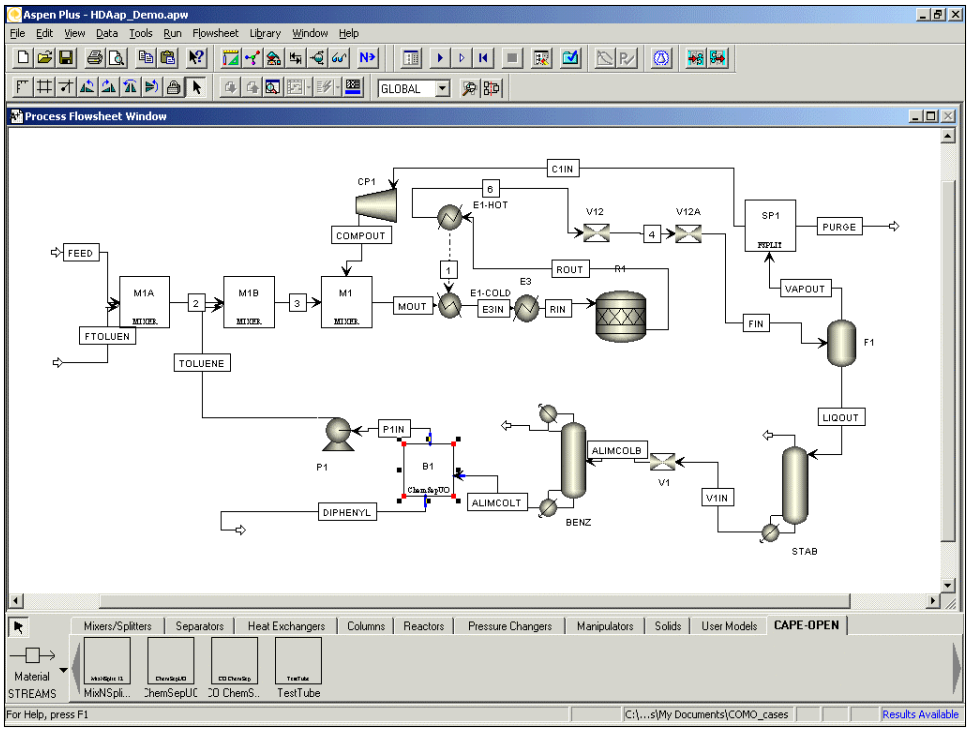
The ChemSep UO wrapper interface appears. We see here that the column itself (not the flowsheet) converged in 9 iterations.



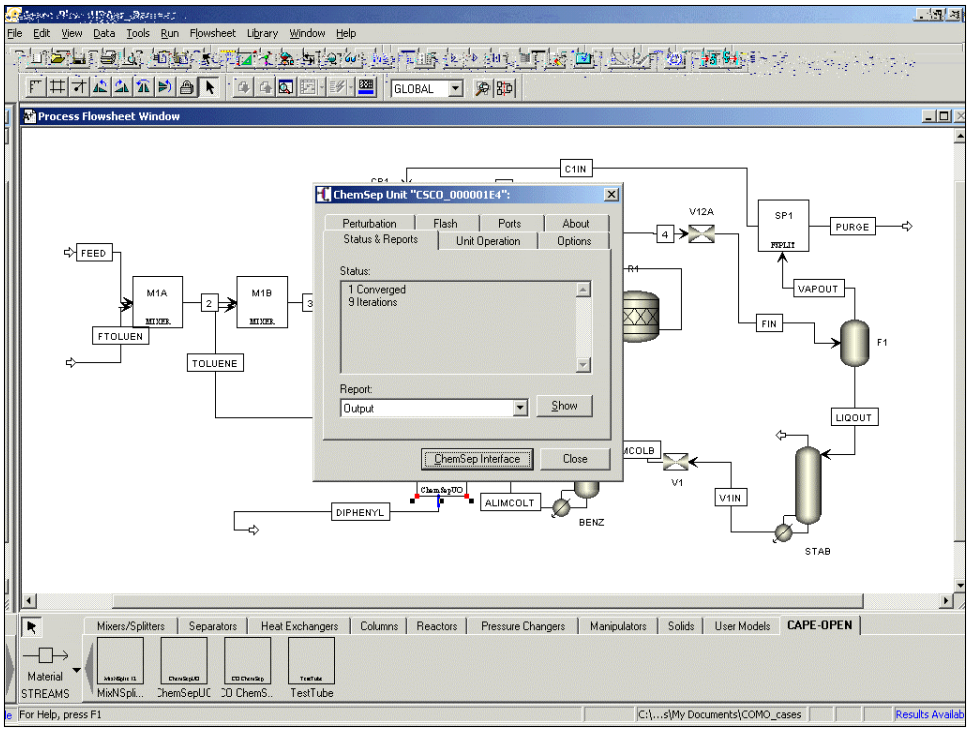
Now we are going to repeat the calculations but use the thermodynamic models available from the COSE (the first check). In this case only K-values and enthalpies will be computed by the COSE (the second check), all other physical properties will be calculated internally. Derivatives will be obtained numerically (the third check).



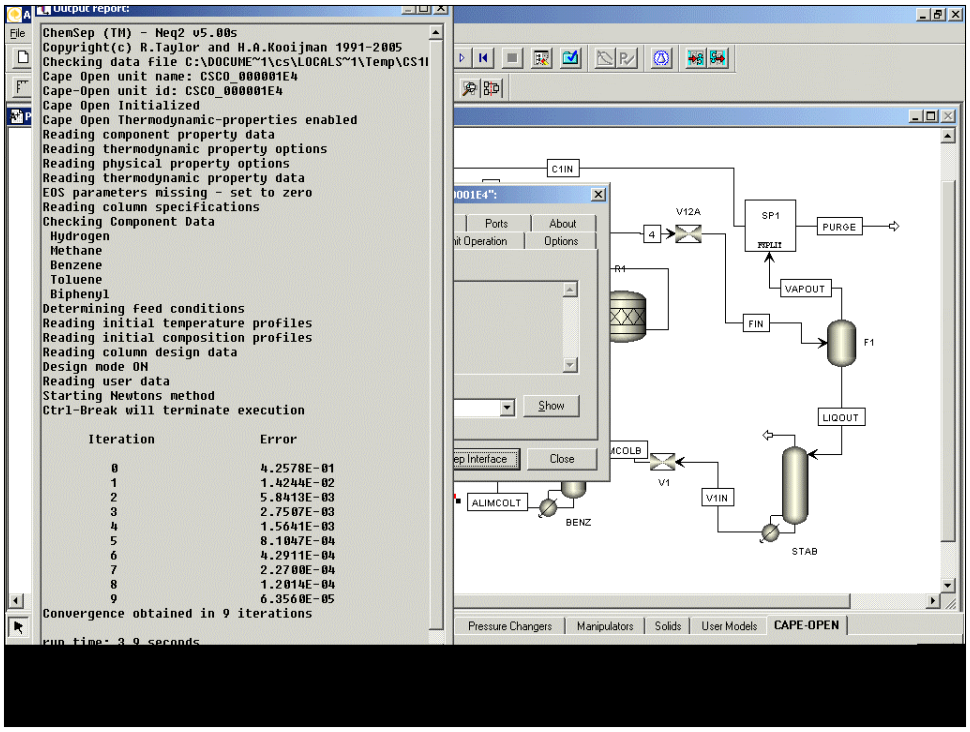
The flowsheet is reinitialized.



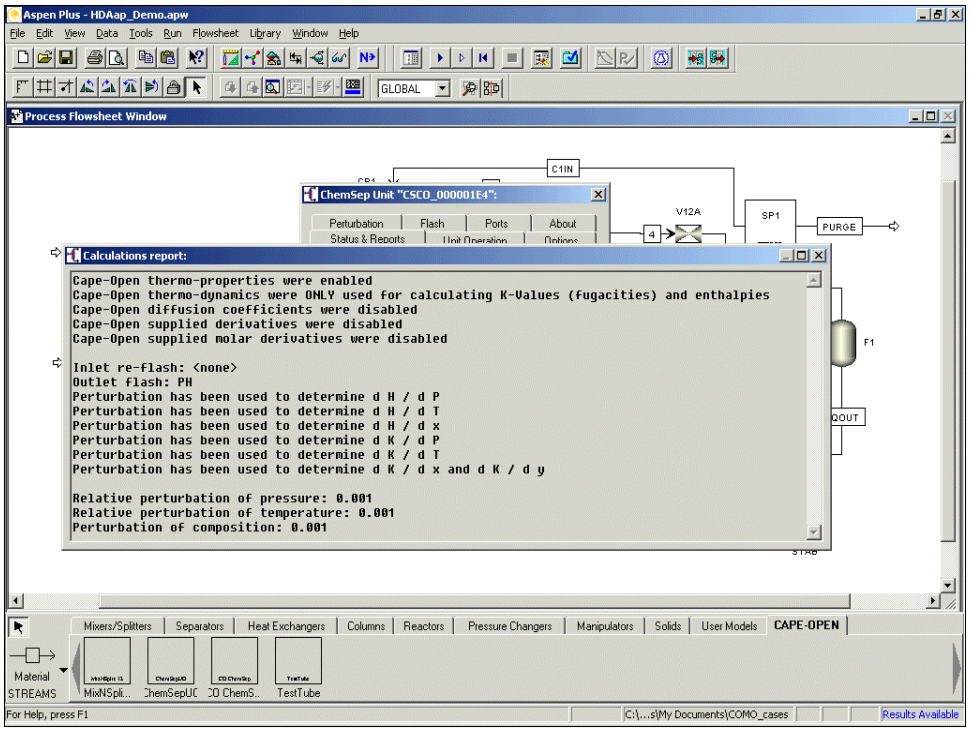
And the flowsheet converged again.



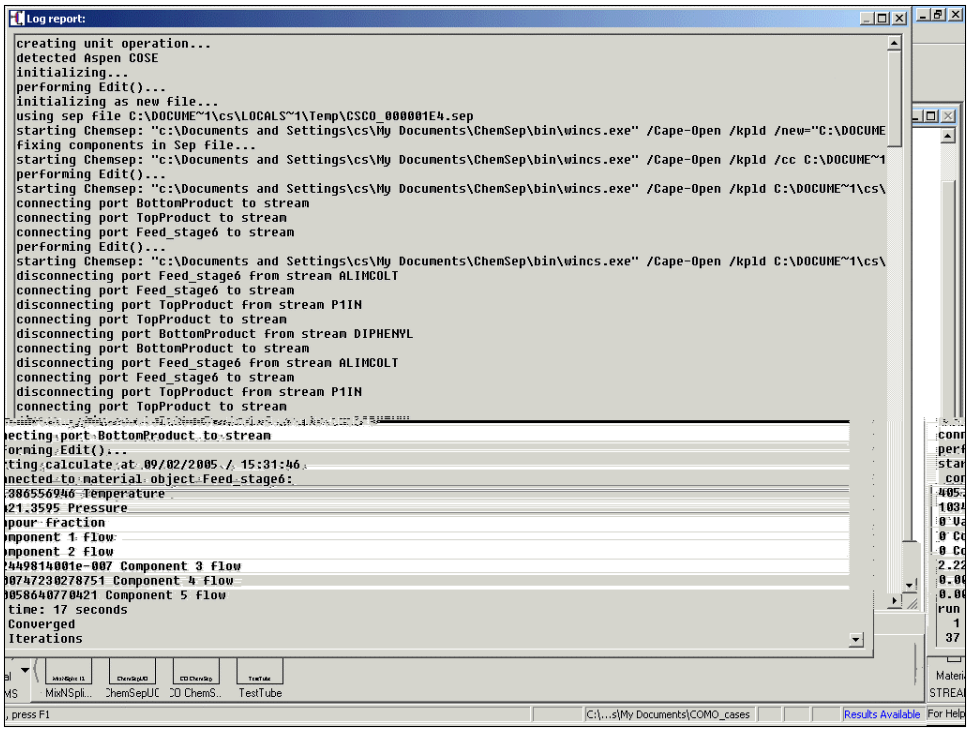
Click on the UO symbol to bring up the UO interface.



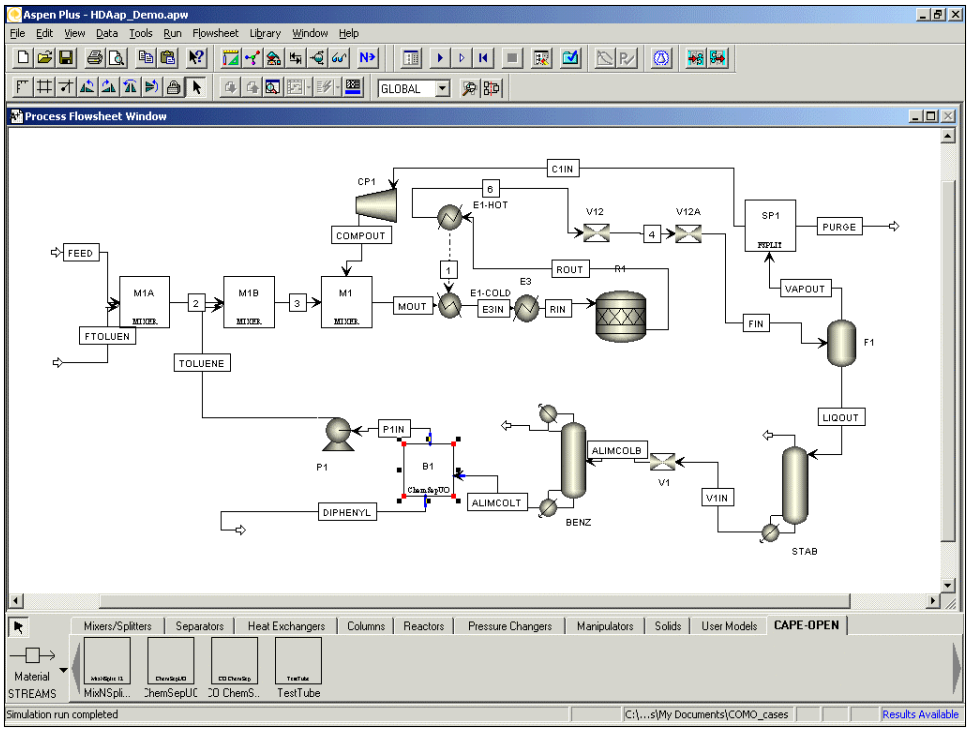
Here we see one of the reports that can be displayed by the UOI. In this case we see the output from the program that would normally be displayed on screen, but in CO model is redirected to a file.



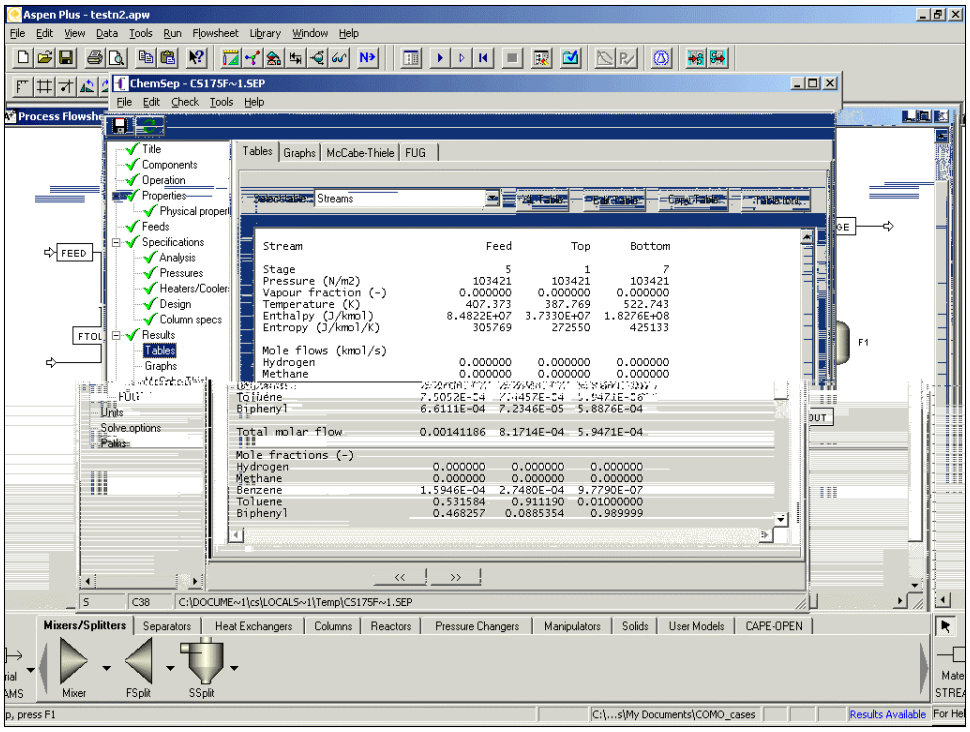
This panel shows a different report; this one indicates that thermodynamic properties were calculated from a CO package.



And this report shows CO calls.

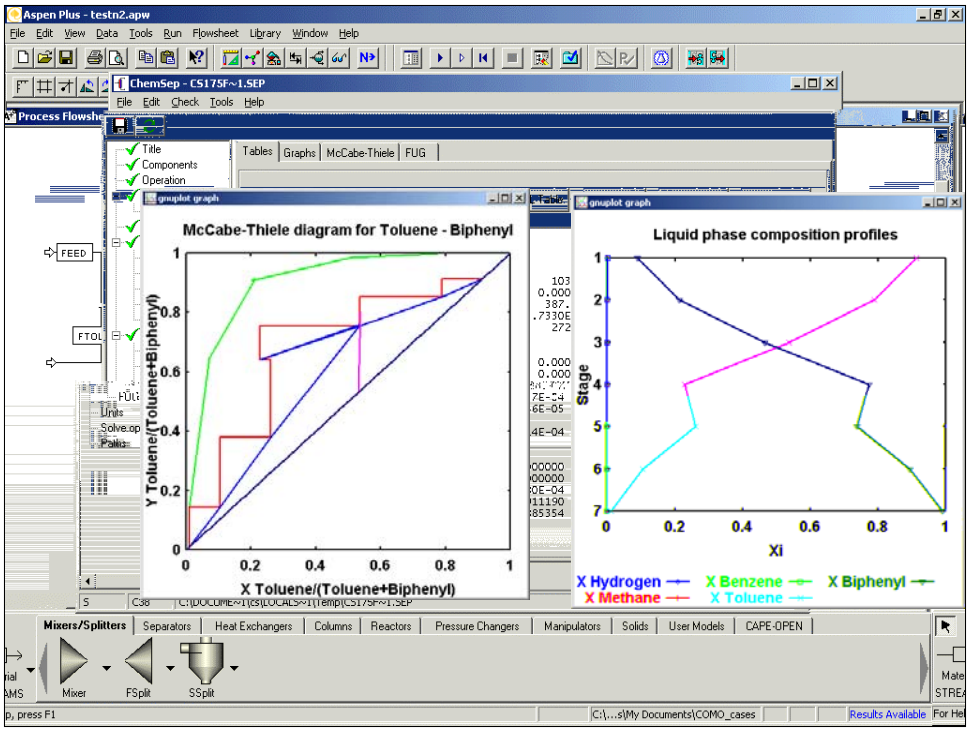


The flowsheet again.



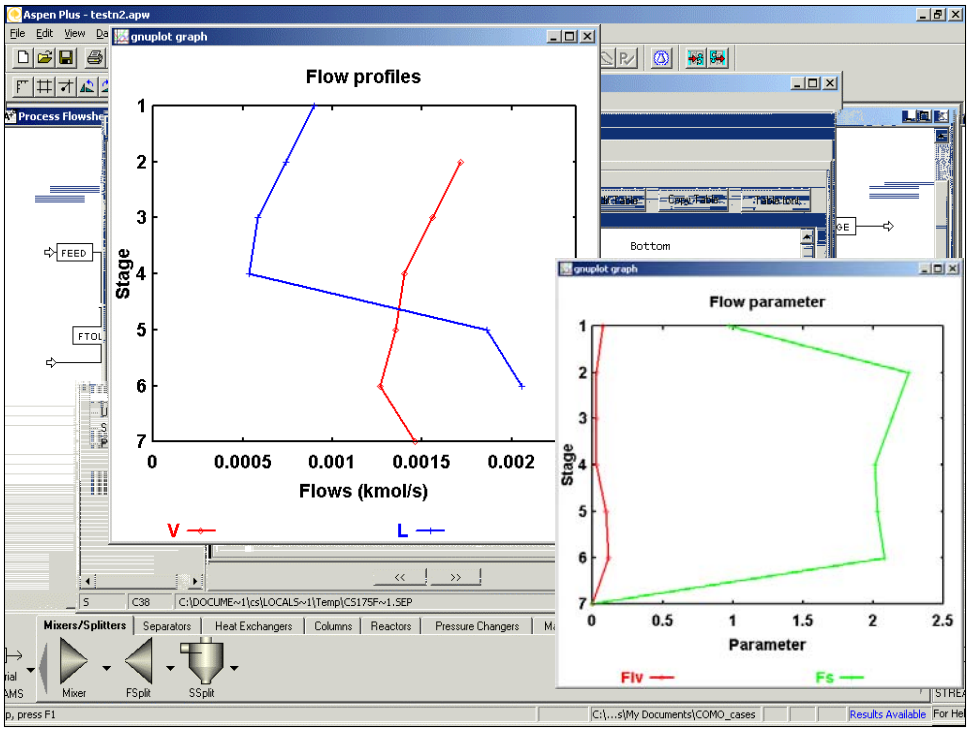
Relaunch the **ChemSep** GUI to inspect the results. This panel shows the stream table, but many other tables are available.

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.



ChemSep has extensive support for plotting almost any kind of column profile including composition, flow, temperature, pressure, K-values and much more. The plots are completely configurable. **ChemSep** uses the Open Source package Gnuplot (for Windows) to display a plot in its own separate window. The illustration shows two open windows with two predefined ChemSep plots. The *Graph settings* checkbox (not visible) allows the user to configure the details of the graph before it is displayed.

McCabe-Thiele diagrams also can be constructed from the results of a nonequilibrium simulation, and are just as useful for understanding column behavior as they are for binary distillation. Note how the triangles do not touch the equilibrium line (as of course, they should not).



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 very many variables that can be plotted). The plot on the right hand side above shows the flow parameter and the superficial F-factor as a function of tray number (height).