**Getting started with the COCO chemical process simulator**

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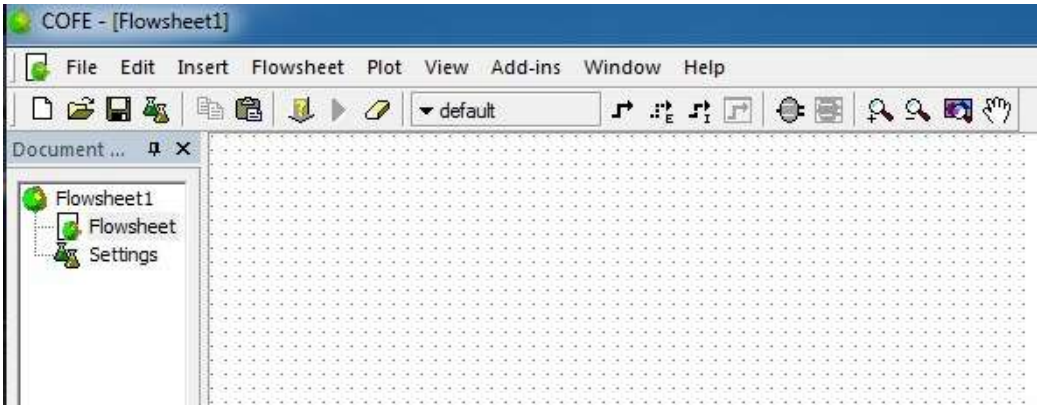
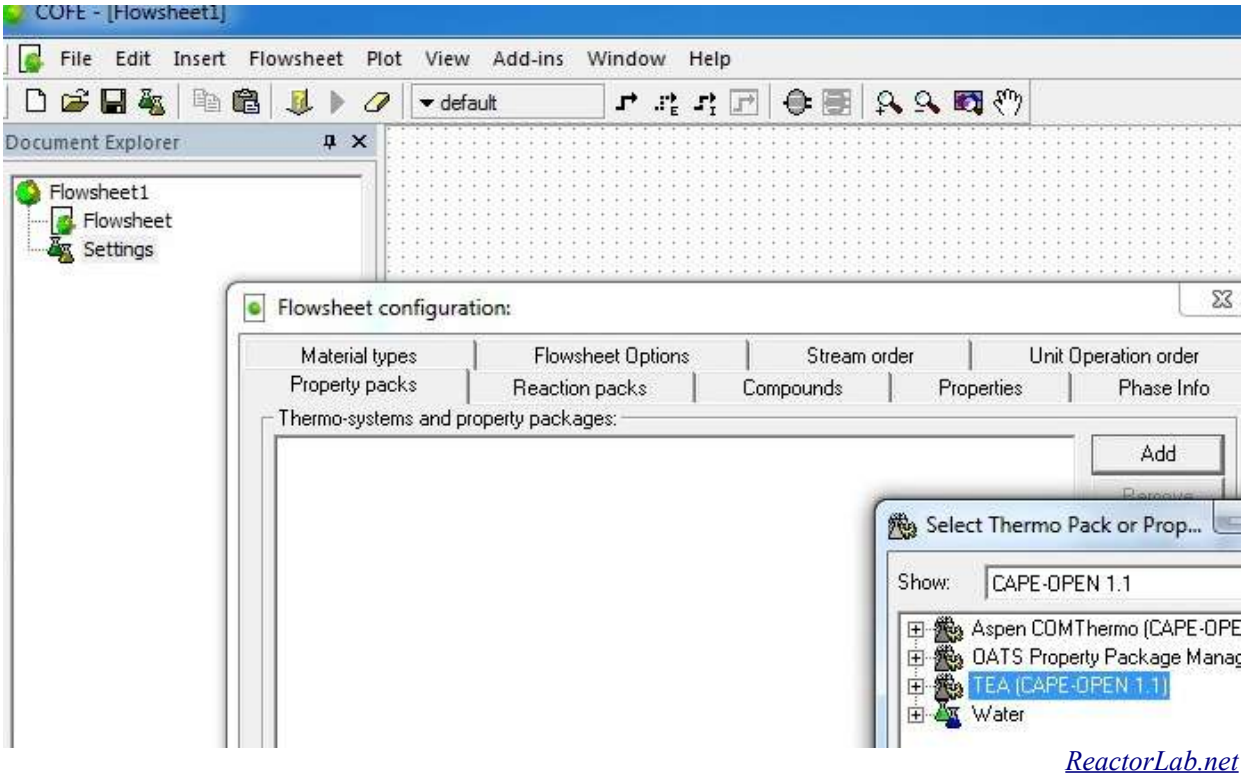
COCO (CAPE-OPEN to CAPE-OPEN) is a free CAPE-OPEN-compliant steady-state chemical process simulator. CAPE-OPEN is a standard that defines rules and interfaces that allow CAPE (Computer-Aided Process Engineering) applications or components to interoperate.

COCO runs on Windows OS computers. To download COCO go to <http://www.cocosimulator.org>
For info about CAPE-OPEN go to <http://www.colan.org>

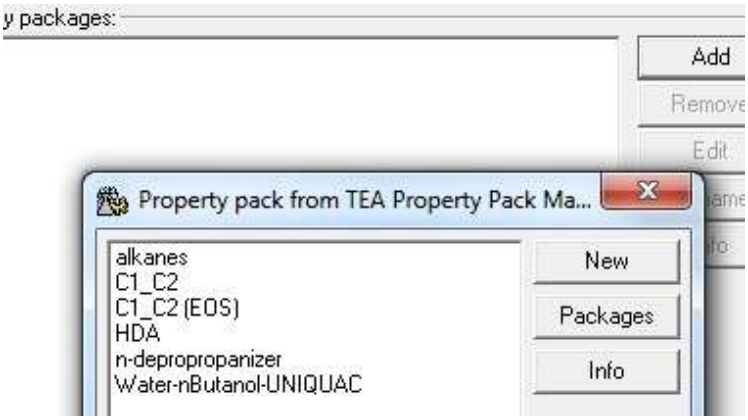
The COCO installer installs several components. One of them is the COFE flowsheet program. Start COFE and you will see something similar to this.




The first thing we will do here is to add components and select a thermodynamic system. Click the Settings button on the left side of the COFE window. The Flowsheet Configuration window will open. With the tab "Property packs" selected, click the Add button. The Select Thermo Pack or Prop... window will open. Select TEA and click the Select button.

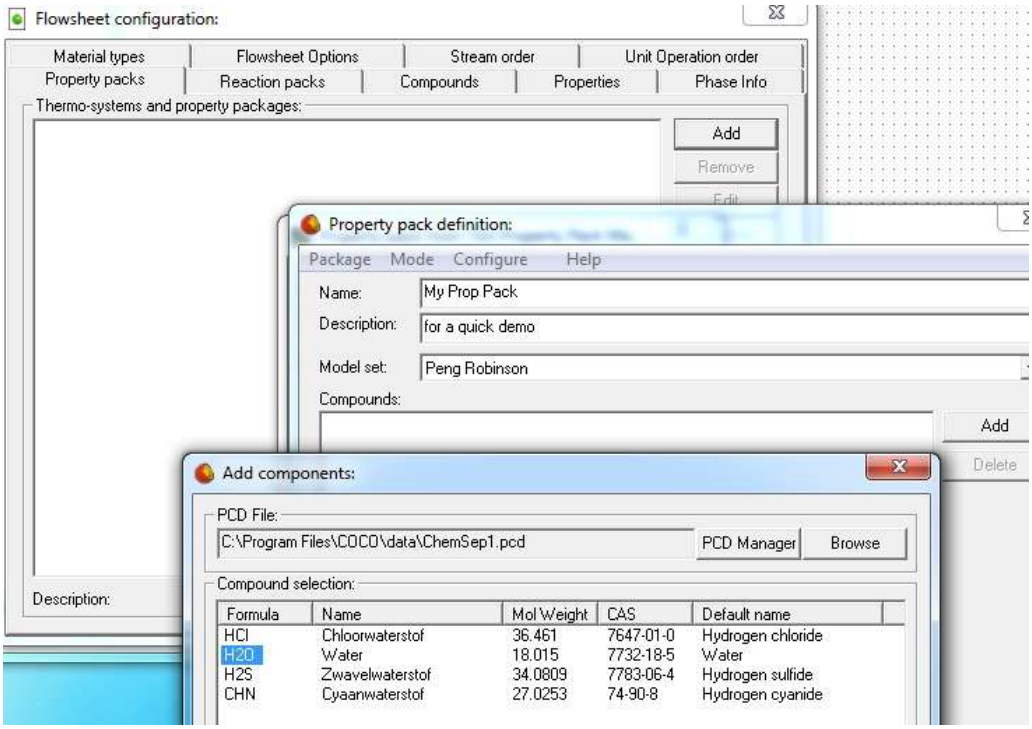


The Property pack from TEA Property Pack... window will open. Click the New button.

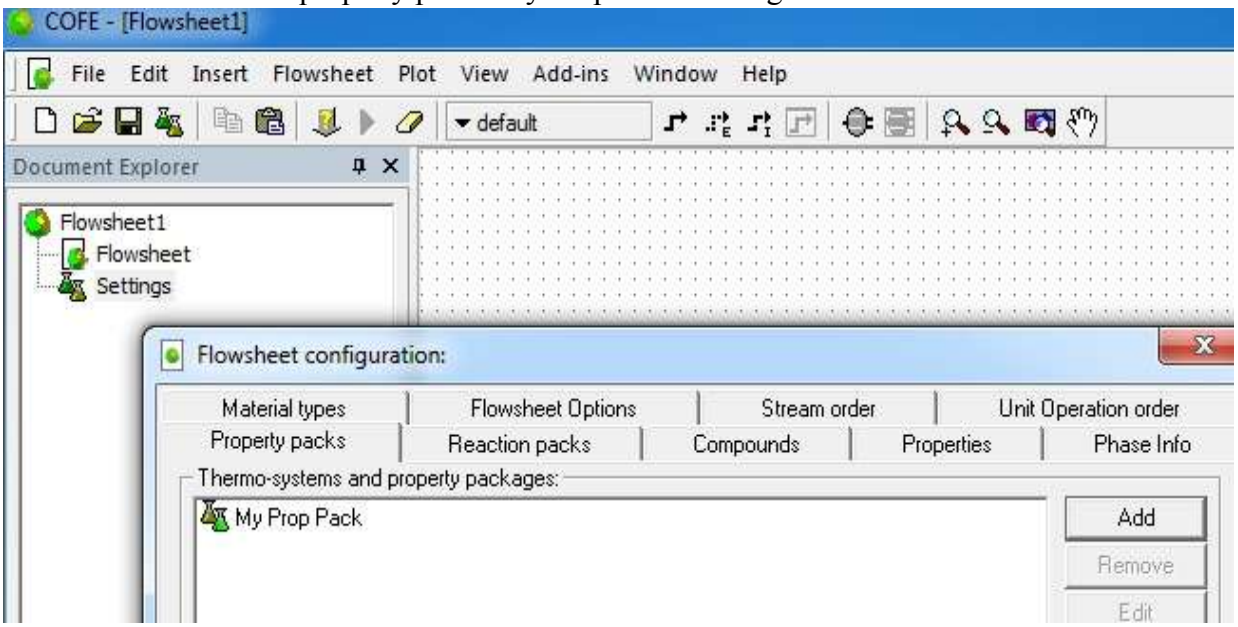



The Property pack definition window will open. Enter a name and select a thermodynamic model set. Here I have selected Peng-Robinson from the drop-down menu. This might not be the best thermo model to use for these components and phases. Do some literature research for yourself. See how your final results change with changes in the thermo model selected.

Then click the Add button to add compounds. Here I add water and methanol.

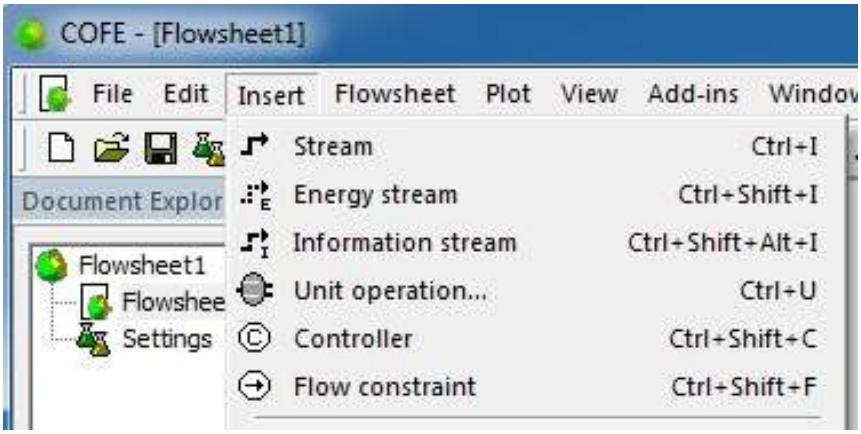


Now we have our new property pack "My Prop Pack" configured for use.



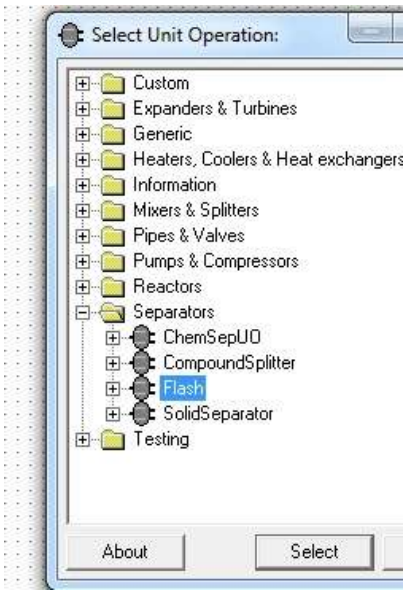

If you find that you are working with the same sets of components to build multiple flowsheets, then you will want to define property pack templates. Then, when starting a new flowsheet, you can select a template. The property pack imported from a template can then be modified for a specific flowsheet without changing the template. You can define templates using the application ConfigureTEA. Or in your flowsheet, you can also select Edit after selecting TEA in the Add Property Pack window, then click Edit Templates button.

Now we will add a unit to the flowsheet. Under the Insert menu, select Unit Operation.

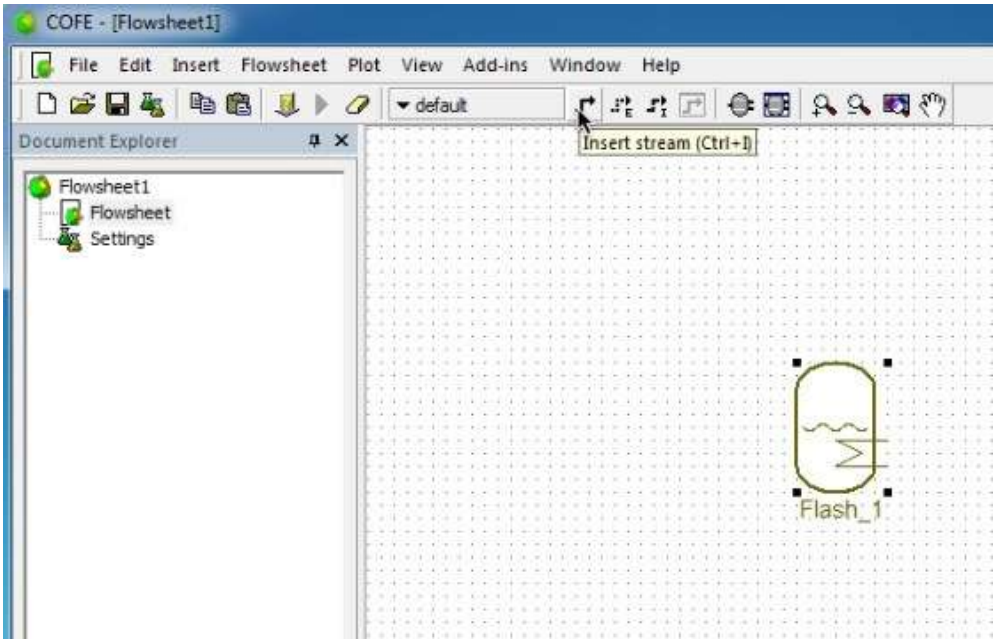



In the Select Unit Operation window, notice the ChemSepUO item. This is a separation unit operation from the program ChemSepLITE that was installed when you installed the COCO package. ChemSep is a CAPE-OPEN compliant program. COCO's COFE can use unit operations from ChemSep.

In the Select Unit Operation window, select Separators, Flash.

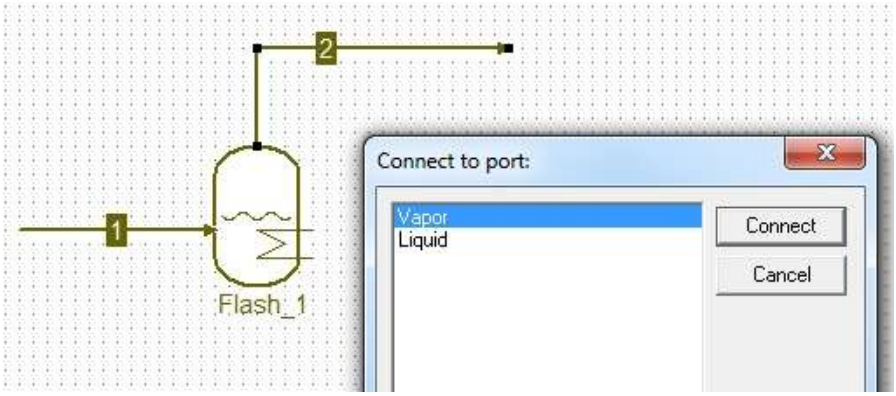



This adds a flash drum to the flowsheet. The click the menu button to insert a material stream as shown, or click the Insert menu and select Stream.

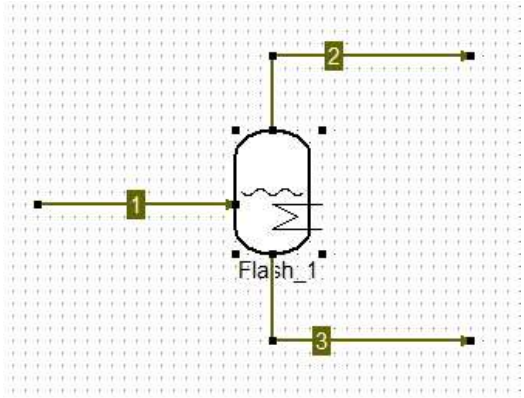



The mouse cursor will change shape to a plus + sign. click on the flowsheet to the left of the flash drum and then click on the left edge of the flash drum to connect a feed stream to the drum. Click again on the insert stream button and click on the top of the drum and then to the top right of the drum to terminate the stream.

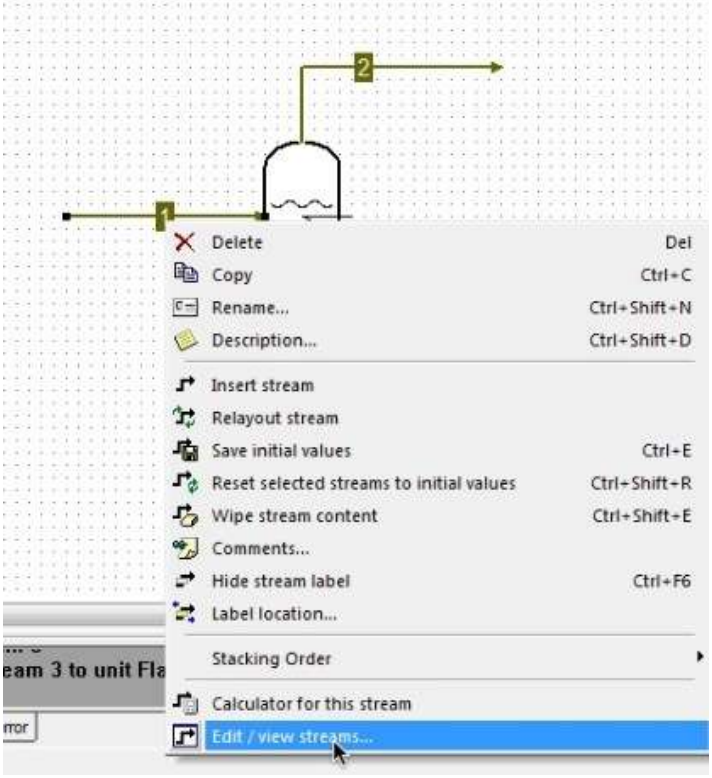
You will be asked if you want to make this the vapor outlet of the drum. You do.



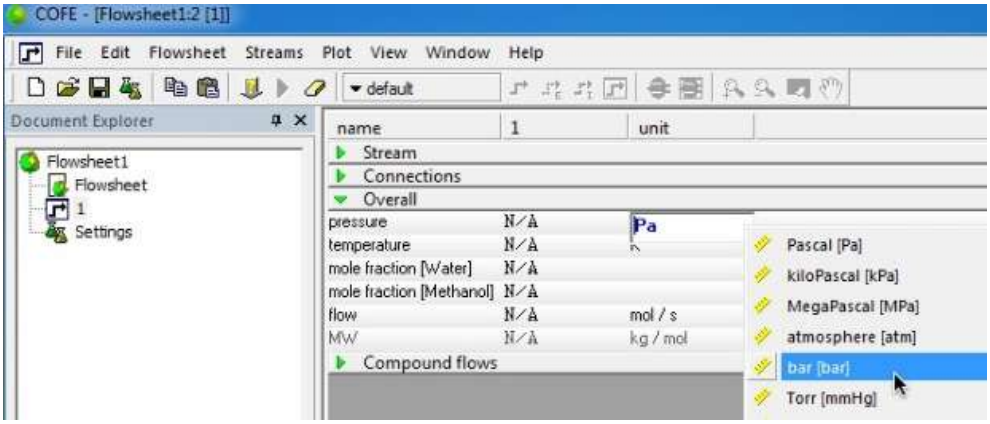

Repeat to connect a stream at the bottom of the drum through which the liquid product will leave.



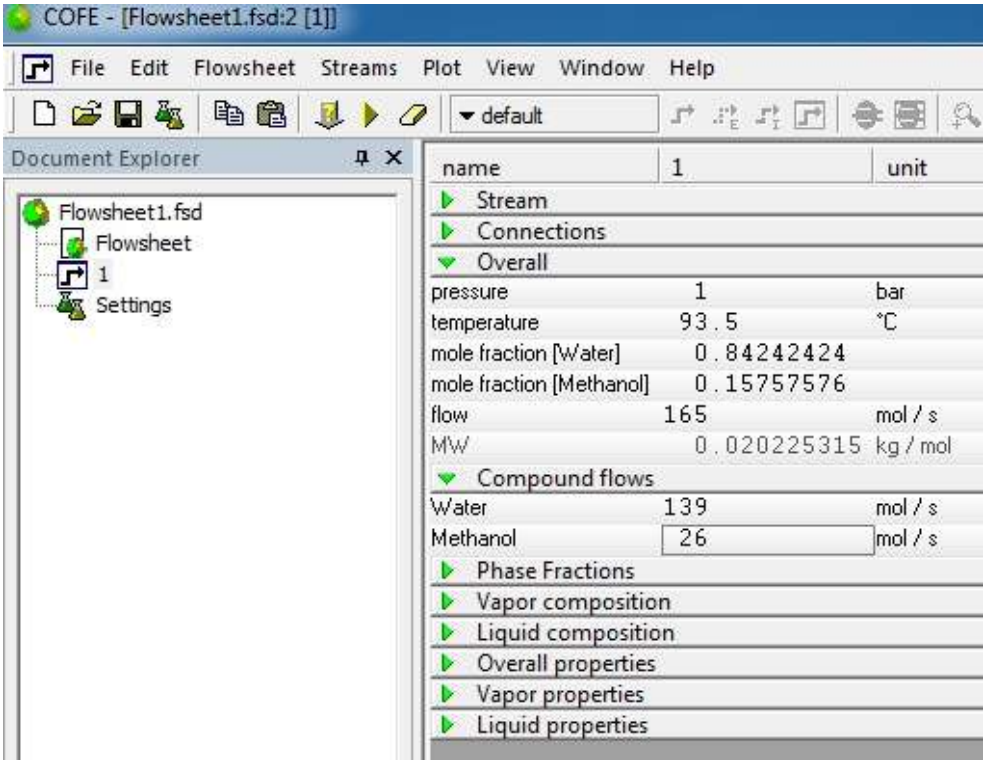

Now we need to define conditions in the feed stream. Right-click on stream 1 and select Edit/view streams.



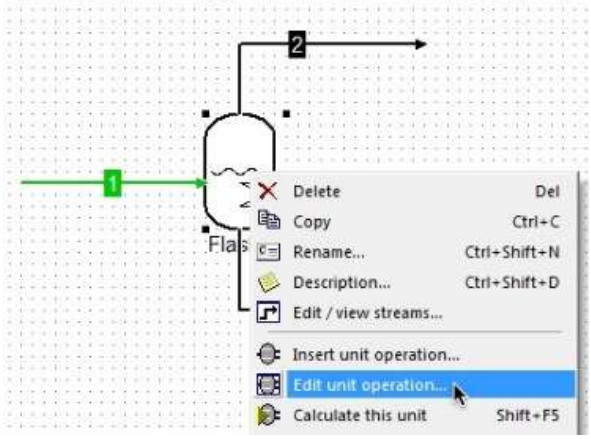
A window opens that allows us to specify stream 1. Here we change the pressure units from Pa to bar.



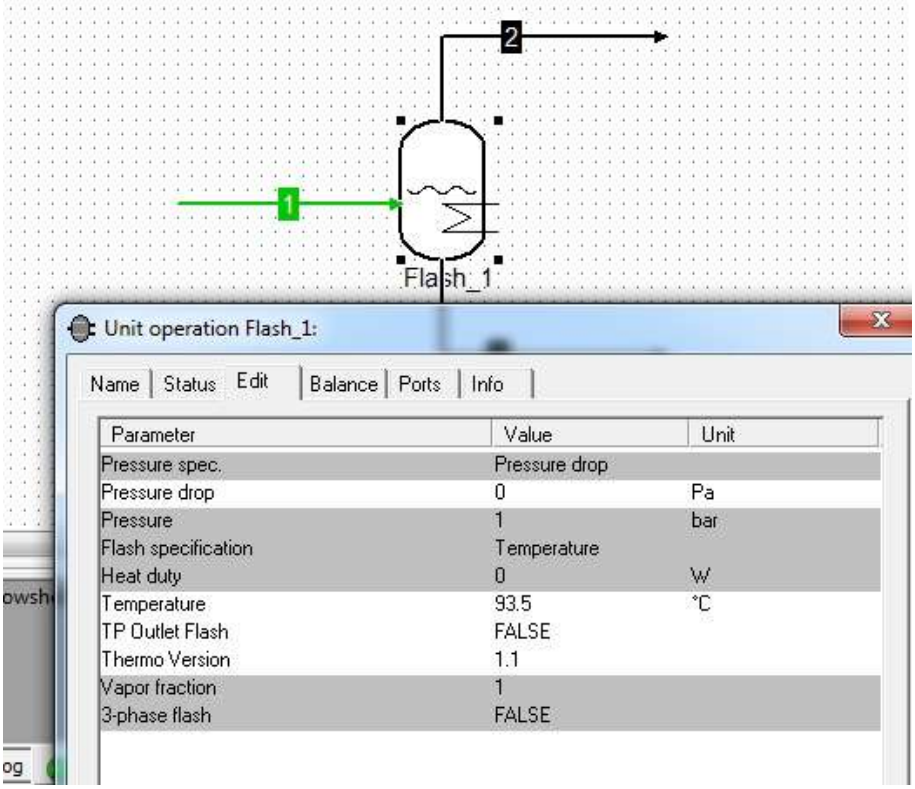

Continue to enter conditions: 1 bar, 93.5 °C, 139 mol/s water, 26 mol/s methanol. Other quantities are computed. You could also enter the total flow rate and the mole fractions and have the individual flow rates computed.



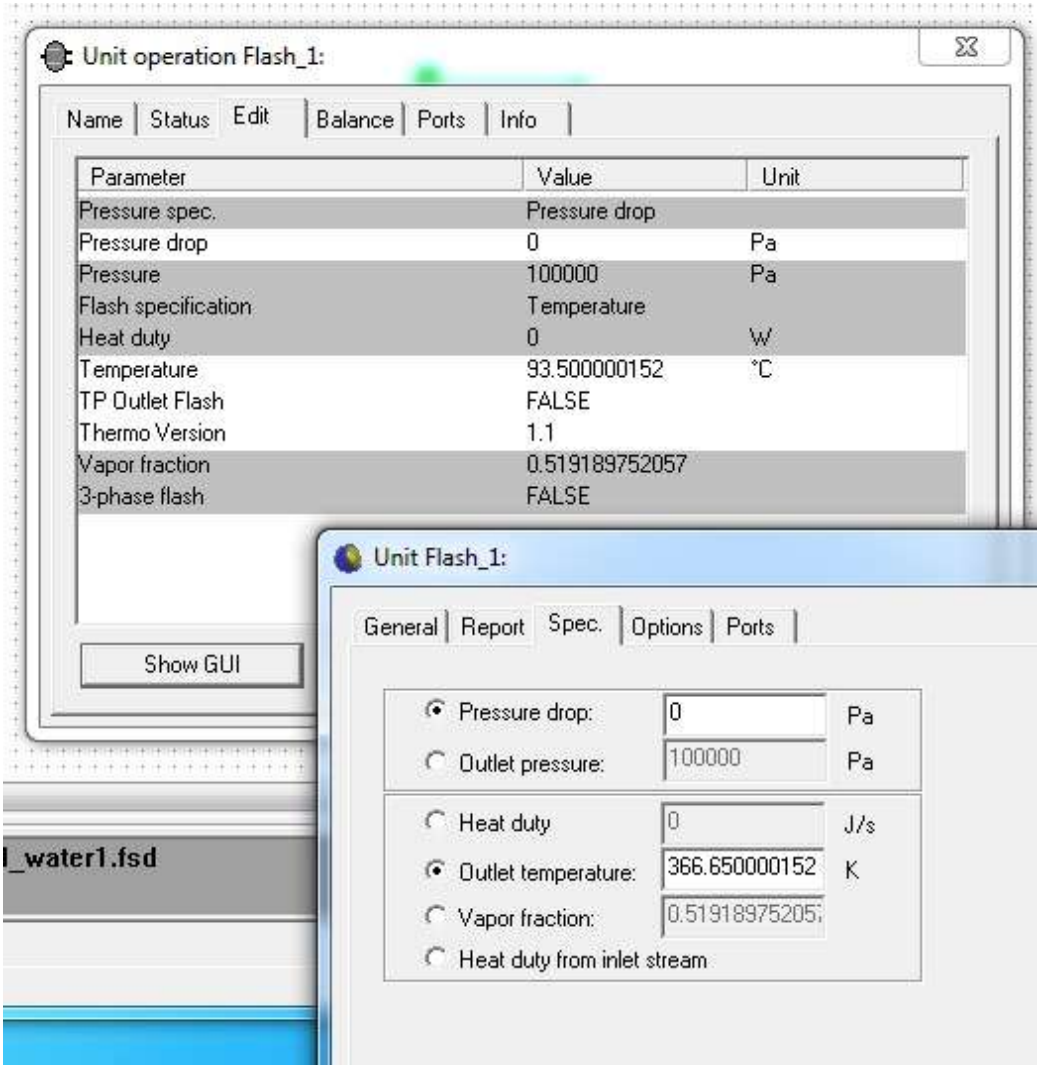
Next, specify conditions for the flash drum. Right-click on the unit and select Edit unit operation...



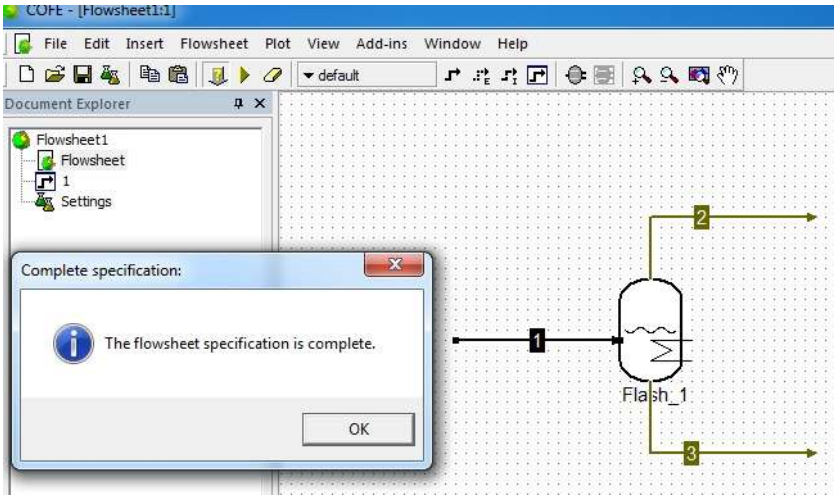

Enter conditions for the unit: Pressure drop of 0 Pa, Temperature of 93.5 °C. Note there are several options for which conditions to specify.



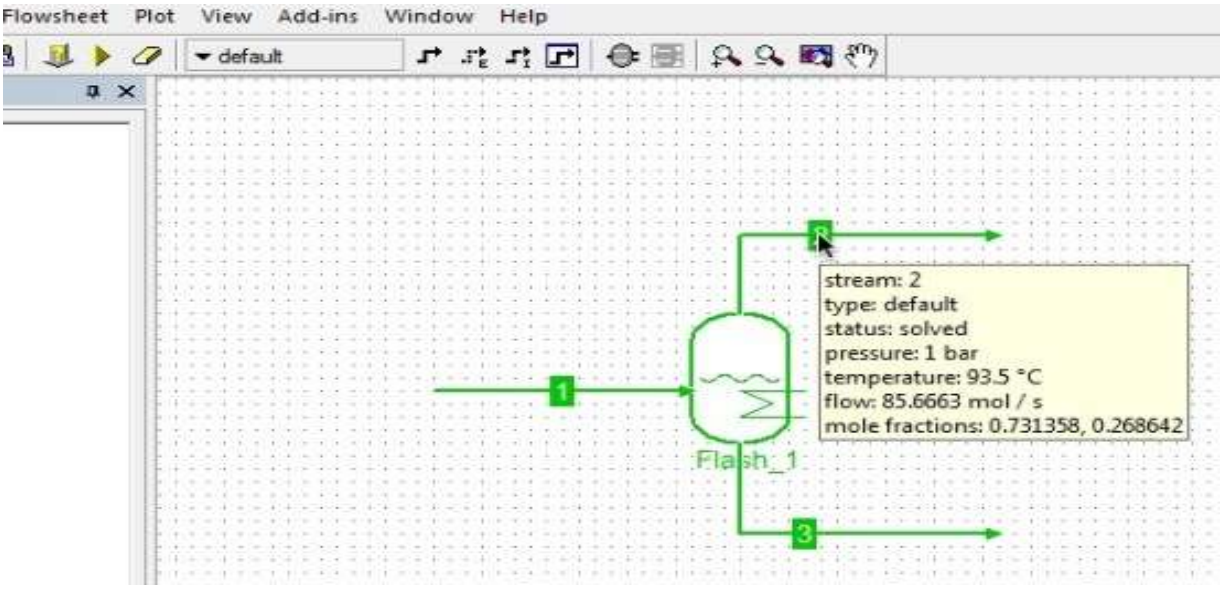
Note the Show GUI (graphical user interface) button at the bottom of the Unit operation window. You may wish to use the GUI interface to specify the unit.



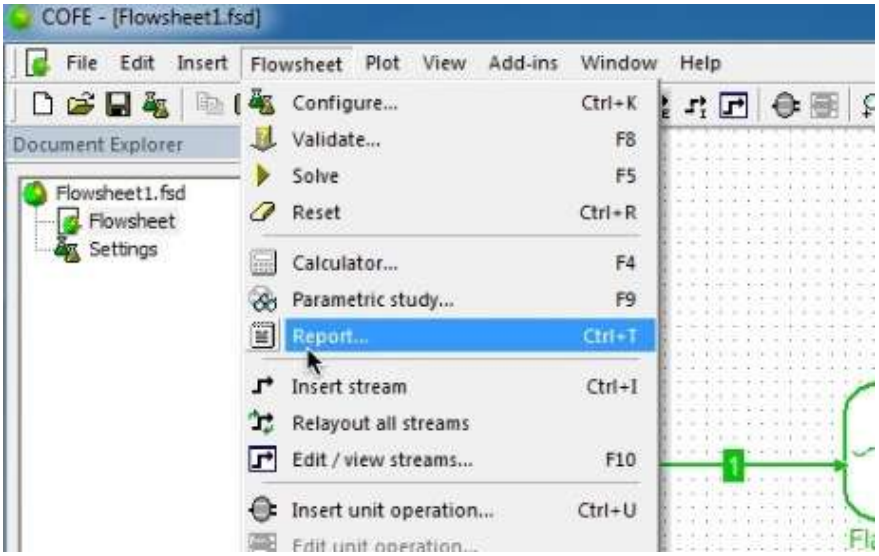

We should have specified enough conditions such that the degrees of freedom of the system are zero. Click the Validate arrow (down arrow with ?) under the Flowsheet menu, or select Validate from that menu. We see a message that we are ready to try to solve or converge the model.



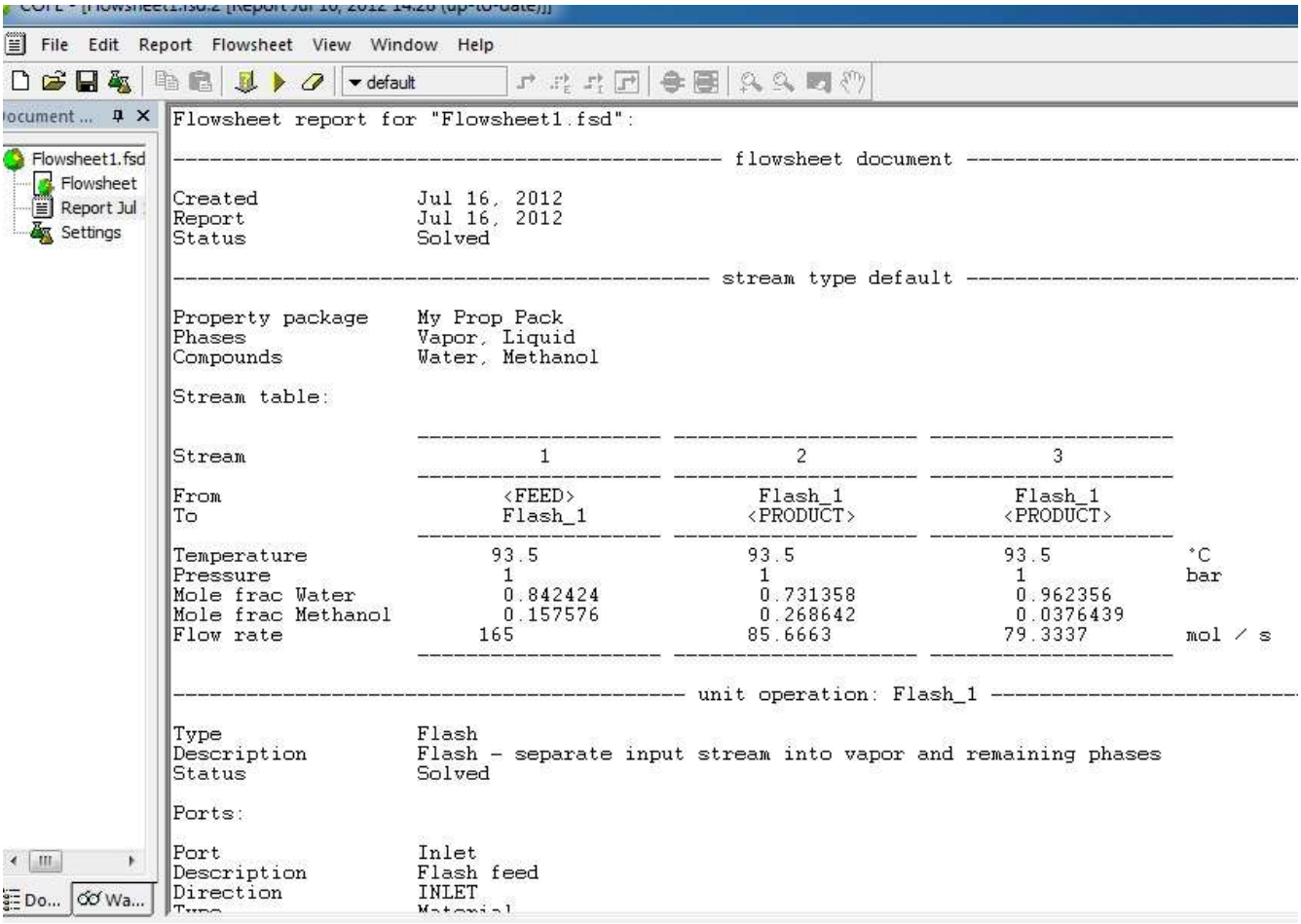
Click the arrow head that points to the right under the Flowsheet menu, or select Solve under that menu.




The model converges to a solution. Move the mouse cursor over stream 2 to see results for that stream.



We can get a full report by selecting Report under the Flowsheet menu.




Is this the correct answer? Not sure at this point. We used the Peng-Robinson thermo model. This might not be the best thermo model to use for these components and phases. Do some literature research for yourself. See how your final results change with changes in the thermo model selected.

For more help and examples, see the example flowsheets and links at the COCO web site <http://www.cocosimulator.org>.

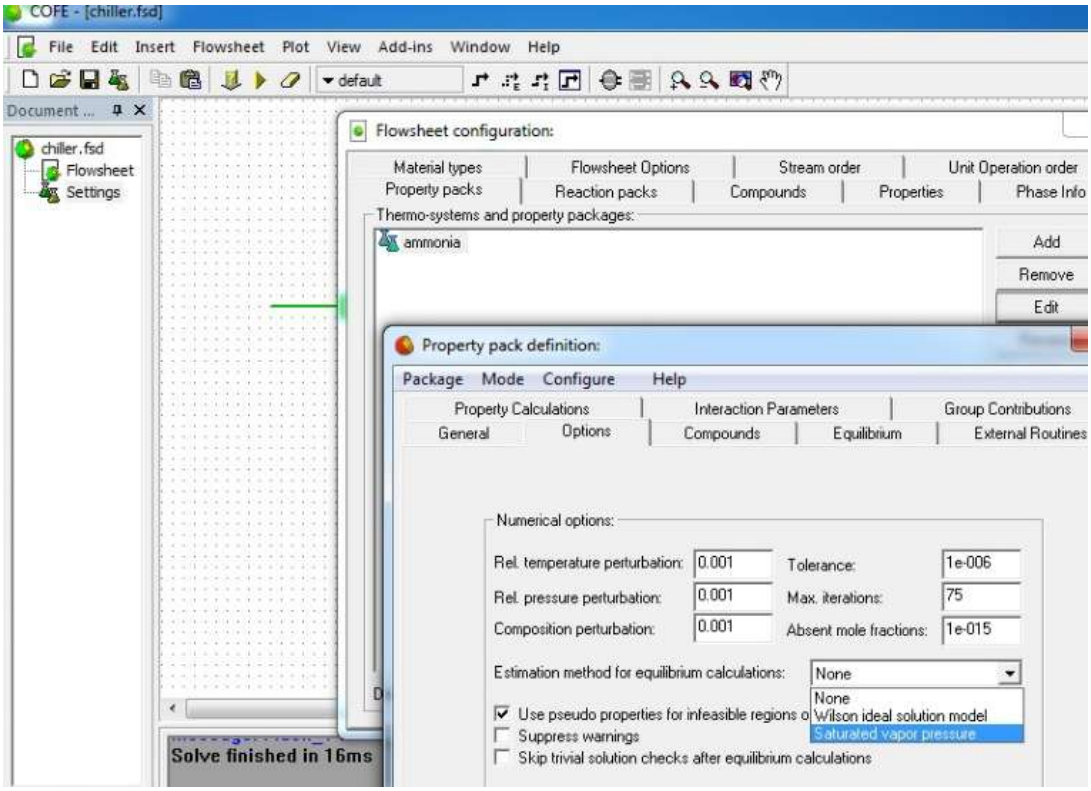
COCO is a free simulator built substantially by one person. Not surprisingly it isn't as robust as a commercial project such as Aspen Plus.

Below is an example as a flash that didn't run with default settings in COCO and required some trouble-shooting to get parameters that allowed a converged solution.

Using both Aspen Plus and COCO, I simulated condensing ammonia from an ammonia synthesis reactor in a flash drum. Peng-Robinson thermo was used in both. Similar results were obtained.

COCO didn't converge when the default setting of "Wilson ideal solution model" was used in the "Estimation method for equilibrium calculations" in Options tab of Property pack definition.

COCO gave good results only when "Saturated vapor pressure" was selected in "Estimation method for equilibrium calculations" in Options tab of Property pack definition. When None or Wilson ideal solution model were selected, all of the feed stream was send overhead as vapor.




COCO gave a warning when the flash drum T was below 250 K, saying this T was outside range of computing properties for $H_2$. However, at least down to 248 K, it gave reasonable results. Aspen had no problem with lower T's.

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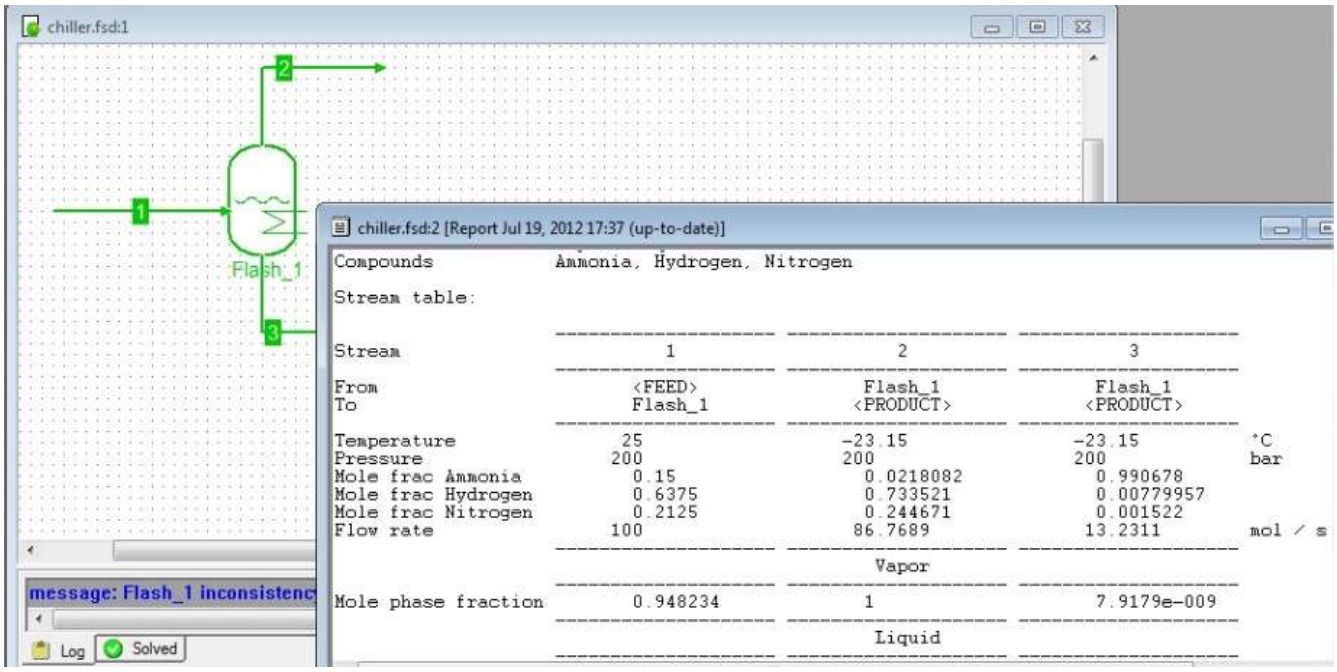
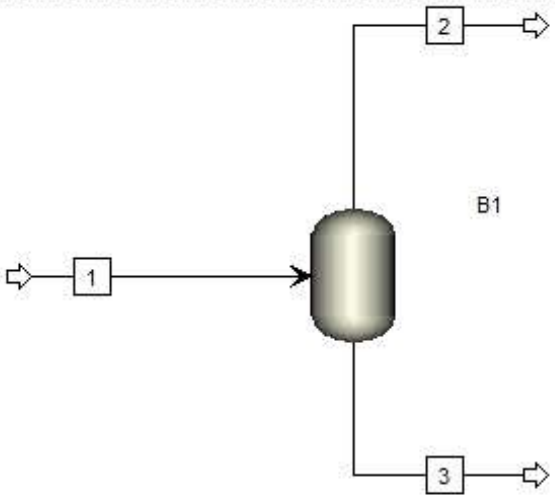



Compounds: Ammonia, Hydrogen, Nitrogen

Stream table:

| Stream | 1 | 2 | 3 | |
|---|---|---|---|---|
| From | <FEED> | Flash_1 | Flash_1 | |
| To | Flash_1 | <PRODUCT> | <PRODUCT> | |
| Temperature | 25 | -23.15 | -23.15 | °C |
| Pressure | 200 | 200 | 200 | bar |
| Mole frac Ammonia | 0.15 | 0.0218082 | 0.990678 | |
| Mole frac Hydrogen | 0.6375 | 0.733521 | 0.00779957 | |
| Mole frac Nitrogen | 0.2125 | 0.244671 | 0.001522 | |
| Flow rate | 100 | 86.7689 | 13.2311 | mol / s |
| | | Vapor | | |
| Mole phase fraction | 0.948234 | 1 | 7.9179e-009 | |
| | | Liquid | | |

COCO results above, Aspen Plus below at -23.15 °C = 250.00 K for both. Note 100 mol/s feed above, 100 kmol/hr feed below.




| Heat and Material Balance Table | | | | |
|---|---|---|---|---|
| Stream ID | | 1 | 2 | 3 |
| Temperature | C | 25.0 | -23.1 | -23.1 |
| Pressure | bar | 200.000 | 200.000 | 200.000 |
| Vapor Frac | | 0.927 | 1.000 | 0.000 |
| Mole Flow | kmol/hr | 100.000 | 86.355 | 13.645 |
| Mass Flow | kg/hr | 979.257 | 747.573 | 231.685 |
| Volume Flow | cum/hr | 12.563 | 9.850 | 0.349 |
| Enthalpy | Gcal/hr | -0.206 | -0.048 | -0.229 |
| Mole Flow | kmol/hr | | | |
| H3N | | 15.000 | 1.439 | 13.561 |
| H2 | | 63.750 | 63.688 | 0.062 |
| N2 | | 21.250 | 21.228 | 0.022 |