First-Pass Distillation Estimates with Aspen Plus® V8.0

1. Lesson Objectives

- DSTWU distillation modeling
- N vs. RR curves
- Initial column sizing

2. Prerequisites

- Aspen Plus V8.0
- Microsoft Excel or similar program
- Experience inserting blocks and connecting streams in Aspen Plus
- Introduction to vapor liquid equilibrium

3. Background

DSTWU Block

The DSTWU block uses equations which are based in theory but are semi-empirical to estimate the separation. The Winn equation, which is a modification of the Fenske equation, is used to estimate the minimum number of theoretical stages. The Underwood equation is used to calculate the minimum reflux ratio. The Gilliland equation is used to calculate the required reflux ratio at a specified number of stages, or the number of stages at a specified reflux ratio. This information is available in the Aspen Help section on DSTWU. View the help page by clicking on the button for DSTWU in the Columns tab of the model palette and then press F1.

Heavy and Light Keys

In two-component distillation, the column splits the feed so a single component is enriched in each exit stream. In multi-component distillation, there are more components than effluent streams, so there are multiple components enriched in at least one of the exit streams. The key components are the components that are split by the column. The light key is the least volatile component enriched in the distillate stream; the heavy key is the most volatile component enriched in the bottoms stream. If there are components A, B, C, and D with decreasing volatility, a column can create the following separations:

Case	1	2	3
Distillate	A	AB	ABC
Bottoms	BCD	CD	D
Light Key	A	B	C
Heavy Key	B	C	D

The examples presented are solely intended to illustrate specific concepts and principles. They may not reflect an industrial application or real situation.

4. Problem Statement and Aspen Plus Solution

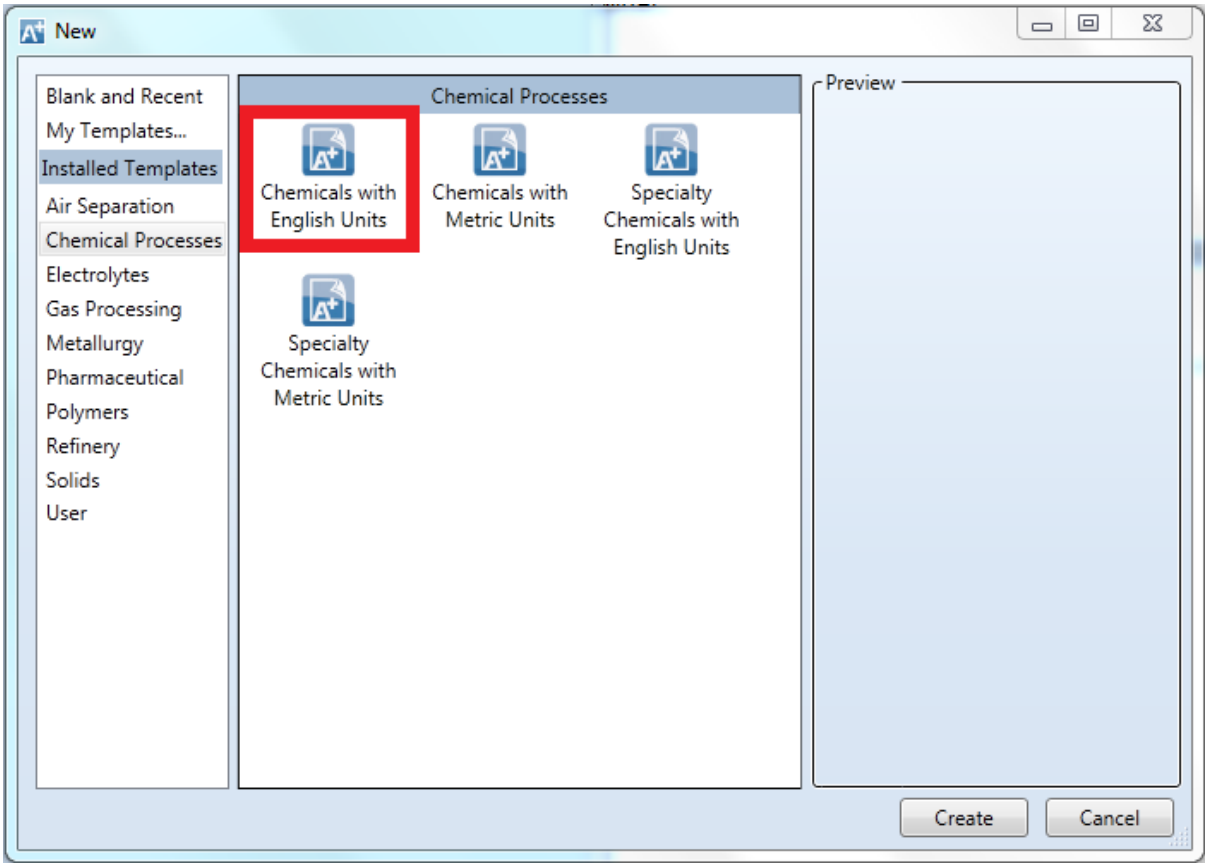
Problem

A stream containing 68.5 wt% ethylene and 31.5 wt% ethane with a total flowrate of 7.3 million lb/day must be separated. Report a reasonable starting point for more detailed design including an estimate of the number of theoretical stages and reflux ratio required to achieve a separation of 99.9% recovery of ethyle ne and 99.0% recovery of ethane.

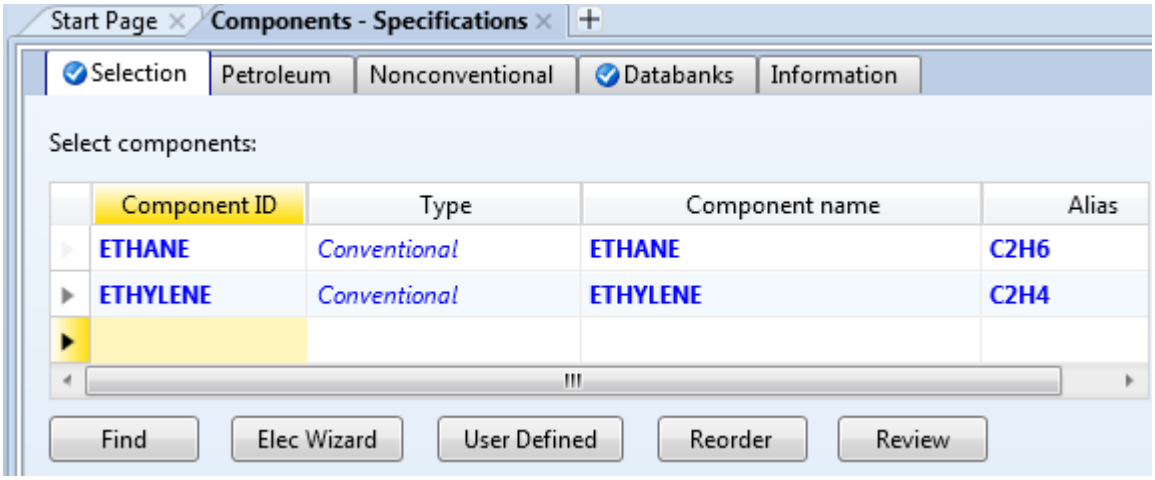
Aspen Plus Solution

Initial estimation for distillation of relatively ideal components like ethane and ethylene can be done using graphical methods and semi-empirical equations like the equations described in the background section. In Aspen Plus, the DSTWU block uses these equations. The user must input which components are the light and heavy keys and the recovery of each of these components, the pressure in the condenser and reboiler, and either the number of stages or reflux ratio. These equations are good starting points, but DSTWU is not a rigorous calculation block; it does not directly use thermodynamics to solve for the reflux ratio or required number of stages. A more rigorous look at this separation problem is available in Dist-001_C2Splitter.

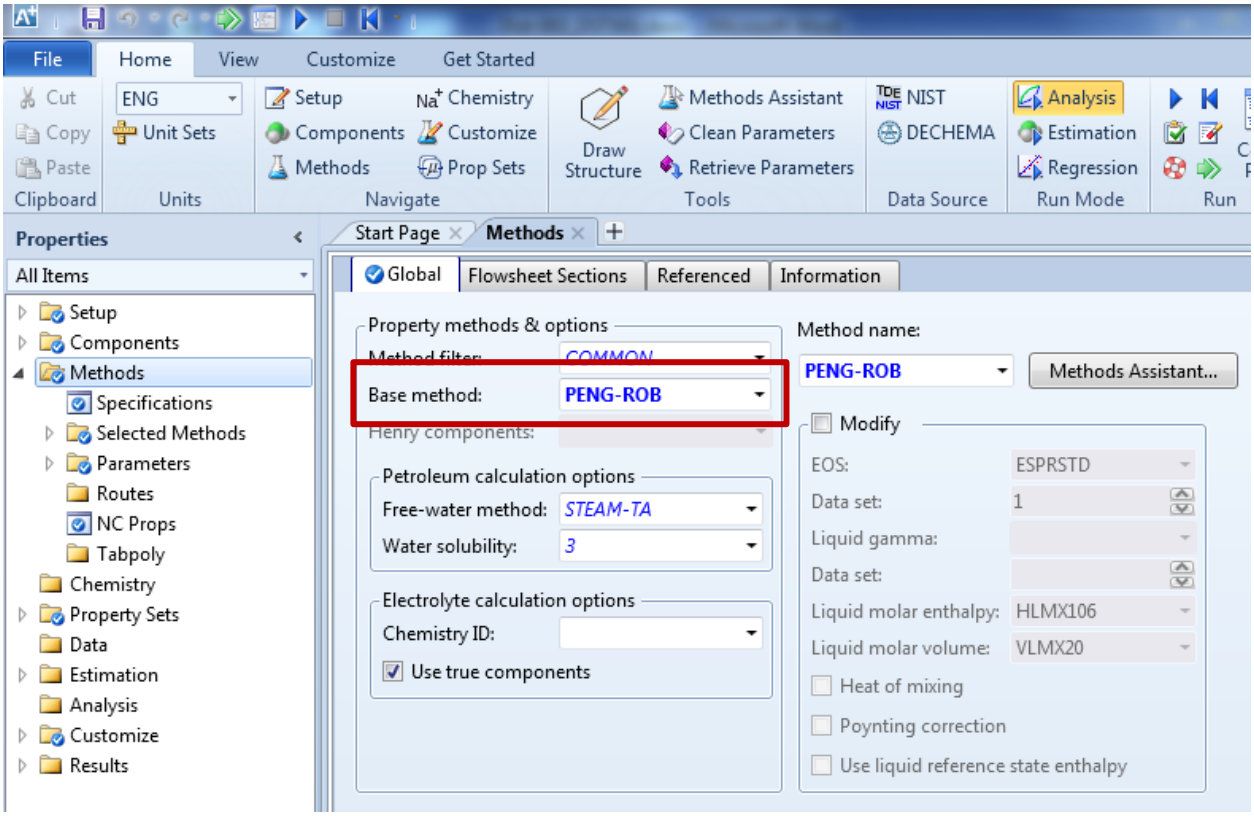
4.01. Open a new Aspen Plus simulation by selecting **New | Chemical Processes | Chemicals with English Units**. Click **Create**.



4.02. In the **Components | Specifications | Selection** tab, enter the components needed for this simulation.

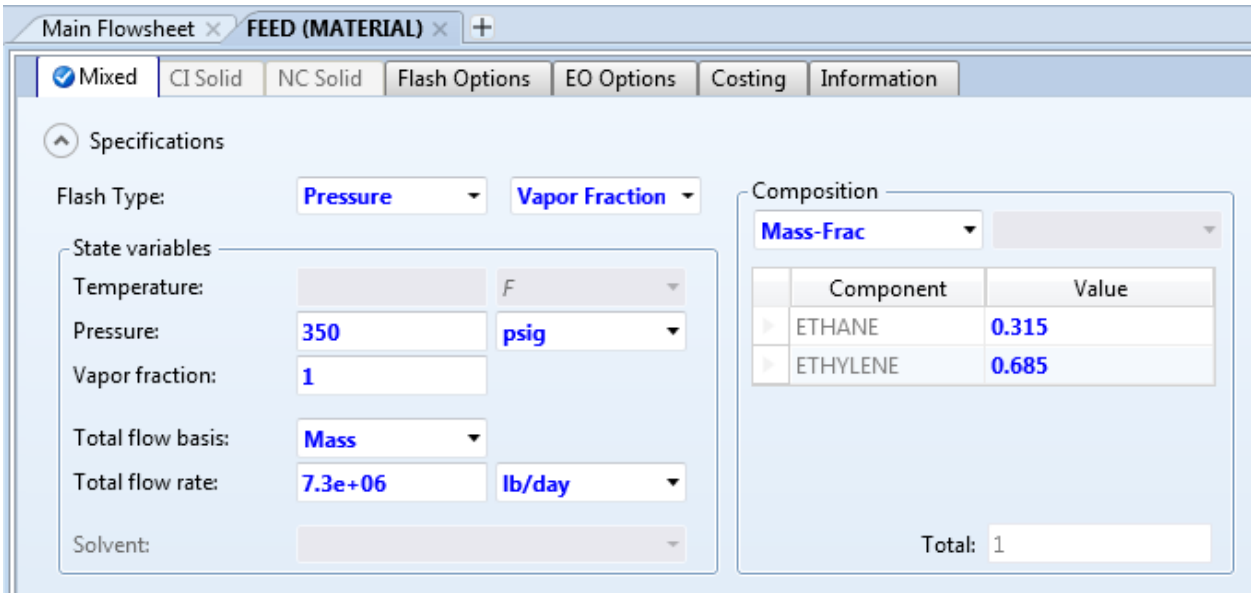


4.03. Define property methods. Click on **Methods** in the navigation pane. Select **Peng-Rob** as the **Base Method**. The Peng-Robinson equation of state is typically used to model systems containing hydrocarbons at high pressures. Populate the binary interaction parameters by clicking **Methods | Parameters | Binary Interaction | PRKBV-1**.

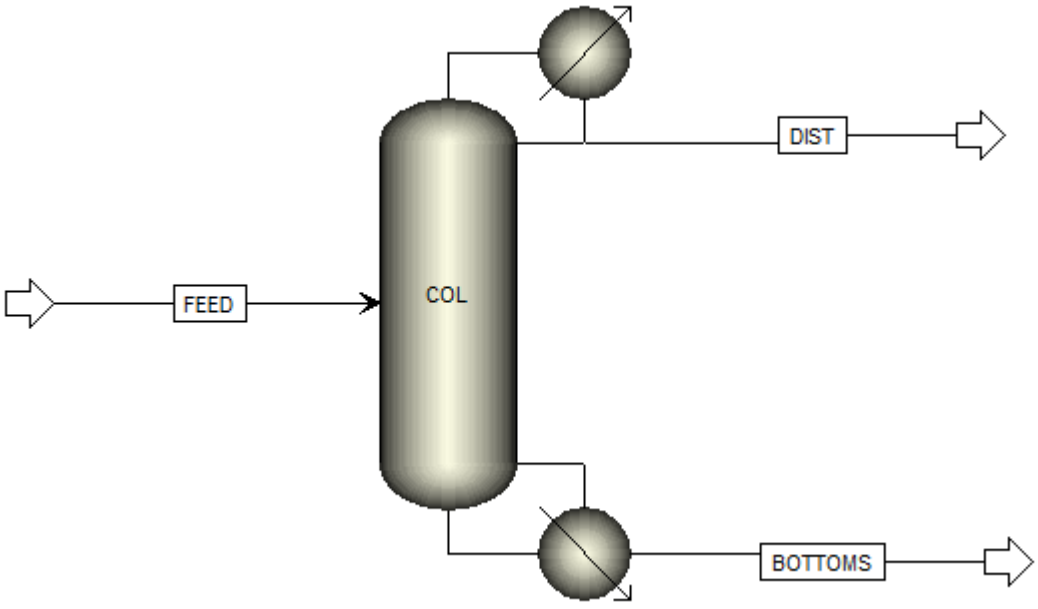


4.04. Go to the simulation environment by clicking on the **Simulation** button below the navigation pane.

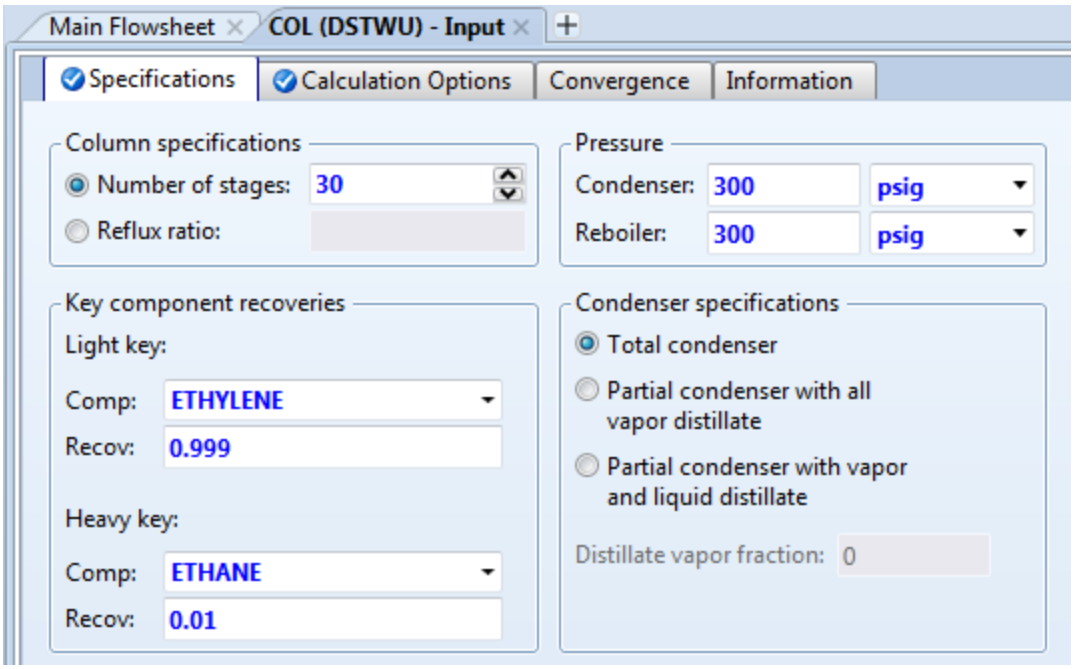
4.05. From the **Model Palette**, add a material stream to the flowsheet, and name it **FEED** (right-click on the stream and click rename, or select the stream and press **Ctrl+M**). Double-click the stream to enter the stream characteristics. Select the **Flash Type** variables to be **Pressure** and **Vapor fraction**. Enter a **Pressure** of **350 psig** and a **Vapor fraction** of **1**. Change the **Total flow basis** to **Mass** and the units to **lb/day**. Enter **7,300,000** into the **Total flow rate** field. Change the **Composition** basis to **Mass-Frac** and enter **0.315** for **ethane** and **0.685** for **ethylene**.



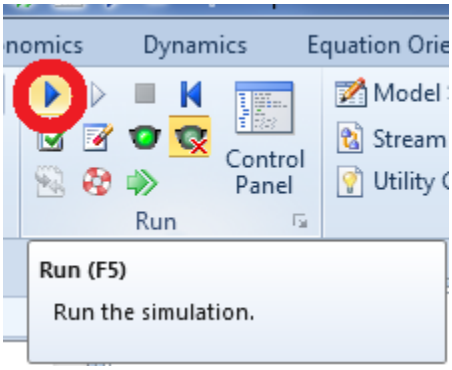
4.06. In the **Columns** section of the **Model Palette**, insert a **DSTWU** block onto the flowsheet and connect the **FEED** stream to the column input. Make a distillate stream and a bottoms stream. Your flowsheet should look like the example below.



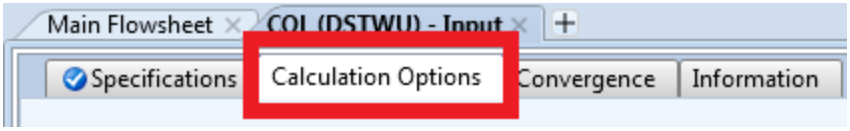
4.07. Double-click on the column to enter the specifications. Enter an initial guess for the **Number of stages**. The **Light key** is **ethylene**, and the **Heavy key** is **ethane**. Enter the desired recoveries for these components in the distillate stream, **99.9%** and **1%** respectively. The condenser and reboiler pressure should both be **300 psig**.



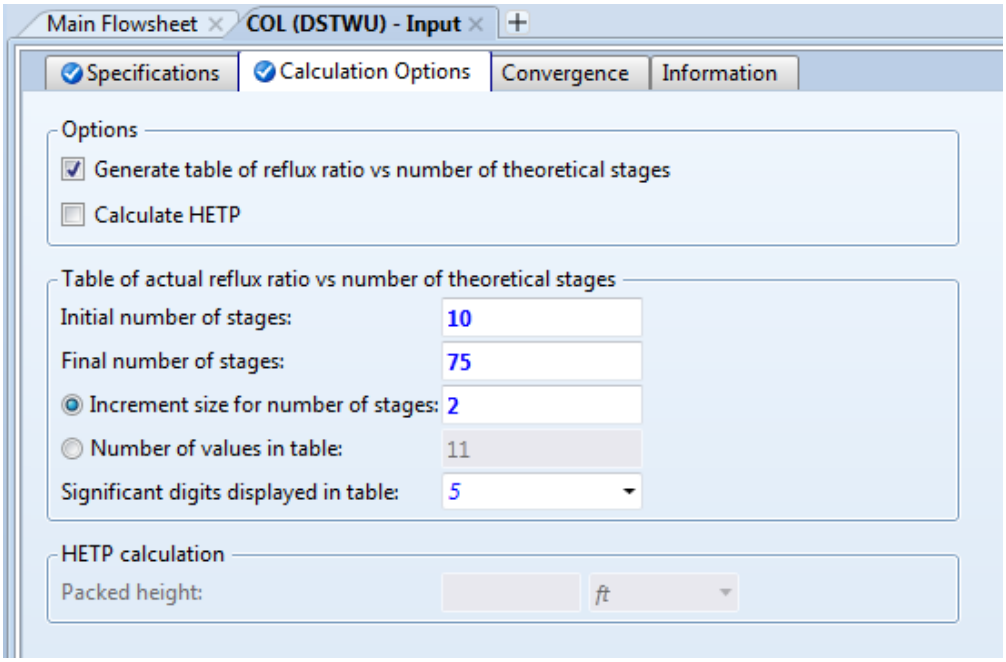
4.08. Open the **Control Panel** and run the simulation by pressing the run button (**F5**).



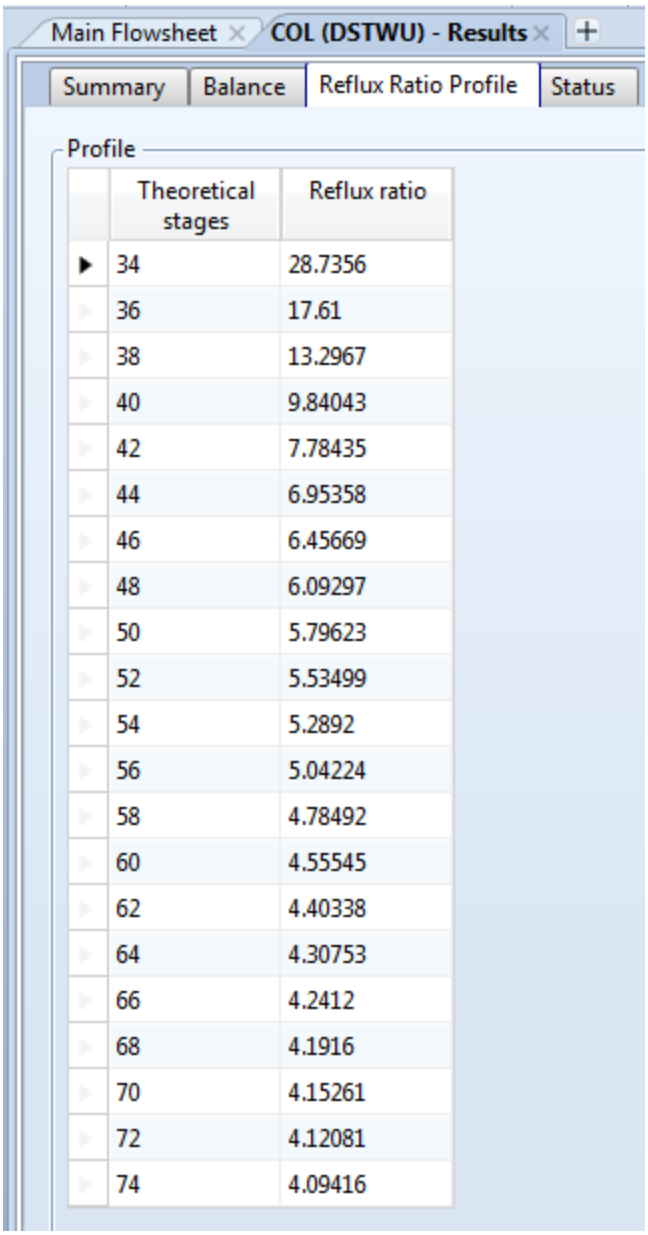
4.09. Create profile of Reflux Ratio versus Number of Stages. Go to the **Calculation Options** tab of the input page for the column.



4.10. Select the **Generate table of reflux ratio vs number of theoretical stages** option. Enter reasonable estimates for the initial and final number of stages, and an increment size that will give you good resolution in the resulting curve.



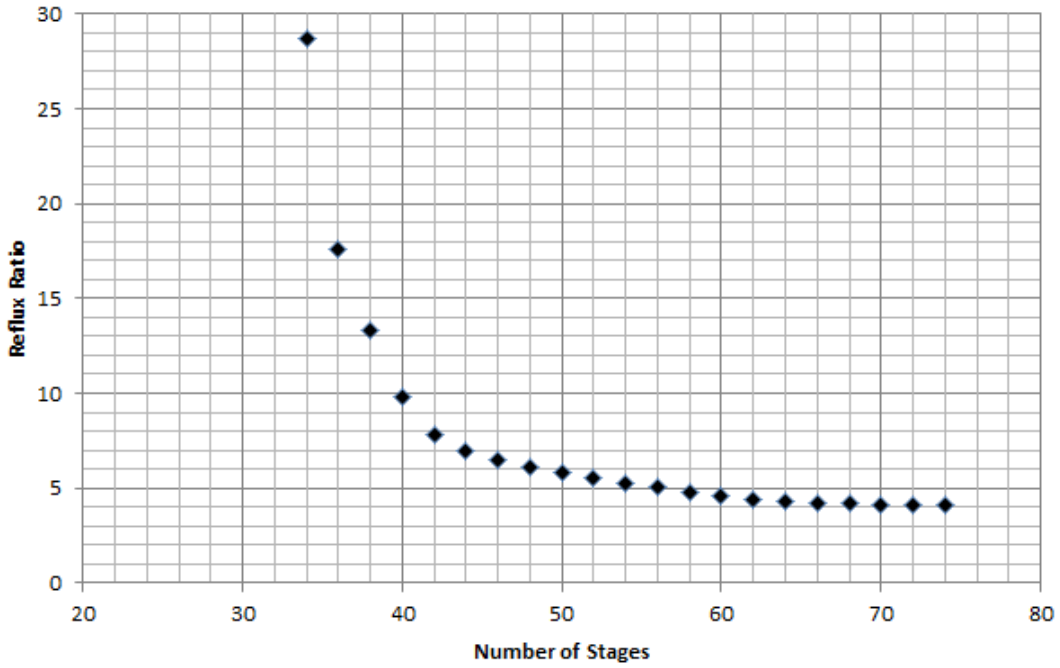
4.11. Run the simulation. The results table for reflux ratio versus number of stages can be found in the **Reflux Ratio Profile** tab of the results page for the column. The column results page is available in the navigation pane or by right-clicking on the column and then clicking **Results**. Your table should resemble the example below.

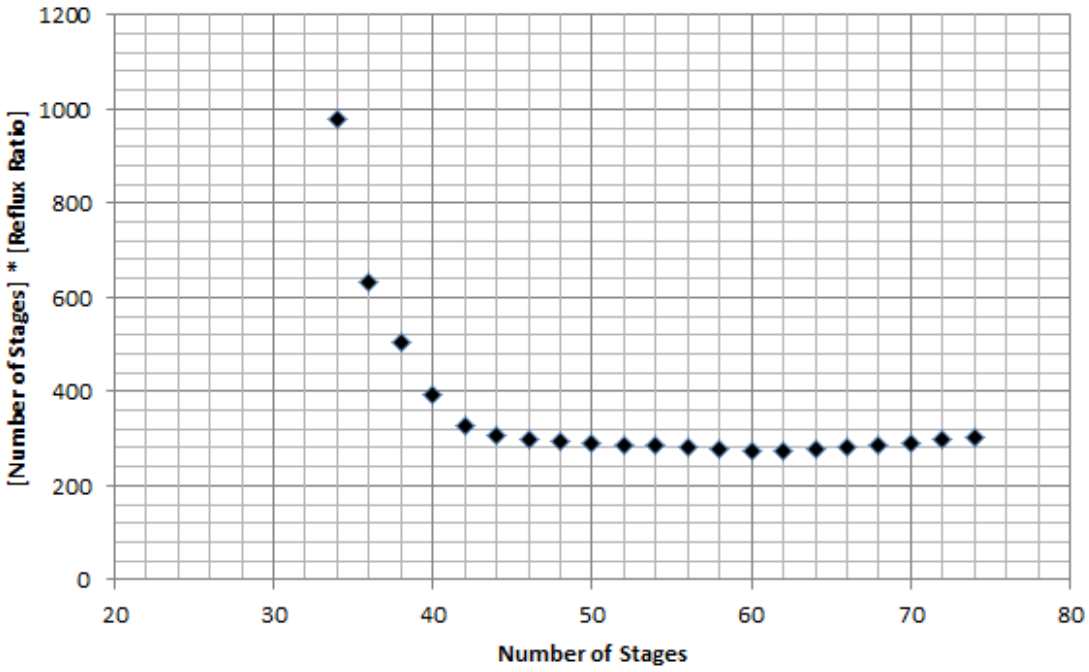


Theoretical stages	Reflux ratio
34	28.7356
36	17.61
38	13.2967
40	9.84043
42	7.78435
44	6.95358
46	6.45669
48	6.09297
50	5.79623
52	5.53499
54	5.2892
56	5.04224
58	4.78492
60	4.55545
62	4.40338
64	4.30753
66	4.2412
68	4.1916
70	4.15261
72	4.12081
74	4.09416

4.12. Copy and paste these values into MS Excel or similar program so you can manipulate and plot them.

4.13. Create a column in the spreadsheet which calculates the product of the number of stages and the reflux ratio. Plot this product and reflux ratio against the number of stages on separate graphs.



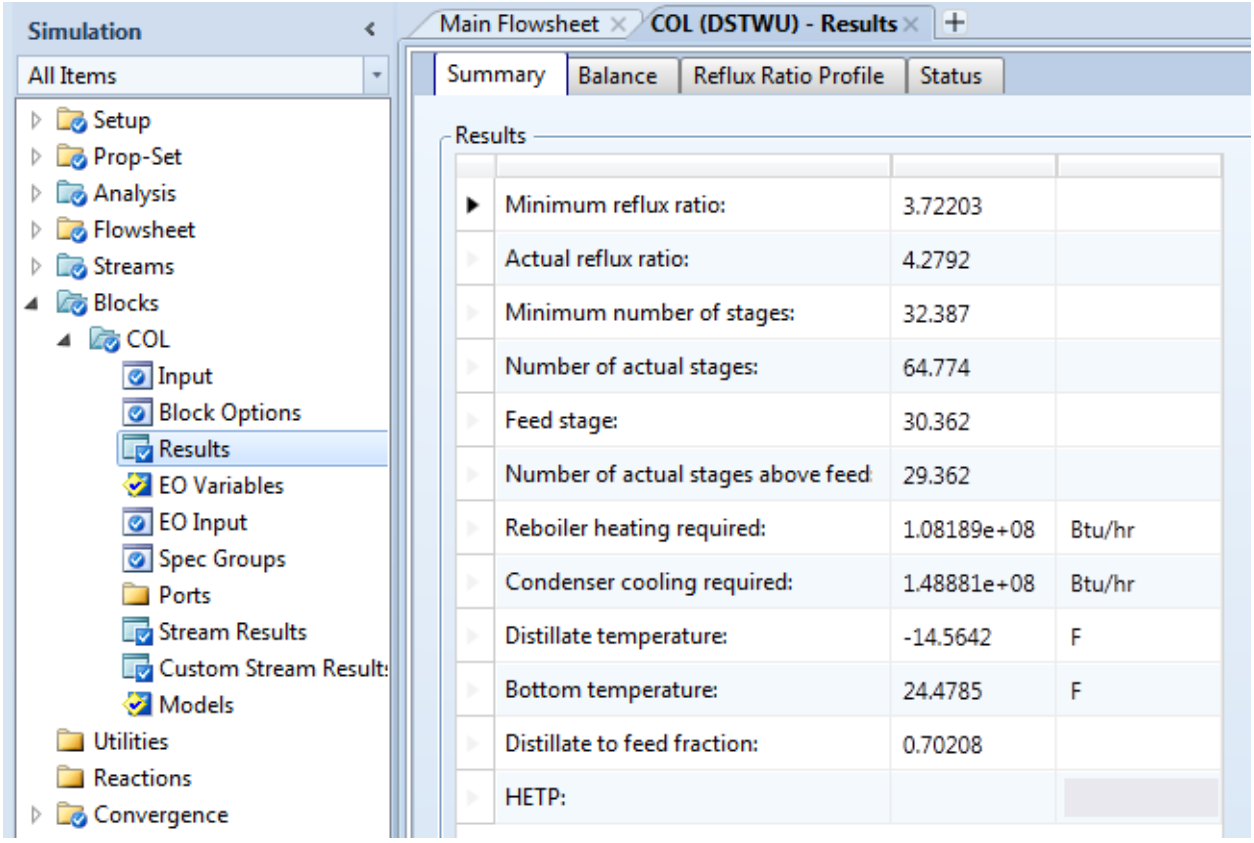


4.14. There is a minimum number of stages for a given separation, the use of which would require infinite reflux. There is a minimum reflux ratio for a given separation, the implementations of which would require an infinite number of stages. Between these extrema, there is a roughly exponential decrease in reflux ratio (RR) with increasing number of stages (N). When the y-axis is N*RR instead of RR, the points will form a curve which has a distinct minimum.

4.15. Increasing the number of stages increases the capital cost of the column. Increasing the reflux ratio increases the operating costs of the column because more material is recycled, and it must be reheated in the reboiler and recondensed in the condenser. Consequently, there is a tradeoff: larger columns have a larger upfront cost but lower operating costs, while smaller columns have smaller capital costs but are more expensive to operate. It turns out that the economic optimum between these tradeoffs often occurs around the minimum of the N*RR vs. N curve. This basic heuristic essentially puts equal weight on the number of stages and reflux ratio.

4.16. A point slightly to the right of the minimum is selected because the DSTWU model assumes complete equilibrium in each stage. In essence, the hand-waiving argument is that a real column will need slightly more stages to achieve the separation modeled in the DSTWU block because a real column cannot achieve the same efficiency as the model.

4.17. Alternatively, you can simply check the Summary tab under results. Here you will see the following.



5. Conclusions

The minimum in the N*RR vs. N curve occurs at 62 theoretical stages, so a guess of around 65-70 stages is a good starting point for more detailed design. This kind of estimation can be done in less than half an hour, even for complex distillation systems, and results in starting points for further analysis.

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