

Distillation of Close Boiling Components with Aspen Plus® V8.0

1. Lesson Objectives

- RadFrac distillation modeling
- Column profiles
- Custom stream results
- Material balance across distillation column

2. Prerequisites

- Aspen Plus V8.0
- Experience inserting blocks and connecting streams in Aspen Plus
- Introduction to vapor liquid equilibrium

3. Background

Ethylene is an important monomer, and is made from ethane. The conversion of the reaction is not perfect, so the ethylene must be separated from the system. Ethane and ethylene are molecularly similar, and so are difficult to separate. The difficulty of the separation is compounded by the fact that polymer production requires extremely pure feedstocks.

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

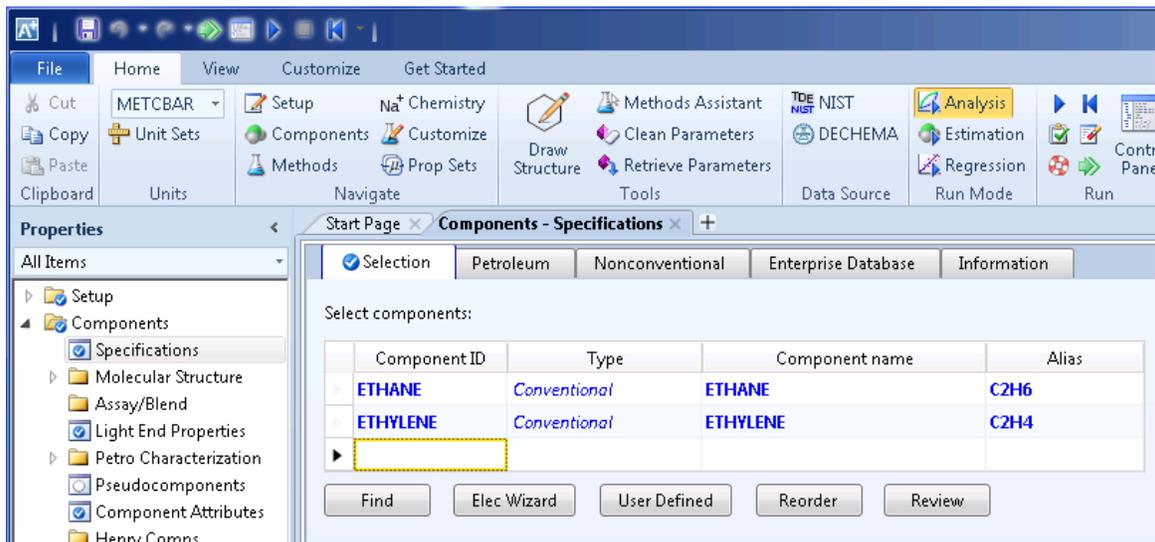
Problem: A stream containing 68.5wt% ethylene with a total flowrate of 7.3 million lb/day is fed into a distillation column consisting of 125 stages. It is desired to produce a distillate product stream containing a minimum of 99.96 wt% ethylene with a total flowrate of 5 million lb/day. It is also desired that the bottoms product contains no more than 0.10wt% ethylene. Determine if this separation is feasible.

Assumptions:

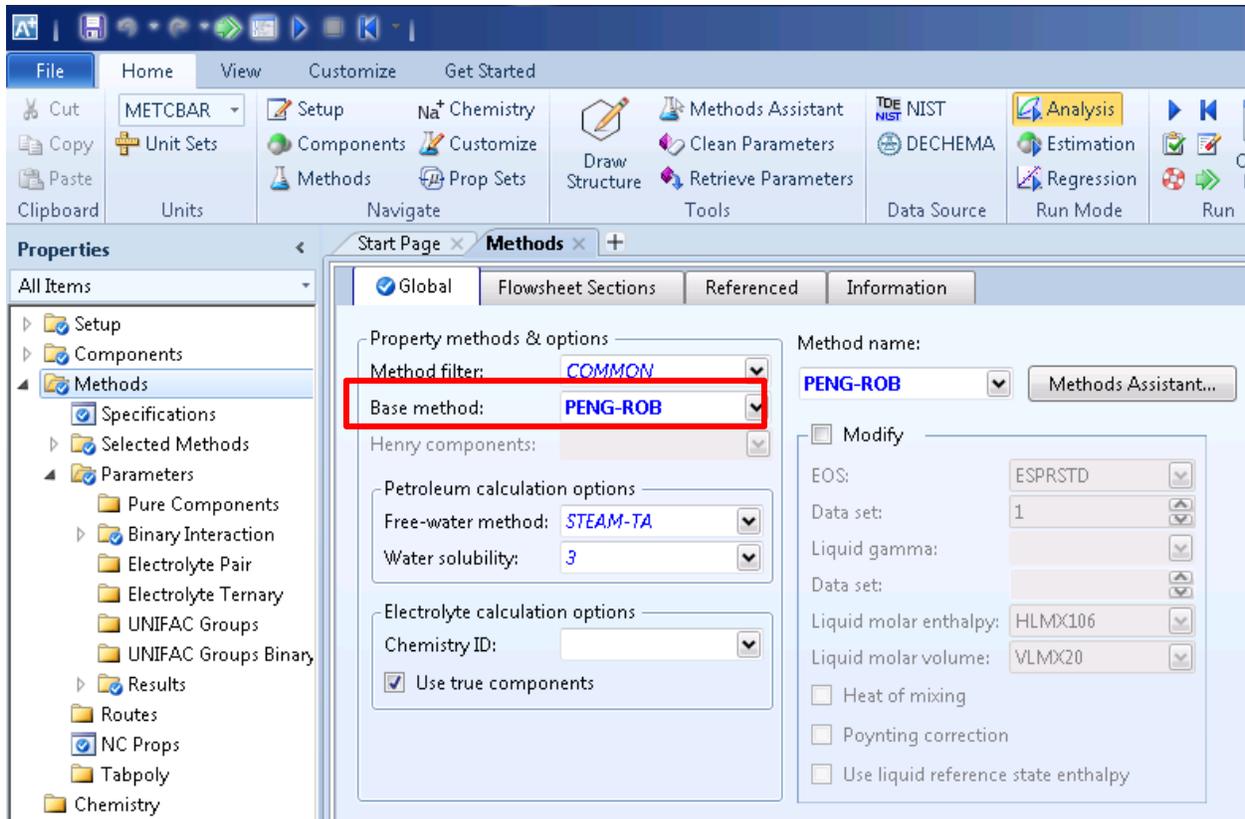
- 100% tray efficiency
- Total condenser
- 300 psig column operating pressure
- A refrigerant utility stream capable of condensing the ethylene mixture (not included in model)
- Feed mixture is at 350 psig and is a vapor
- 125 stages
- Feed enters column at stage 90
- Peng-Robinson equation of state

Aspen Plus Solution:

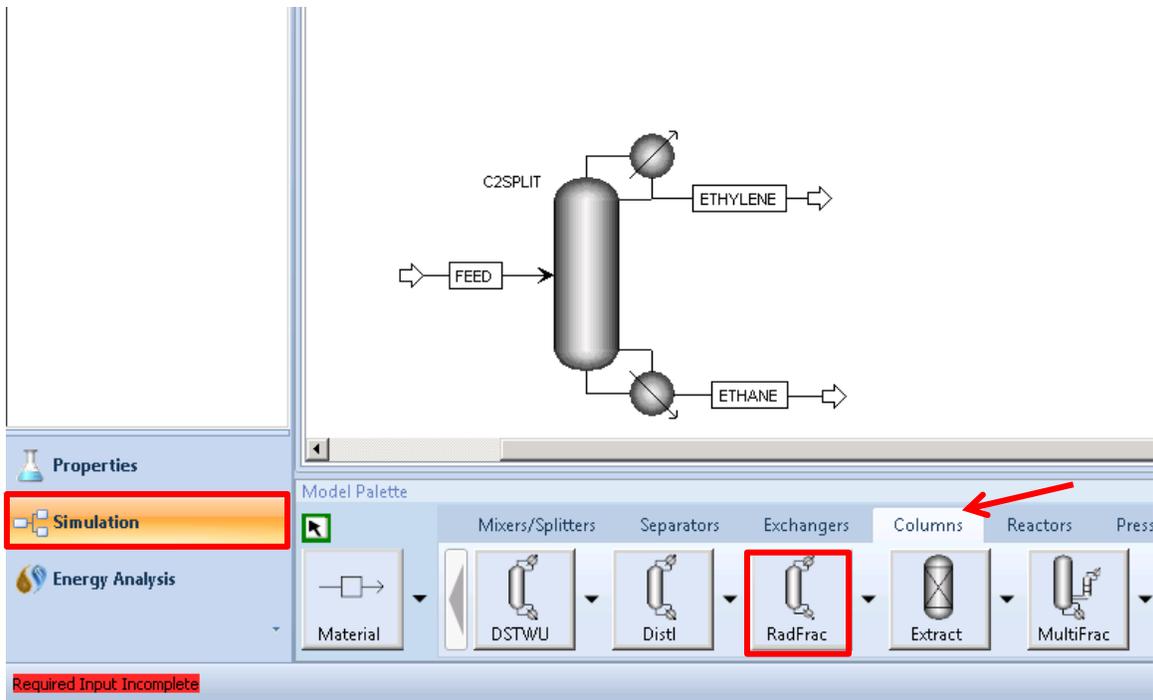
- 4.01. Start **Aspen Plus V8.0**. Select **New | Blank and Recent | Blank Simulation**. Click Create.
- 4.02. Define **Components**. Enter **ethane** and **ethylene** as **Component ID's**, Aspen Plus will recognize these components and will fill in the remaining component information.



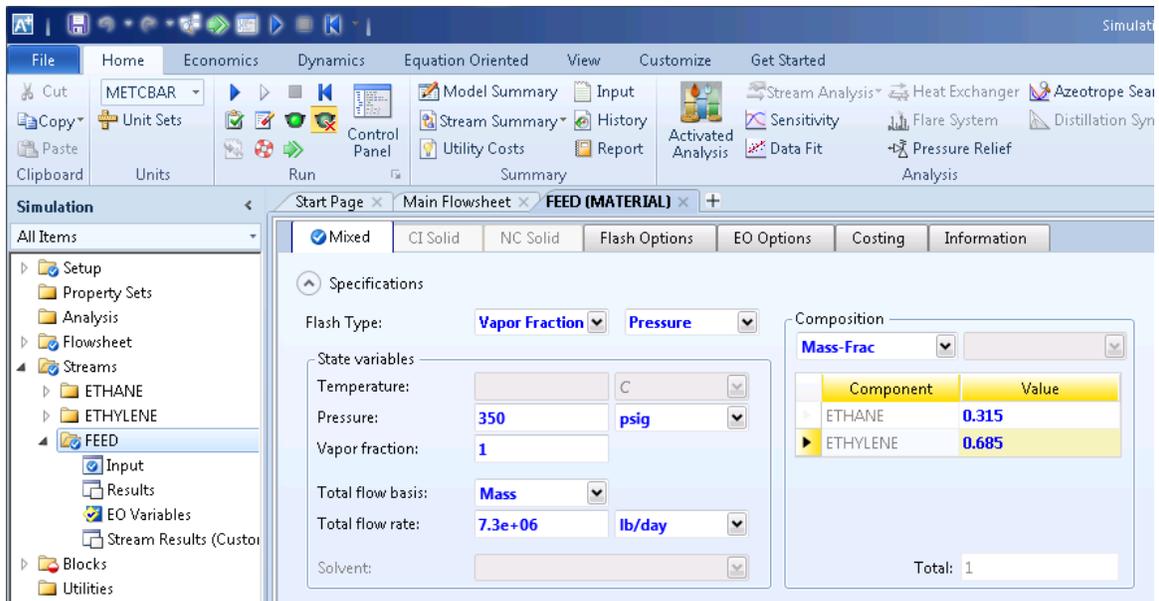
- 4.03. Define **Property Methods**. Click on **Methods** in the navigation pane. Select **PENG-ROB** as the **Base Method**. The Peng-Robinson equation of state is typically used to model systems containing hydrocarbons at high pressures. Populate the model parameters by clicking **Methods | Parameters | Binary Interaction | PRKBV-1**. You can check the accuracy of these parameters by comparing predicted values against data from the **NIST Thermo Data Engine**. You can also define new parameter values by doing a data regression of experimental data.



- 4.04. Construct the Flowsheet. Go to the simulation environment by clicking the **Simulation** button at the bottom left of the screen. Place a **RadFrac** block onto the flowsheet and connect the feed, distillate, and bottoms ports with material streams. The **RadFrac** block is in the **Columns** section of the **Model Palette**; it is a rigorous distillation model which can model multi-phase, non-ideal liquids, and rate-controlled mixing. Rename streams as appropriate.



- 4.05. Specify the **Feed** stream. Double click on the feed stream on the main flowsheet, or go to **Streams** | **FEED** in the navigation pane. Enter the feed composition, flowrate, and state variables as shown below.



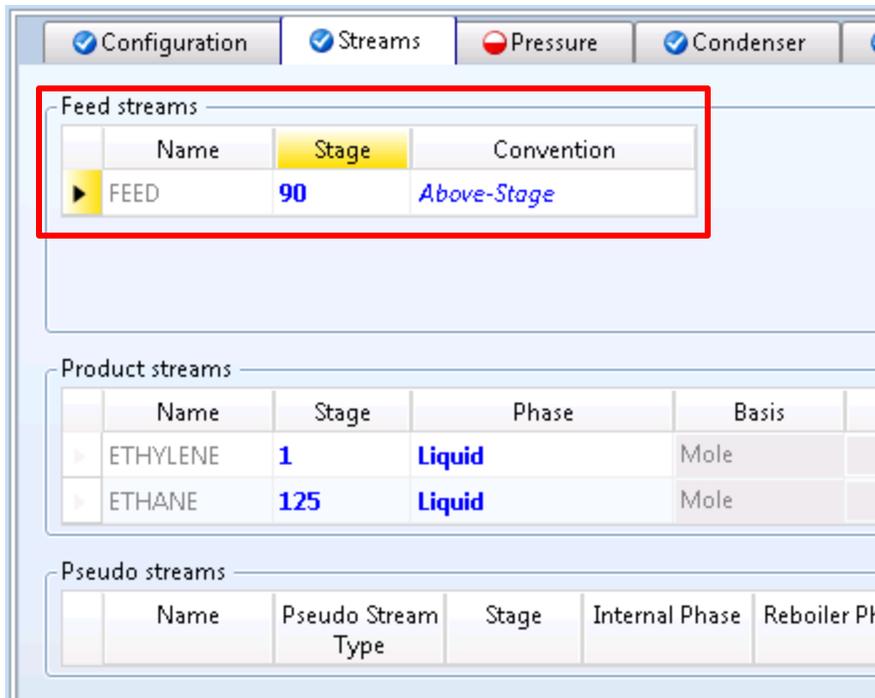
- 4.06. Specify column operating conditions. Go to **Blocks | C2SPLIT | Specifications | Setup**. Enter **125** for **Number of stages** and select **Total** for **Condenser**. The operating specifications must be determined before you can run the simulation. It is common to specify **Distillate to feed ratio** and **Reflux ratio**. Initial estimations will be used as first approximations, which can then be refined in order to meet product specifications. We know what our feed flowrate is, and we know what our desired distillate flowrate is, therefore we can specify the **Distillate to feed ratio**. In this case it is **0.684932** by mass. A **Reflux ratio** of **4** will be entered as a first guess. This is shown below.

The screenshot shows the Aspen Plus C2SPLIT Specifications Setup dialog box. The Configuration tab is selected. The Setup options section includes: Calculation type: Equilibrium; Number of stages: 125; Condenser: Total; Reboiler: Kettle; Valid phases: Vapor-Liquid; Convergence: Standard. The Operating specifications section includes: Distillate to feed ratio: Mass, 0.684932; Reflux ratio: Mole, 4; Free water reflux ratio: 0. A Feed Basis button is also present.

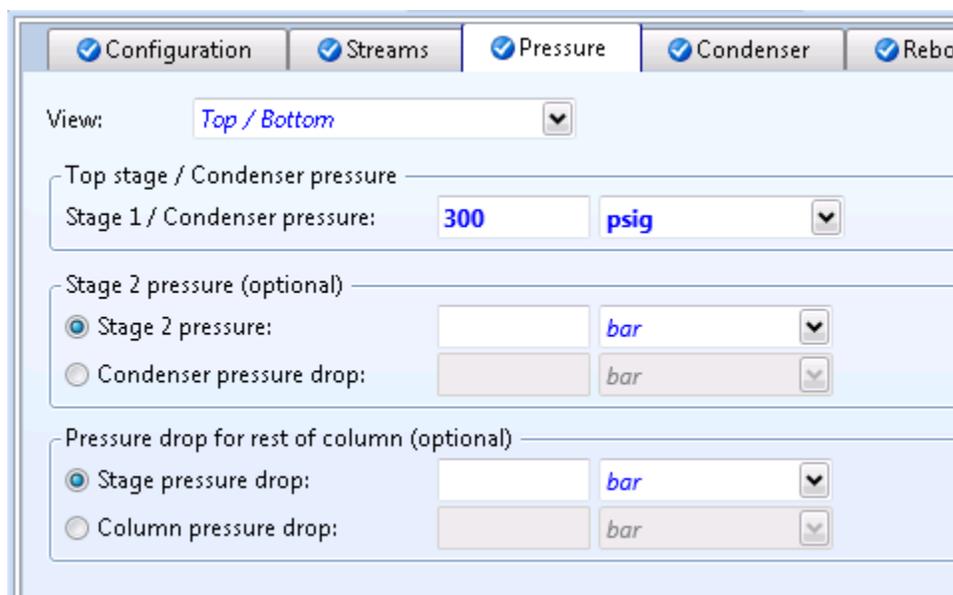
- 4.07. Next, go to the **Streams** tab and enter the stage number at which the feed stream will enter the column. In this case, specify a stage number of **90**.

(FAQ) Useful Option To Know: Convention for stage numbering

The numbering convention in Aspen Plus is that the condenser is stage 1, with stage numbers increasing down the column.



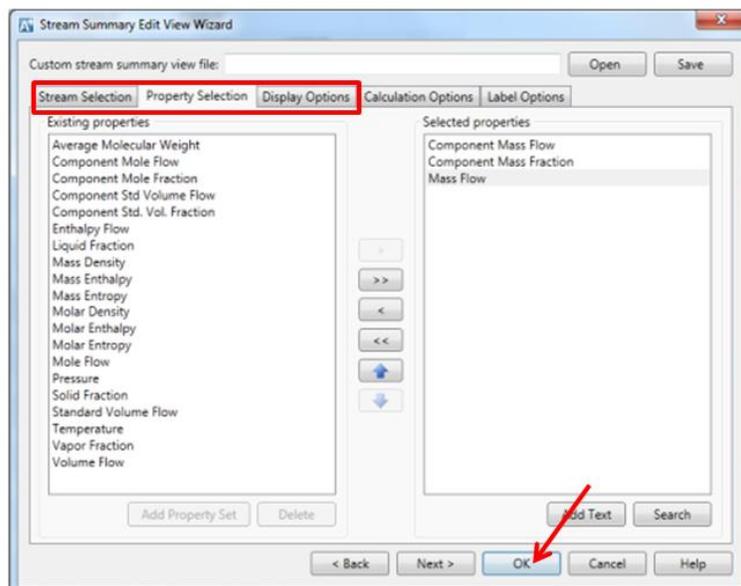
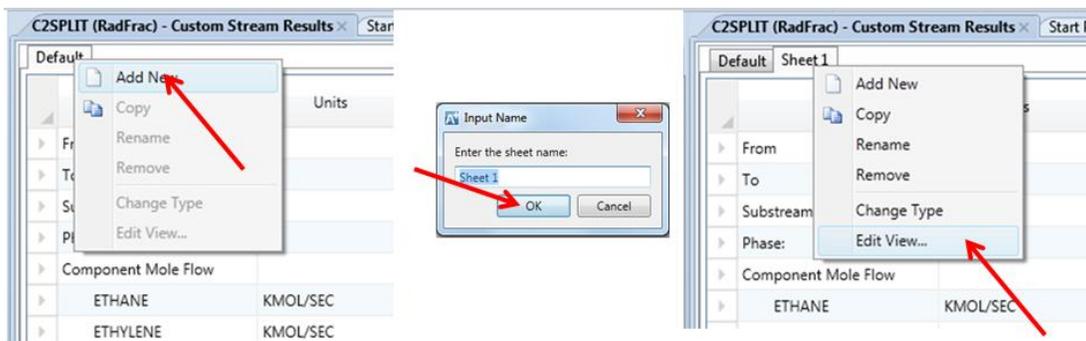
4.08. Next, go to the **Pressure** tab and enter a **Stage 1/condenser pressure** of **300 psig**. For this problem, we will assume that there are no pressure gradients throughout the column. If no pressure drop is entered into Aspen Plus, the top stage pressure will be assumed to be the operating pressure of the entire column. Note that in real life situations there will be a pressure drop throughout the column.



4.09. Open the Control Panel and run the simulation (**F5**).



4.10. Create a custom stream table to view your results. Go to **Blocks | C2SPLIT | Stream Results (Custom)**. Right click on the **Default** tab and select **Add New**. Enter the sheet name for the new results table. Next, right click on the new sheet tab that you just created and select **Edit View**. In the **Stream Summary Edit View Wizard** that appears, select the streams, the properties, and the units you wish to display. This process is shown below.



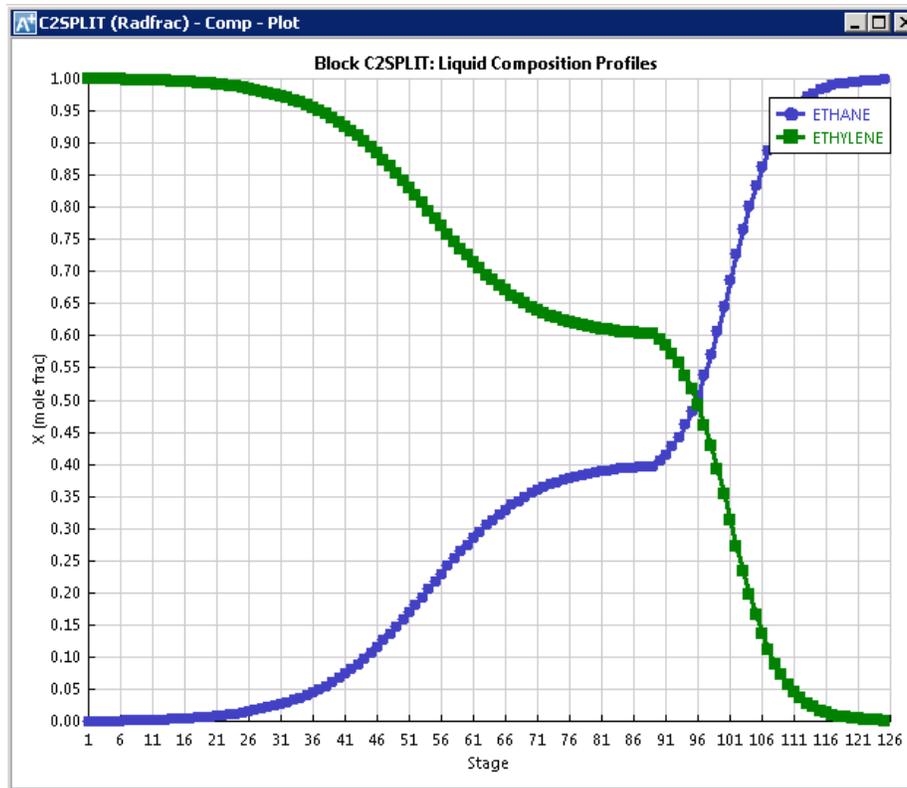
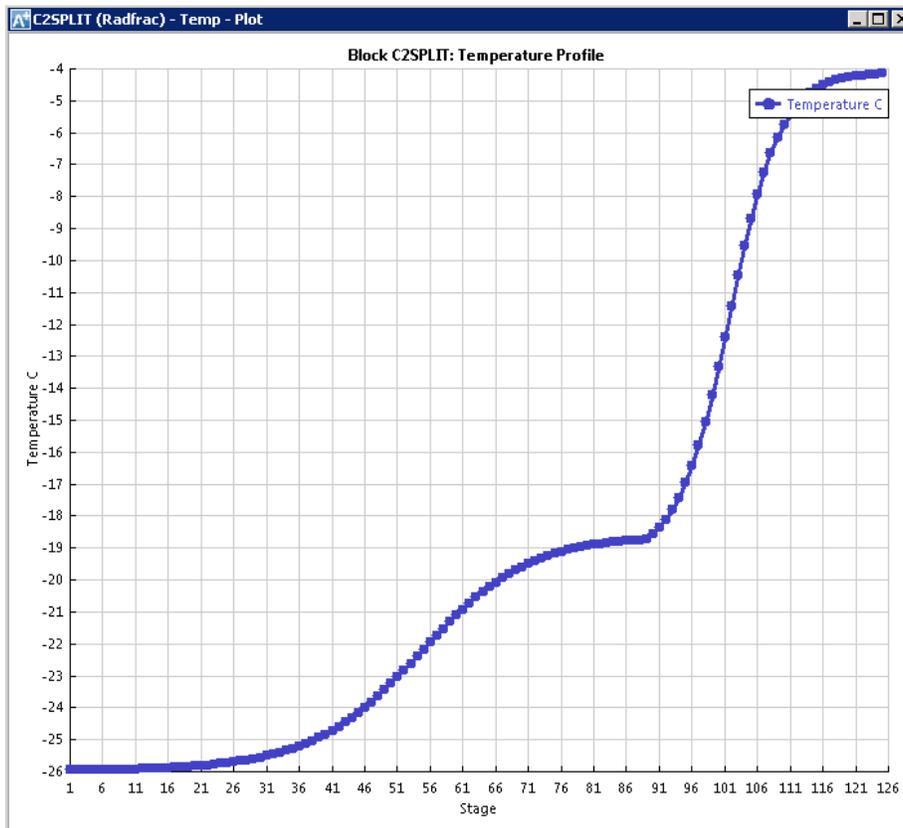
- 4.11. Check results. In the new data sheet you created you can see that both ethylene and ethane streams meet the product specifications.

		Units	ETHANE	ETHYLENE	FEED	
From			C2SPLIT	C2SPLIT		
To					C2SPLIT	
Substream: MIXED						
Phase: All						
Component Mass Flow						
ETHANE	LB/DAY		2.29786e+06	1639.18	2.2995e+06	
ETHYLENE	LB/DAY		2135.58	4.99836e+06	5.0005e+06	
Component Mass Fraction						
ETHANE			0.999072	0.000327835	0.315	
ETHYLENE			0.000928514	0.999672	0.685	
Mass Flow	LB/DAY		2.3e+06	5e+06	7.3e+06	

- 4.12. View column profile. Go to **Blocks | C2SPLIT | Profiles**. Here you can view Temperature, Pressure, Heat, and Material profiles over the column. Clicking the **Compositions** tab will display the compositions at each stage in the column. You can choose to display either vapor or liquid compositions, and you can choose to display mole or mass fractions. You can then graph these profiles by using the plot tool located on the Home ribbon. Temperature and composition profile plots are shown below.

The screenshot shows the Aspen Plus interface with the 'C2SPLIT (RadFrac) - Profiles' window open. The 'Compositions' tab is selected, showing a table of stage data. A red box highlights the 'Custom' and 'Temp' plot icons in the top right corner of the software interface.

Stage	Temperature (C)	Pressure (bar)	Heat duty (cal/sec)	Liquid from (Mole) (kmol/hr)	Vapor from (Mole) (kmol/hr)	Liquid feed (Mole) (kmol/hr)	Vapor feed (Mole) (kmol/hr)
1	-25.9344	21.6975	-9.81193e+...	16842	0	0	0
2	-25.9324	21.6975	0	13473.4	16842	0	0
3	-25.9301	21.6975	0	13473.2	16841.8	0	0
4	-25.9276	21.6975	0	13473	16841.6	0	0
5	-25.9249	21.6975	0	13472.7	16841.4	0	0
6	-25.9218	21.6975	0	13472.4	16841.1	0	0
7	-25.9183	21.6975	0	13472.1	16840.8	0	0
8	-25.9144	21.6975	0	13471.7	16840.5	0	0
9	-25.9101	21.6975	0	13471.3	16840.1	0	0



5. Conclusions

The 125 stage column was able to exceed the specification of 99.96wt% ethylene at 5 million lb/day, as well as the bottoms having less than 0.10wt% ethylene. It could then be concluded that this column is capable of completing the desired separation. Aspen Plus allows engineers to model existing equipment and see if it is possible to repurpose it or, otherwise, design new equipment that would meet very specific criteria.

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