



## Distillation Column Simulation





Example:  $100 \text{ kmol}\cdot\text{h}^{-1}$  of a mixture containing 10, 20, 30, and 40 mol% of propane, *n*-butane, *n*-pentane, and *n*-hexane, respectively, is preheated before entering a distillation tower. Initial temperature of the mixture is  $25^\circ\text{C}$ , and the pressure drop can be neglected. The preheated vapor fraction is 0.2. The preheated mixture has to be separated in a distillation tower. The mole fraction of *n*-pentane in the distillate product is 0.05 and that of *n*-butane in the bottom product is also 0.05. Using the Fenske–Underwood–Gilliland method, calculate the minimum reflux ratio and the minimum number of theoretical stages needed. Assuming a reflux ratio 1.5 times higher than the minimum reflux ratio, calculate the actual number of trays, optimal feed stage, condenser and reboiler temperature, and distribution of non-key components into the distillate and bottom. Consider a uniform pressure in the column of 700 kPa.

How to simulate:

1. Add components to the component list.

Source Databank: HYSYS

Select: **Pure Components** Filter: **All Families**

Search for: Search by: **Full Name/Synonym**

Component	Type	Group
Propane	Pure Component	
n-Hexane	Pure Component	
n-Pentane	Pure Component	
n-Butane	Pure Component	

< Add Replace Remove

Simulation Name	Full Name / Synonym	Formula
Methane	C1	CH4
Ethane	C2	C2H6
i-Butane	i-C4	C4H10
i-Pentane	i-C5	C5H12
n-Heptane	C7	C7H16
n-Octane	C8	C8H18
n-Nonane	C9	C9H20
n-Decane	C10	C10H22
n-C11	C11	C11H24
n-C12	C12	C12H26
n-C13	C13	C13H28
n-C14	C14	C14H30

Status: OK

2. Select Peng-Robinson as the Fluid Package.

Set Up Binary Coeffs StabTest Phase Order Tabular Notes

Package Type: HYSYS Component List Selection: **Component List - 1 [HYSYS Databanks]** View

Property Package Selection:

- Glycol Package
- Grayson Streed
- IAPWS-IF97
- Kabadi-Danner
- Lee-Kesler-Plöcker
- MBWR
- NBS Steam
- NRTL
- Peng-Robinson**
- PR-Twu
- PRSV
- Sour PR
- Sour SRK
- Sour Water
- SRK
- SRK-Twu
- Sulsim (Sulfur Recovery)
- Twu-Sim-Tassone

Options:

Enthalpy	Property Package EOS
Density	Costald
Modify Tc, Pc for H2, He	Modify Tc, Pc for H2, He
Viscosity Method	HYSYS Viscosity
Peng-Robinson Options	HYSYS
EOS Solution Methods	Cubic EOS Analytical Method
Phase Identification	Default
Surface Tension Method	HYSYS Method
Thermal Conductivity	API 12A3.2-1 Method

Parameters:

Property Pkg: OK Edit Properties



3. Enter Simulation Environment and define streams and set-up the heater.

Material Stream: 1

Worksheet Attachments Dynamics

**Worksheet**

Conditions Properties Composition Oil & Gas Feed Petroleum Assay K Value User Variables Notes Cost Parameters Normalized Yields Emissions

Stream Name	1	Liquid Phase
Vapour / Phase Fraction	0.0000	1.0000
Temperature [C]	25.00	25.00
Pressure [kPa]	700.0	700.0
Molar Flow [kgmole/h]	100.0	100.0
Mass Flow [kg/h]	7215	7215
Std Ideal Liq Vol Flow [m3/h]	11.50	11.50
Molar Enthalpy [kJ/kgmole]	-1.730e+005	-1.730e+005
Molar Entropy [kJ/kgmole-C]	80.73	80.73
Heat Flow [kJ/h]	-1.730e+007	-1.730e+007
Liq Vol Flow @Std Cond [m3/h]	11.40	11.40
Fluid Package	Basis-1	
Utility Type		

OK

Delete Define from Stream... View Assay

Material Stream: 1

Worksheet Attachments Dynamics

**Worksheet**

Conditions Properties Composition Oil & Gas Feed Petroleum Assay K Value User Variables Notes Cost Parameters Normalized Yields Emissions

	Mole Fractions	Liquid Phase
Propane	0.1000	0.1000
n-Hexane	0.4000	0.4000
n-Pentane	0.3000	0.3000
n-Butane	0.2000	0.2000

Total 1.00000

Edit... View Properties... Basis...

OK

Delete Define from Stream... View Assay



Heater: E-100

Design Rating Worksheet Performance Dynamics

**Design**

Name **E-100**

Connections  
Parameters  
User Variables  
Notes

Inlet **1** Energy **Energy**

Outlet **Preheat**

Fluid Package **Basis-1**

Delete OK Ignored

Heater: E-100

Design Rating Worksheet Performance Dynamics

**Design**

Connections  
**Parameters**  
User Variables  
Notes

Delta P **0.0000 kPa**

Delta T **72.34 C** Duty **1.67566e+006 kJ/h**

Delete OK Ignored



Heater: E-100

Design Rating Worksheet Performance Dynamics

**Worksheet**

Conditions Properties Composition PF Specs

Name	1	Preheat	Energy
Vapour	0.0000	0.2000	<empty>
Temperature [C]	25.00	97.34	<empty>
Pressure [kPa]	700.0	700.0	<empty>
Molar Flow [kgmole/h]	100.0	100.0	<empty>
Mass Flow [kg/h]	7215	7215	<empty>
Std Ideal Liq Vol Flow [m3/h]	11.50	11.50	<empty>
Molar Enthalpy [kJ/kgmole]	-1.730e+005	-1.562e+005	<empty>
Molar Entropy [kJ/kgmole-C]	80.73	129.9	<empty>
Heat Flow [kJ/h]	-1.730e+007	-1.562e+007	1.676e+006

Delete OK Ignored

4. Select a Short-cut from Model Palette/Separators. Act like below:

Shortcut Column: T-100

Design Rating Worksheet Performance Dynamics

**Design**

Connections Parameters User Variables Notes

Name T-100

Condenser Duty Qc

Distillate D

Reboiler Duty Qr

Bottoms B

Inlet Preheat

Fluid Package Basis-1

Top Product Phase Liquid Vapour

Delete Unknown Key Components Ignored



5. On the Parameters tab, under Design, complete the requirements for key component distribution and column pressure; when these parameters are specified, HYSYS calculates the minimum reflux ratio. Calculate the value of the external reflux ratio by multiplication of this value with the given coefficient and enter it as value of External Reflux Ratio.

Shortcut Column: T-100

Design Rating Worksheet Performance Dynamics

**Design**

Connections  
Parameters  
User Variables  
Notes

Components

	Component	Mole Fraction
Light Key in Bottoms	n-Butane	0.0500
Heavy Key in Distillate	n-Pentane	0.0500

Pressures

Condenser Pressure	700.000 kPa
Reboiler Pressure	700.000 kPa

Reflux Ratios

External Reflux Ratio	2.200
Minimum Reflux Ratio	1.463

Delete OK Ignored

6. On the Performance page, check the distillation column parameters; on the Composition tab, under Worksheet, check the composition of products.



Shortcut Column: T-100

Design Rating Worksheet Performance Dynamics

**Performance**

Trays

Minimum Number of Trays	5.474
Actual Number of Trays	10.463
Optimal Feed Stage	5.959

Temperatures

Condenser [C]	40.64
Reboiler [C]	122.4

Flows

Rectify Vapour [kgmole/h]	88.916
Rectify Liquid [kgmole/h]	61.130
Stripping Vapour [kgmole/h]	68.916
Stripping Liquid [kgmole/h]	141.130
Condenser Duty [kJ/h]	-1752095.376
Reboiler Duty [kJ/h]	1540652.723

Delete OK Ignored

Shortcut Column: T-100

Design Rating Worksheet Performance Dynamics

**Worksheet**

Conditions Properties Composition

Name	Preheat	D	B
Vapour	0.2000	0.0000	0.0000
Temperature [C]	97.34	40.64	122.4
Pressure [kPa]	700.0	700.0	700.0
Molar Flow [kgmole/h]	100.0	27.79	72.21
Mass Flow [kg/h]	7215	1495	5720
Std Ideal Liq Vol Flow [m3/h]	11.50	2.665	8.838
Molar Enthalpy [kJ/kgmole]	-1.562e+005	-1.370e+005	-1.665e+005
Molar Entropy [kJ/kgmole-C]	129.9	78.72	135.4
Heat Flow [kJ/h]	-1.562e+007	-3.808e+006	-1.203e+007
Name	Qr	Qc	
Vapour	<empty>	<empty>	
Temperature [C]	<empty>	<empty>	
Pressure [kPa]	<empty>	<empty>	
Molar Flow [kgmole/h]	<empty>	<empty>	
Mass Flow [kg/h]	<empty>	<empty>	
Std Ideal Liq Vol Flow [m3/h]	<empty>	<empty>	
Molar Enthalpy [kJ/kgmole]	<empty>	<empty>	
Molar Entropy [kJ/kgmole-C]	<empty>	<empty>	
Heat Flow [kJ/h]	1.541e+006	-1.752e+006	

Delete OK Ignored



Shortcut Column: T-100

Design Rating Worksheet Performance Dynamics

**Worksheet**

Conditions  
Properties  
Composition

	Preheat	D	B
Propane	0.1000	0.3592	0.0003
n-Hexane	0.4000	0.0009	0.5536
n-Pentane	0.3000	0.0500	0.3962
n-Butane	0.2000	0.5899	0.0500

Delete OK Ignored

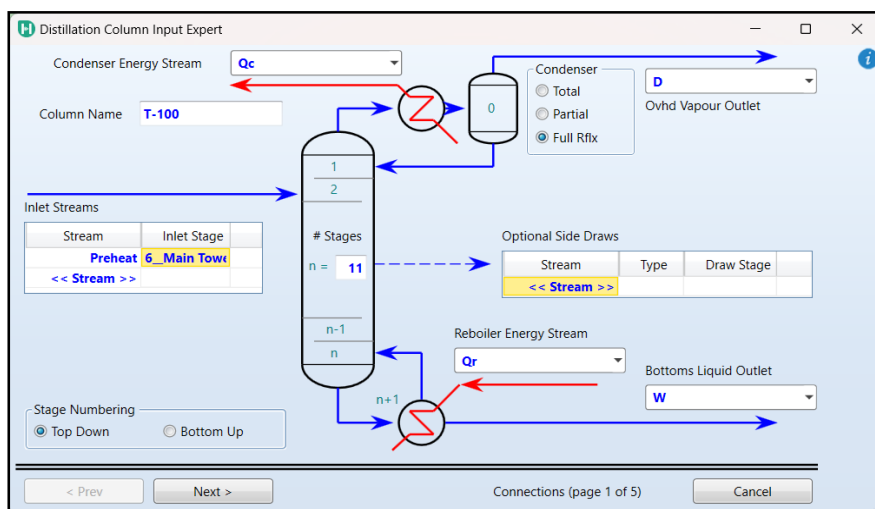




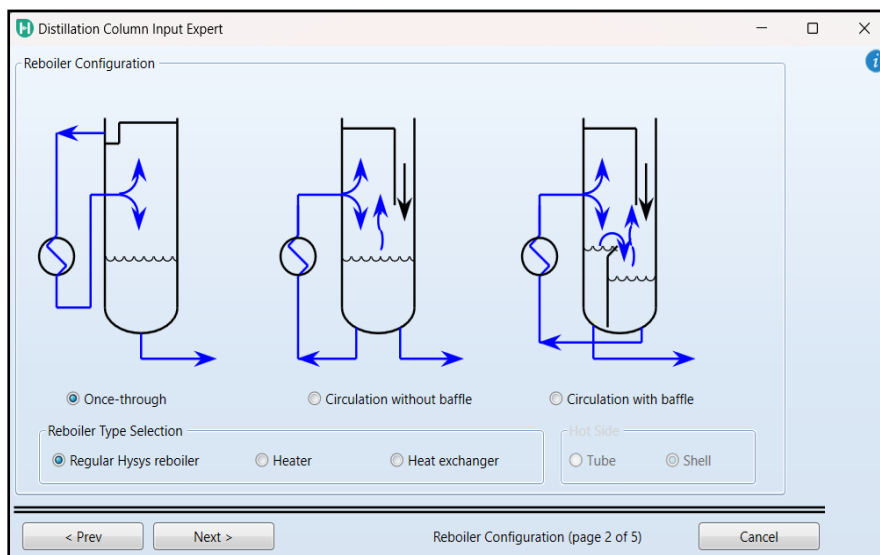
Example 2: Using the rigorous inside-out method, calculate the dependence between the number of theoretical stages and the reflux ratio, if the preheated mixture from Example 1 is separated in a distillation tower, the distillate contains 99 mol% of light components (propane and n-butane) and at the same time common recovery of propane and n-butane is more than 99%. Use the Full Reflux condenser type and neglect the pressure drop in the column and heat exchangers.

How to simulate:

1. Connect Preheat stream as the inlet, define D and W as the outlet streams and Qc and Qr as the energy required for condenser and reboiler. Then click Next.



2. Select the reboiler configuration, you can use the default selected reboiler type.





3. Enter condenser and reboiler pressure of 700 kPa for both equipment.

The screenshot shows the 'Distillation Column Input Expert' window, page 3 of 5, titled 'Pressure Profile'. The window displays a schematic of a distillation column with a condenser at the top and a reboiler at the bottom. The condenser is represented by a vertical cylinder with a zigzag line inside, and the reboiler is a similar cylinder. Blue arrows indicate the flow of liquid and vapor. The interface includes the following fields and values:

- Condenser Pressure: 700.0 kPa
- Condenser Pressure Drop: 0.0000 kPa
- Reboiler Pressure Drop: 0.0000 kPa
- Reboiler Pressure: 700.0 kPa

At the bottom of the window, there are navigation buttons: '< Prev', 'Next >', and 'Cancel'. The page number 'Pressure Profile (page 3 of 5)' is also displayed.

4. On the next page, the condenser and reboiler optimum temperature can be specified, but it is not mandatory, click Next and allow HYSYS to estimate the condenser and reboiler temperature.

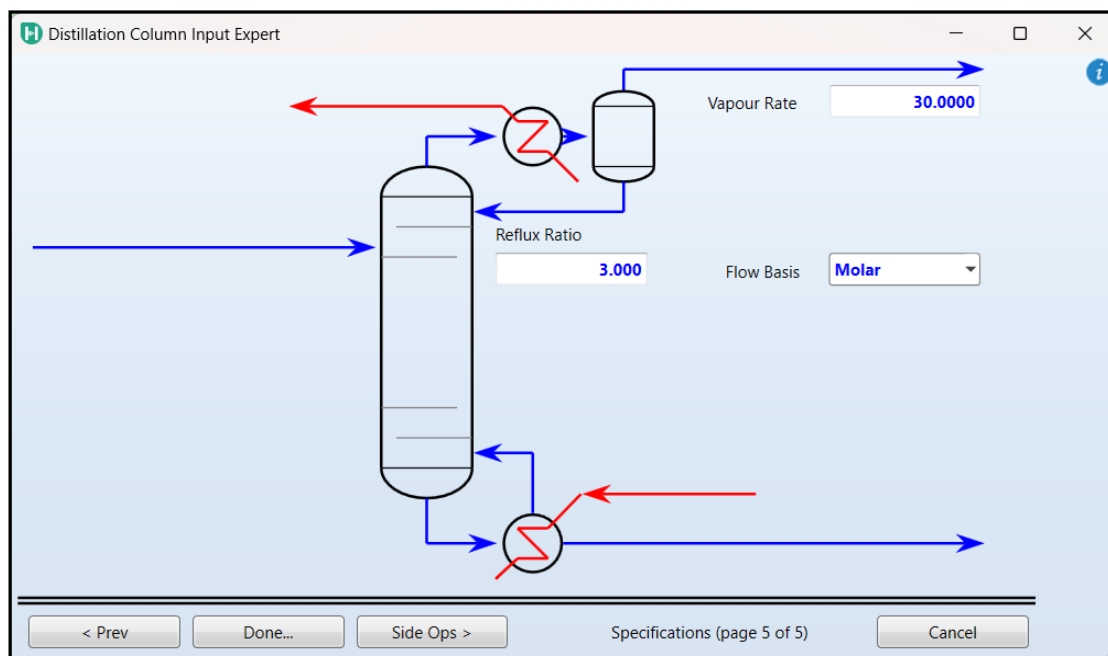
The screenshot shows the 'Distillation Column Input Expert' window, page 4 of 5, titled 'Optional Estimates'. The window displays the same schematic of the distillation column as the previous page. The interface includes the following fields for optional temperature estimates:

- Optional Condenser Temperature Estimate: (empty field)
- Optional Top Stage Temperature Estimate: (empty field)
- Optional Reboiler Temperature Estimate: (empty field)

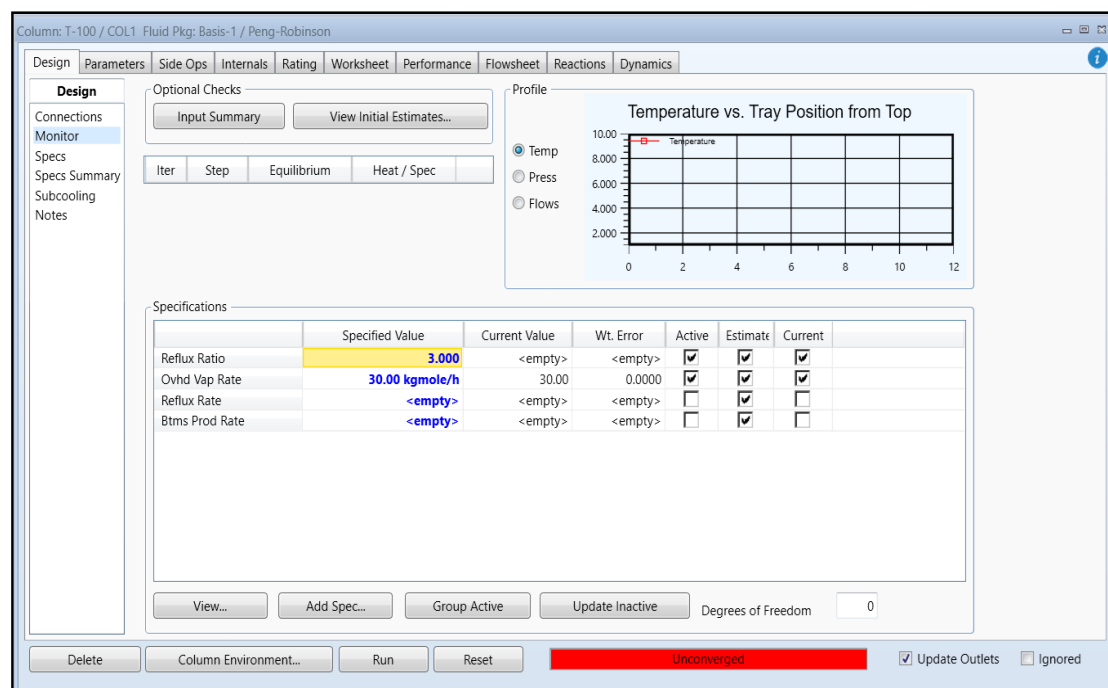
At the bottom of the window, there are navigation buttons: '< Prev', 'Next >', and 'Cancel'. The page number 'Optional Estimates (page 4 of 5)' is also displayed.



5. On the next page, check if flow basis is set to Molar and enter the initial values of the distillation rate (vapor rate) and the reflux ratio. The total amount of propane and n-butane in the feed is 30 kmol·h<sup>-1</sup>, so this value can be chosen as the vapor rate. Finally click Done.



6. Before running the column, check if the value of the degrees of freedom is zero and the values of activated specifications are specified.





7. Move to the Solver tab, under Parameters, and check if the HYSIM inside-out method is set as the solving method;

Column: T-100 / COL1 Fluid Pkg: Basis-1 / Peng-Robinson

Design Parameters Side Ops Internals Rating Worksheet Performance Flowsheet Reactions Dynamics

**Parameters**

Profiles  
Estimates  
Efficiencies  
Solver  
2/3 Phase  
Fluid Pkgs

**Solving Options**

Maximum Number of Iterations: 10000  
Equilibrium Error Tolerance: 1.0000e-05  
Heat / Spec Error Tolerance: 5.0000e-04  
Save Solutions as Initial Estimate: ☒  
Super Critical Handling Model: Simple K Low  
Trace Level:   
Initialise from Ideal K's: ☐  
Two Liquids Check: 2 Liquid Check  
Tighten Water Tolerance: ☐  
Use Estimates for Single Staged Tower: ☐

**Solving Method**

HYSIM Inside-Out  
Control...

General purpose solution method. Good for most problems.

Advanced Solving Options

**Acceleration**

☐ Accelerate K Value & H Model Parameters

**Damping**

☒ Fixed ☐ Adaptive ☐ Azeotropic  
Fixed Damping Factor: 1.000

**Standard Initialization**

☒ Standard Initialization  
☐ Program Generates Estimations

**Initial Estimate Generator Parameters**

☐ Dynamic Integration for IEG  
Dynamic Estimates Integrator...

Delete Column Environment... Run Reset Unconverged ☒ Update Outlets ☐ Ignored

8. Run the column; if the calculations converge, HYSYS indicates it by green color and converged.

Column: T-100 / COL1 Fluid Pkg: Basis-1 / Peng-Robinson

Design Parameters Side Ops Internals Rating Worksheet Performance Flowsheet Reactions Dynamics

**Design**

Connections  
Monitor  
Specs  
Specs Summary  
Subcooling  
Notes

**Optional Checks**

Input Summary View Initial Estimates...

Iter	Step	Equilibrium	Heat / Spec
1	1.0000	1.59399e-02	2.74945e-02
2	1.0000	2.59003e-05	1.03976e-03
3	1.0000	5.09558e-07	1.03846e-04

**Specifications**

	Specified Value	Current Value	Wt. Error	Active	Estimate	Current
Reflux Ratio	3.000	3.000	0.0002	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
Ovhd Vap Rate	30.00 kgmole/h	30.00	0.0000	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
Reflux Rate	<empty>	90.01	<empty>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>
Btms Prod Rate	<empty>	70.00	<empty>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>

View... Add Spec... Group Active Update Inactive Degrees of Freedom 0

Delete Column Environment... Run Reset Converged ☒ Update Outlets ☐ Ignored

**Profile**

Temperature vs. Tray Position from Top

Temp Press Flows

Temperature

120.0  
100.0  
80.0  
60.0

0 2 4 6 8 10 12



9.Result:

Name	Preheat @COL1	D @COL1	W @COL1
Vapour	0.2000	1.0000	0.0000
Temperature [C]	97.34	56.34	125.6
Pressure [kPa]	700.0	700.0	700.0
Molar Flow [kgmole/h]	100.0	30.00	70.00
Mass Flow [kg/h]	7215	1621	5594
Std Ideal Liq Vol Flow [m3/h]	11.50	2.883	8.620
Molar Enthalpy [kJ/kgmole]	-1.562e+005	-1.177e+005	-1.669e+005
Molar Entropy [kJ/kgmole-C]	129.9	138.5	137.7
Heat Flow [kJ/h]	-1.562e+007	-3.532e+006	-1.169e+007

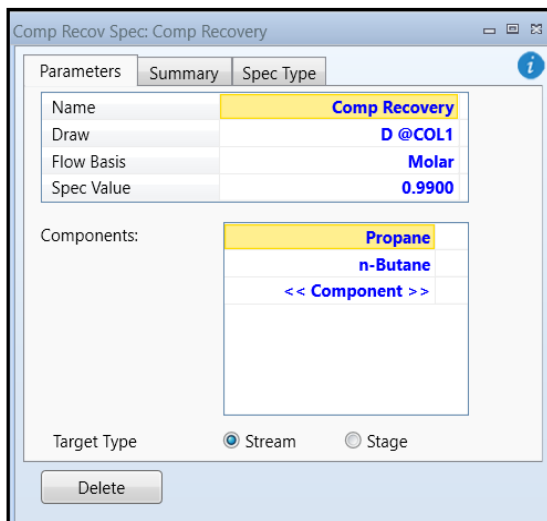
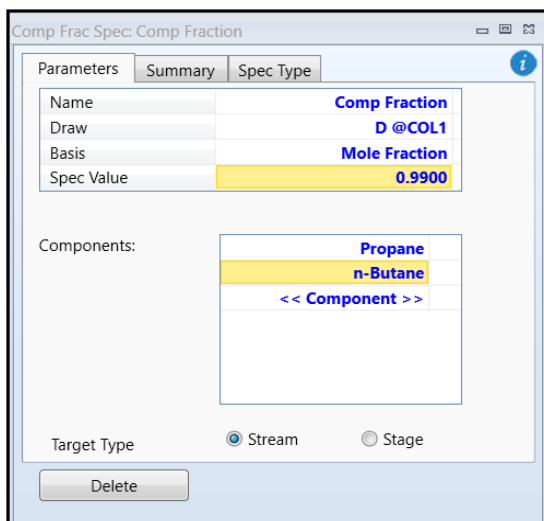
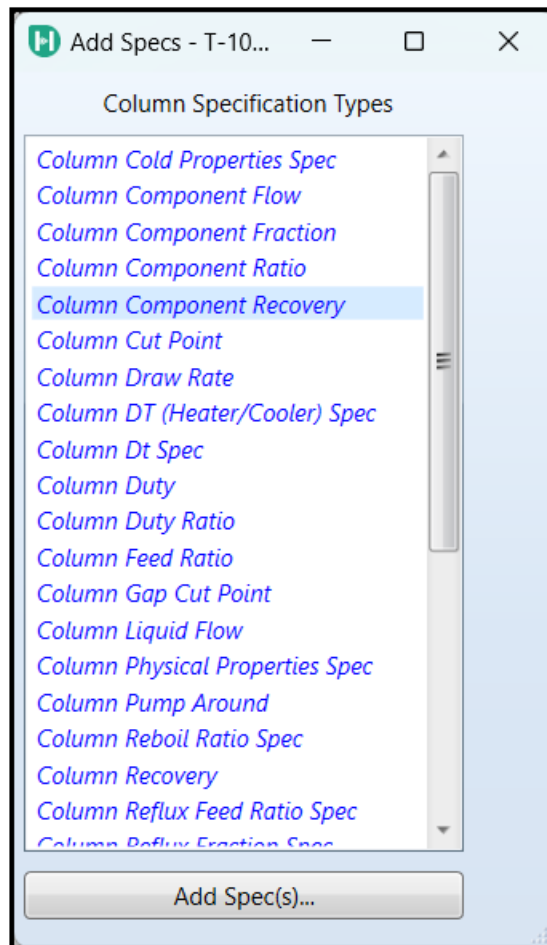
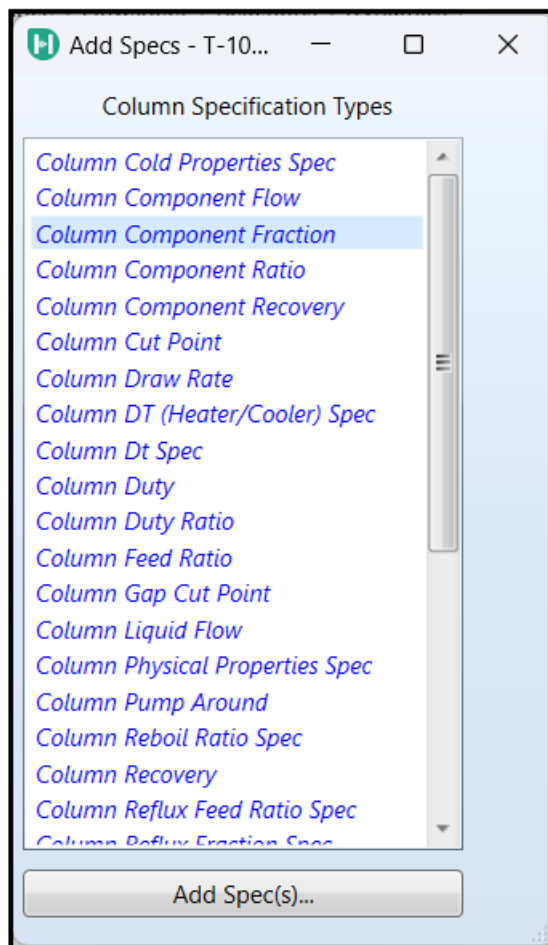
	Preheat	D	W
Propane	0.1000	0.3332	0.0000
n-Hexane	0.4000	0.0001	0.5714
n-Pentane	0.3000	0.0421	0.4105
n-Butane	0.2000	0.6246	0.0180

Condenser	
Type	Total reflux
Temperature	56.34 C
Pressure	700.0 kPa
Duty	1.822e+006 kJ/h
Reflux Flowrate	90.01 kgmole/h

Reboiler	
Type	Regular
Temperature	125.6 C
Pressure	700.0 kPa
Duty	2.227e+006 kJ/h
Outlet Flowrate	70.00 kgmole/h



## 10. Changing the specs.





	Preheat	D	W
Propane	0.1000	0.3333	0.0000
n-Hexane	0.4000	0.0000	0.5714
n-Pentane	0.3000	0.0100	0.4243
n-Butane	0.2000	0.6567	0.0043