



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 $25 \text{ }^\circ\text{C}$, 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

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

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

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

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

Property	Value	Unit
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

Component	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

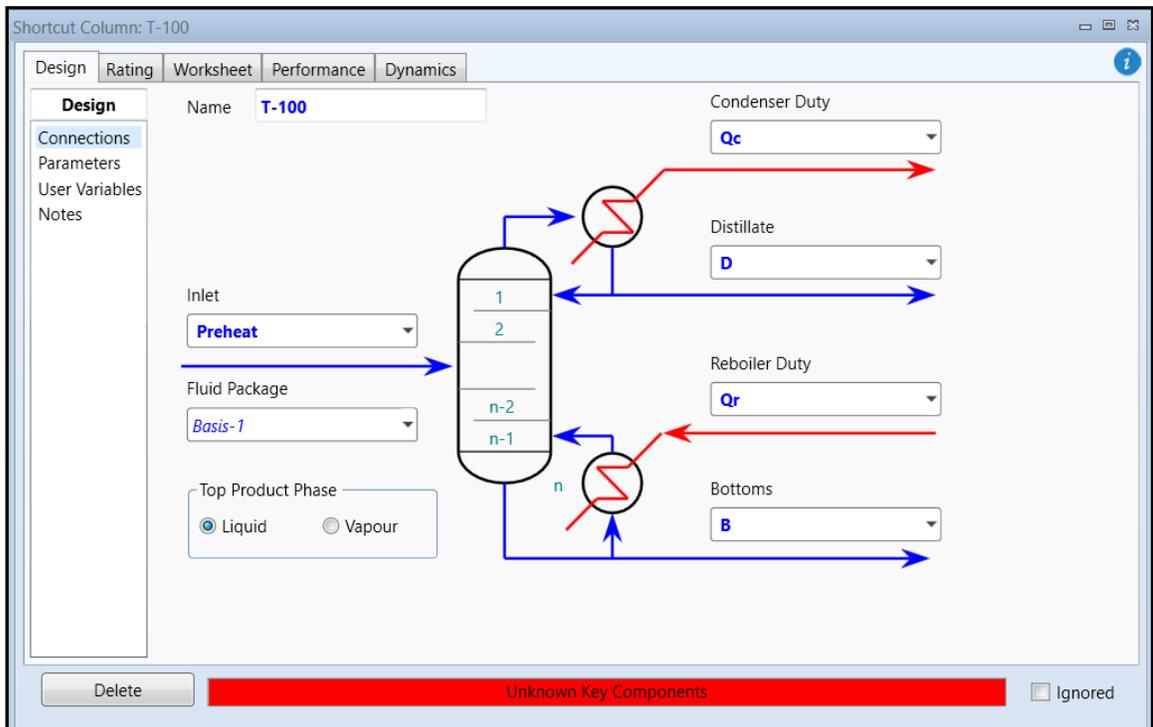
Design Rating Worksheet Performance Dynamics

Worksheet

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:





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.

The screenshot shows the 'Design' tab for a Shortcut Column (T-100). The interface is divided into several sections:

- Design** (selected tab)
- Rating**
- Worksheet**
- Performance**
- Dynamics**

On the left sidebar, the following options are listed: Connections, Parameters (selected), User Variables, and Notes.

The main content area is divided into three sections:

- Components**: A table showing the mole fractions of key components.
- Pressures**: Input fields for Condenser Pressure and Reboiler Pressure.
- Reflux Ratios**: Input fields for External Reflux Ratio and Minimum Reflux Ratio.

Component	Mole Fraction
n-Butane	0.0500
n-Pentane	0.0500

Condenser Pressure	700.000 kPa
Reboiler Pressure	700.000 kPa

External Reflux Ratio	2.200
Minimum Reflux Ratio	1.463

At the bottom of the window, there are buttons for 'Delete', 'OK', and '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	

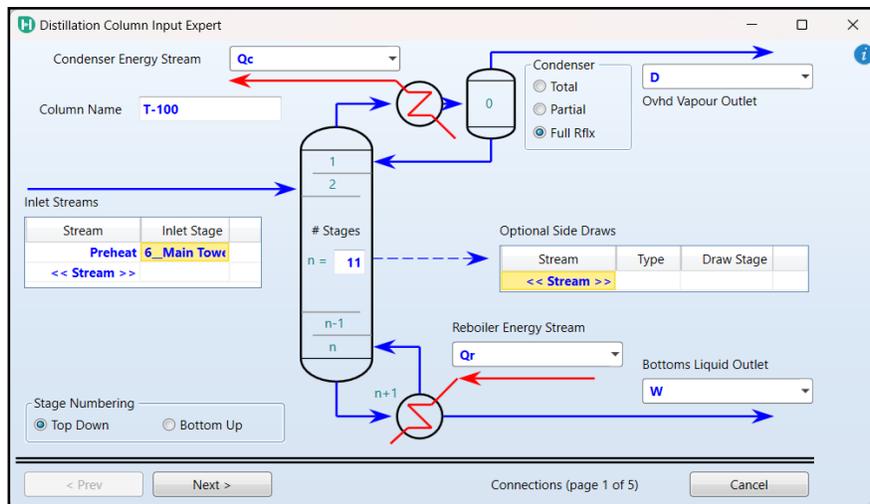
Delete OK Ignored



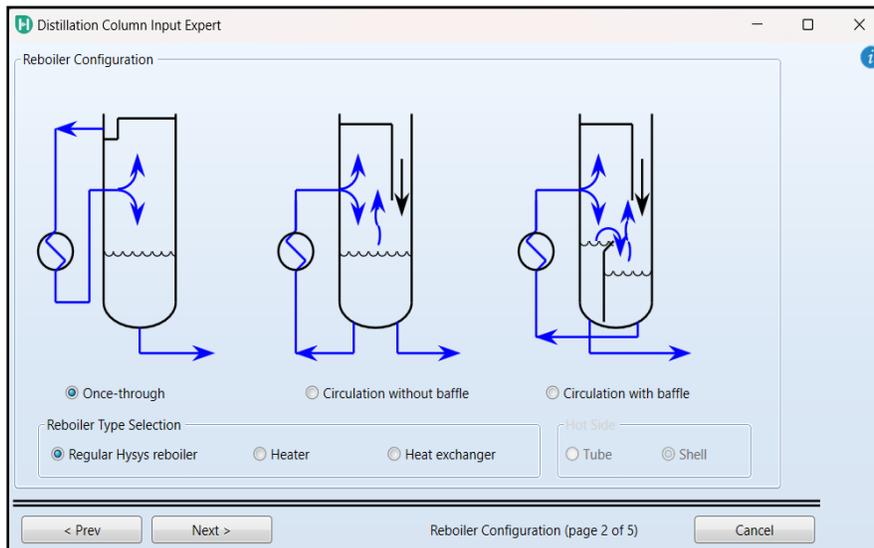
Example 2: Using the rigorous inside-out method, calculate the dependence between the number of theoretical stages and the reflux ratio, if the preheated mixture from Example 1 is separated in a distillation tower, the distillate contains 99 mol% of light components (propane and n-butane) and at the 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.

Distillation Column Input Expert

Condenser Pressure
700.0 kPa

Condenser Pressure Drop
0.0000 kPa

Reboiler Pressure Drop
0.0000 kPa

Reboiler Pressure
700.0 kPa

< Prev Next >

Pressure Profile (page 3 of 5) Cancel

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.

Distillation Column Input Expert

Optional Condenser Temperature Estimate

Optional Top Stage Temperature Estimate

Optional Reboiler Temperature Estimate

< Prev Next >

Optional Estimates (page 4 of 5) Cancel



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⁻¹, so this value can be chosen as the vapor rate. Finally click Done.

Distillation Column Input Expert

Vapour Rate: 30.0000

Reflux Ratio: 3.000

Flow Basis: Molar

< Prev Done... Side Ops > Specifications (page 5 of 5) Cancel

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

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

Design Parameters Side Ops Internals Rating Worksheet Performance Flowsheet Reactions Dynamics

Design

Optional Checks: Input Summary View Initial Estimates...

Profile: Temperature vs. Tray Position from Top

Specifications	Specified Value	Current Value	Wt. Error	Active	Estimate	Current
Reflux Ratio	3.000	<empty>	<empty>	<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>	<empty>	<empty>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>
Btms Prod Rate	<empty>	<empty>	<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 Unconverged Update Outlets Ignored



7. Move to the Solver tab, under Parameters, and check if the HISIM 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

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
- Trace Level: Low
- 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 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

Profile: Temp Press Flows

Temperature vs. Tray Position from Top

Spec	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



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

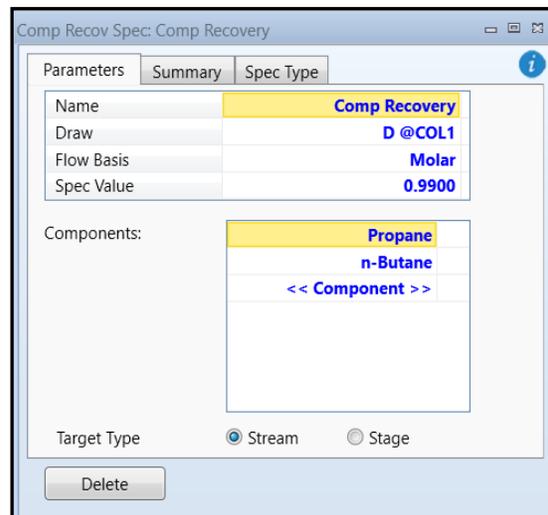
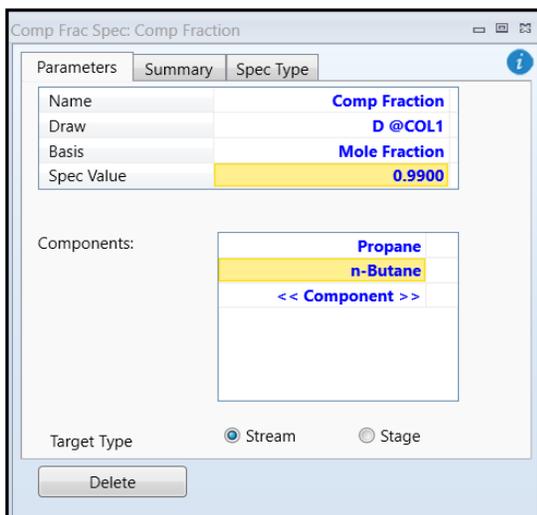
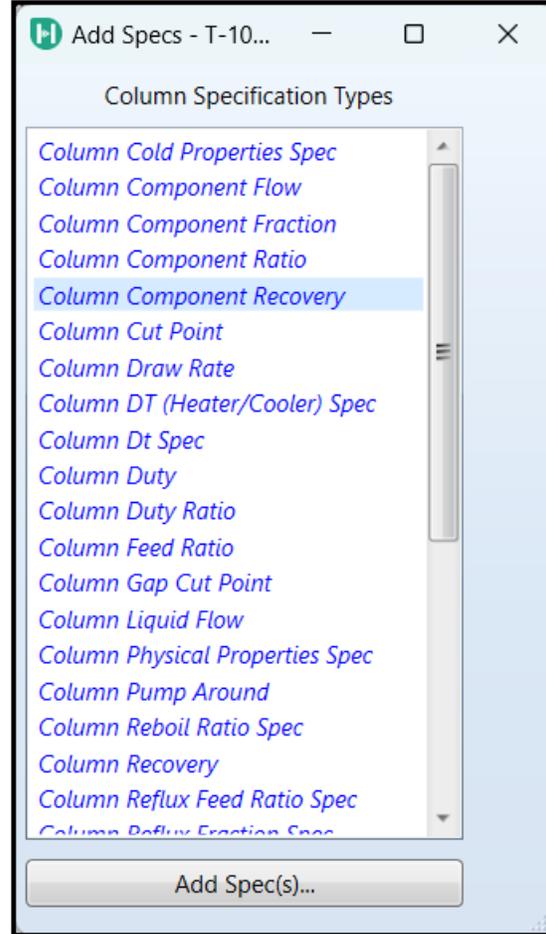
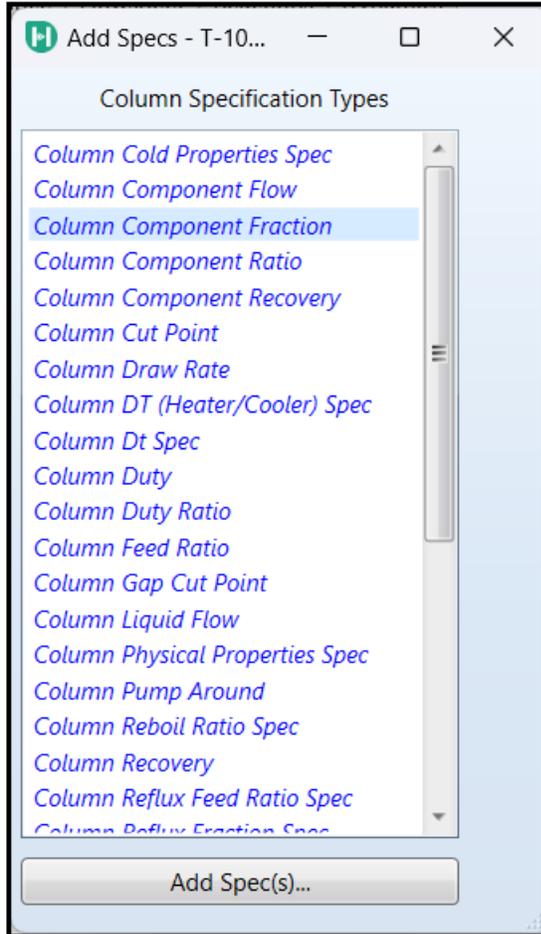
	Preheat	D	W
Propane	0.1000	0.3332	0.0000
n-Hexane	0.4000	0.0001	0.5714
n-Pentane	0.3000	0.0421	0.4105
n-Butane	0.2000	0.6246	0.0180

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