Distillation Column Simulation Using DWSIM:

A Free and Open-Source Chemical Process Simulator

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Level: Intermediate

Version: 0.00

Oct 2022

PREFACE

The manual "DISTILLATION COLUMN SIMULATION USING DWSIM" presents a set of Pump Sizing exercise using a free and open-source chemical process simulator "DWSIM" and can be utilized to establish process simulation laboratory as part of undergraduate chemical engineering degree or in allied degree curriculum. The problem statements are of intermediate level.

Prerequisite

- Must know about DWSIM UI/UX.
- Flow sheeting in DWSIM
- Selection of Thermodynamic Packages.
- Manipulating variables
- Basic Modules

Thanks

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P.E. O&G

Disclaimer

All the exercises are strictly restricted to learning only and not meant to be used in real world application.

PROCESS SIMULATION USING DWSIM: A FREE AND OPEN-SOURCE CHEMICAL PROCESS SIMULATOR

PREAMBLE

DWSIM is an open-source CAPE-OPEN compliant chemical process simulator. It features a Graphical User Interface (GUI), advanced thermodynamics calculations, reactions support and petroleum characterization / hypothetical component generation tools. DWSIM can simulate steady-state, vapor–liquid, vapor–liquid-liquid, solid–liquid and aqueous electrolyte equilibrium processes and has built-in thermodynamic models and unit operations (https://en.wikipedia.org/wiki/DWSIM). It is available for Windows, Linux and Mac OS.

The objective of the course is to create awareness of the open-source process simulator “DWSIM” among prospective graduates and practicing process engineers. The course will cover Intermediate aspects of create flow sheet in DWSIM and simulation of simple Pressure changing module like shortcut column, energy streams, material streams etc.

Target Audience

- Junior Interns in Process Firms
- III / Final year B. Tech. Chemical Engineering students
- M. Tech. Chemical Engineering students
- Practicing Process Engineers

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1 BACKGROUND

Distillation is a widely used technique in chemical analysis for characterizing materials by establishing an index of purity and for separating selected components from a complete matrix. The technique is even more widely used in preparative chemistry and throughout manufacturing industry as a means of purifying products and chemical intermediates. Distillation operations differ enormously in size and complexity from the semimicro scale to the 'thousands of tons per annum' production operations. For analytical purposes the scale employed is usually bench-level.

Distillation is the process that occurs when a liquid sample is volatilized to produce a vapor that is subsequently condensed to a liquid richer in the more volatile components of the original sample. The volatilization process usually involves heating the liquid, but it may also be achieved by reducing the pressure or by a combination of both. This can be demonstrated in a simple laboratory distillation apparatus comprising a flask, distillation head, condenser, and sample collector.

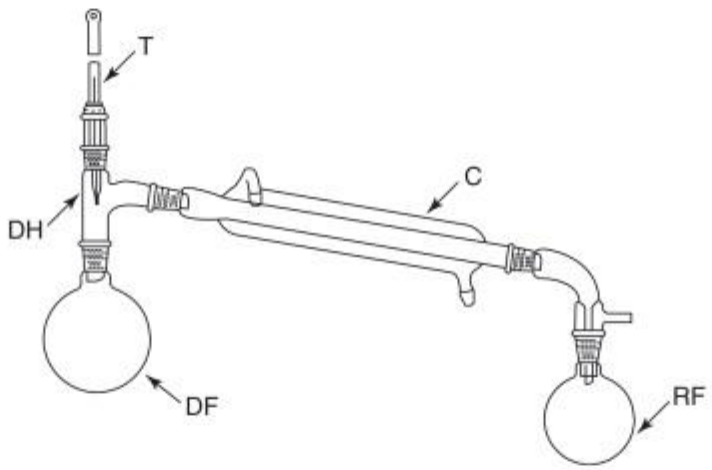


Figure 1 Simple distillation apparatus comprising distillation flask (DF), distillation head (DH), thermometer (T), condenser (C), and receiver (or collection) flask (RF).

A thermometer is included in the apparatus as shown to monitor the progress of the operation. In its simplest form this procedure results in a separation into a volatile fraction collected in the receiver flask and a non-volatile residue in the distillation flask. When a distillation column is incorporated in the equipment, the evaporation and condensation processes occur continuously. This results in a progressive fractionation of the volatiles as they pass up the column. The most volatile components emerge from the top of the column initially and the less volatile components emerge later. By changing the receivers throughout the course of the distillation a separation or fractionation is affected. Eventually, all the volatiles will have passed over into the sample collectors and any involatile residue present will remain in the distillation flask.

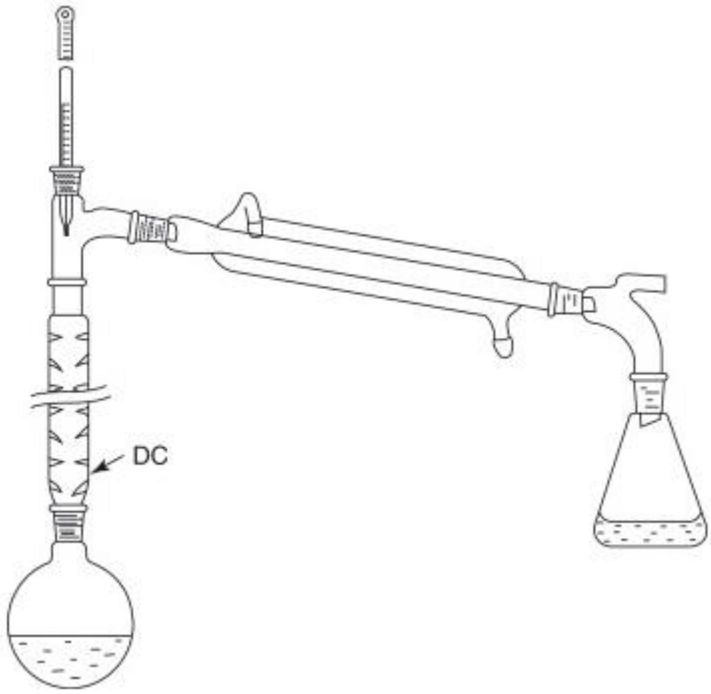


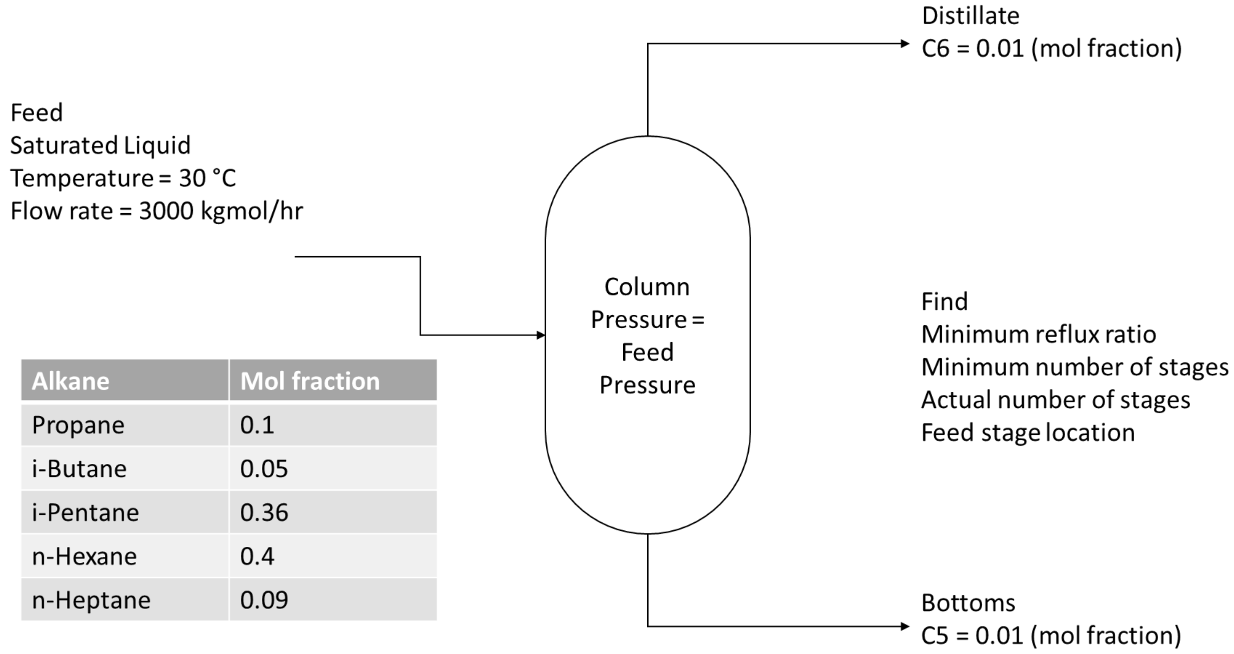
Figure 2 Distillation apparatus including distillation column (DC).

2 SIMPLE DISTILLATION COLUMN

Objective

- Find Minimum reflux ratio
- Minimum number of stages
- Actual number of stages
- Feed stage location

Data



Alkane	Mol fraction
Propane	0.1
i-Butane	0.05
i-Pentane	0.36
n-Hexane	0.4
n-Heptane	0.09

Figure 3 Problem Statement

DWSIM Blocks Used

- Shortcut Column
- Material Stream
- Energy Stream
- Indicators (Digital or Analog)

Procedure

1. Start a new DWSIM Simulation (DWSIM VER 8.3.1 - CLASSIC UI). Click on “New steady state Simulation” as a template for new simulation
2. The simulation configuration window will be opened. It shows a specification page. Add components required to solve the problem statement. In the present case, add Isobutane, Isopentane, Propane, N-hexane & N-heptane. Ensure all components are added from the same property database. For instance, in this case, both components are added from “ChemSep” database.
3. Specify the thermodynamic package as Peng-Robinson (PR).

4. Customize the system of units to C5 for the simulation and click “Next”.
5. The flow sheeting section of simulation window will be opened. First, let provide input and output streams for the unit operation to be performed. Drag and drop three Material streams available at the right, in the object palette. Rename them stream as “Feed”, “Top” and “Bottom”.
6. Drag and drop two Energy streams available at the right, in the object palette. Rename them stream as “R-Duty”, “C-Duty”.
7. On clicking the “Feed” stream, general information about the stream will be displayed on the left side of screen. Specify the feed compositions, temperature, and pressure for the inlet streams. Once credentials are specified for the inlet streams, the color of stream turns blue.

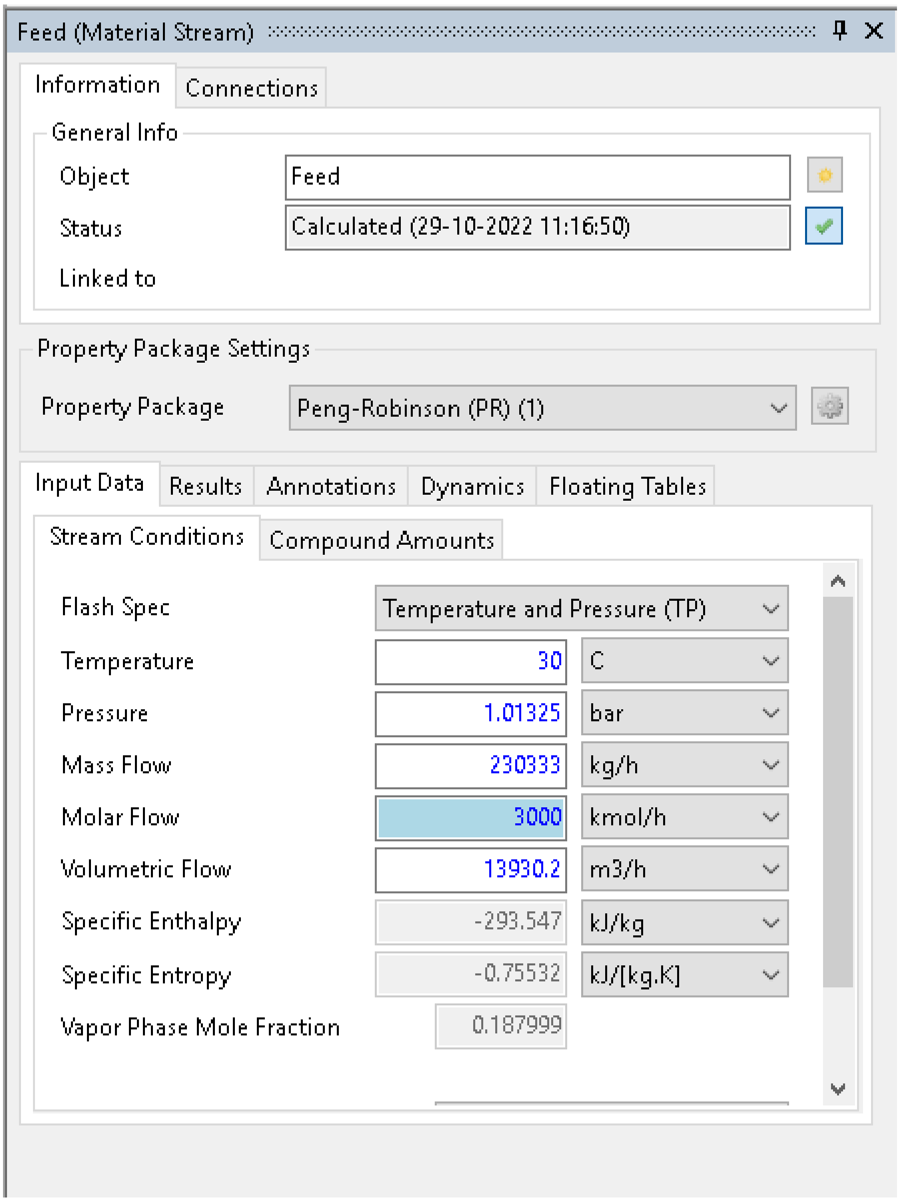


Figure 4 Feed Stream Specs

8. Below the Unit Operation tab on left, locate the shortcut column (SC) block. Drag and drop into the flow sheet. Rename it as "ADU".

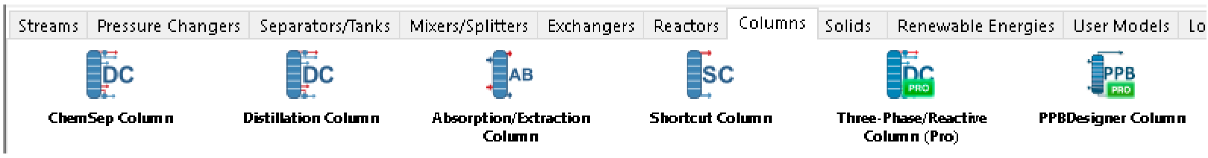


Figure 5 Shortcut Column

9. Under specification for shortcut column add the data as follows.

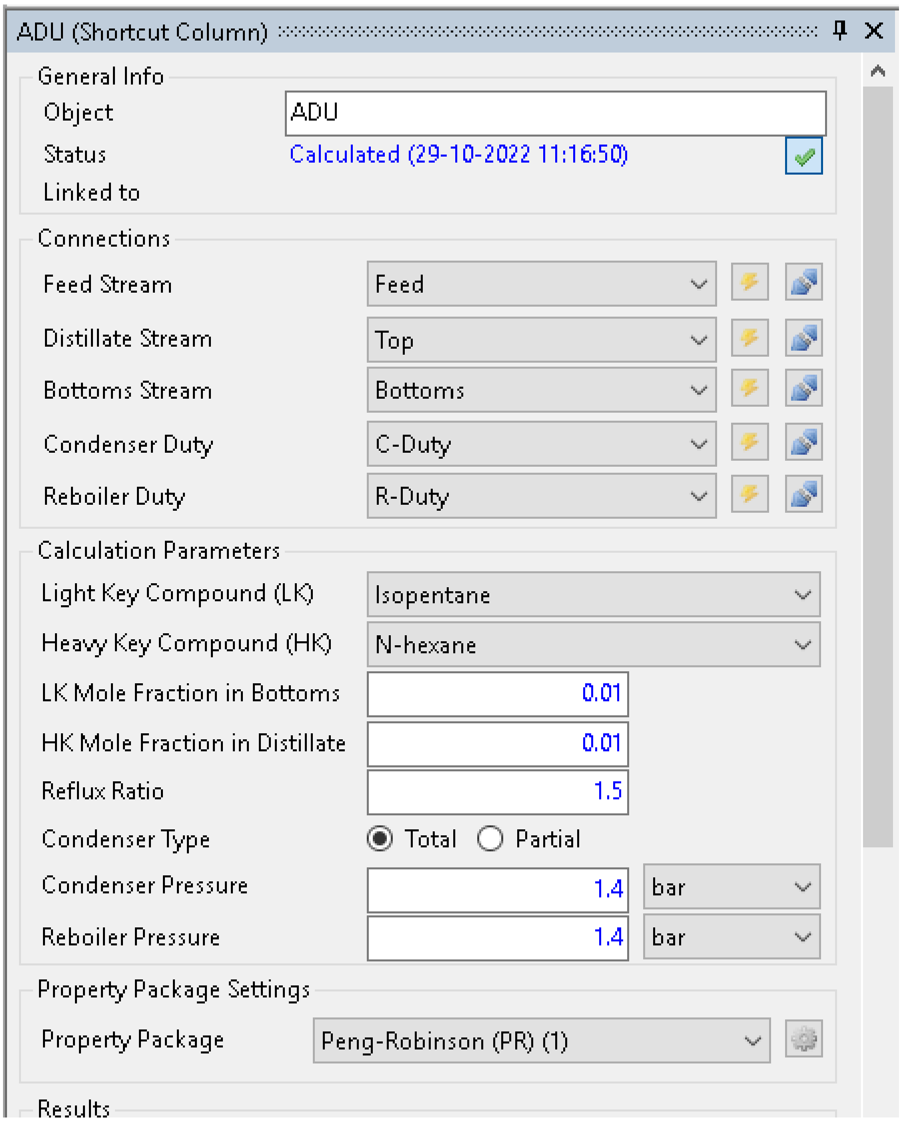


Figure 6 Shortcut Column Specs

10. Provide appropriate connections to the shortcut column as shown

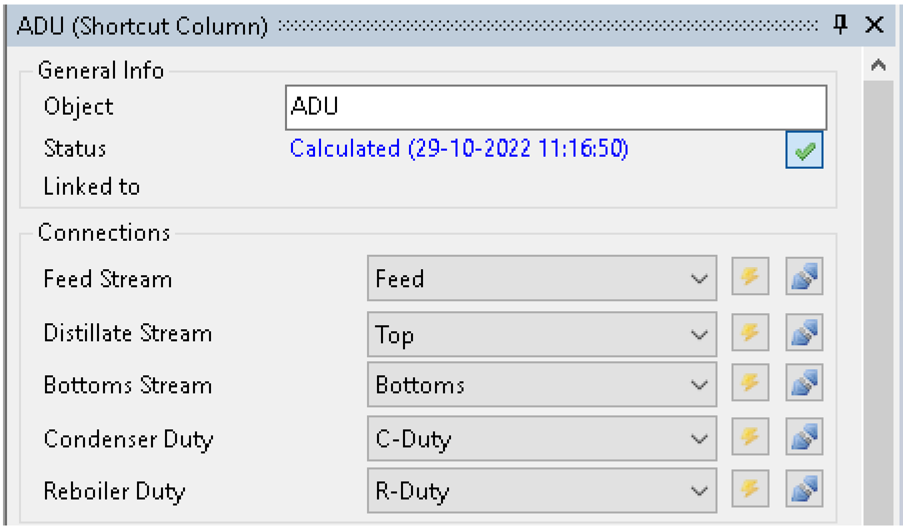


Figure 7 Connections to shortcut column

11. Run the simulation by pressing "Solve flow sheet" button on the top corner of the screen.

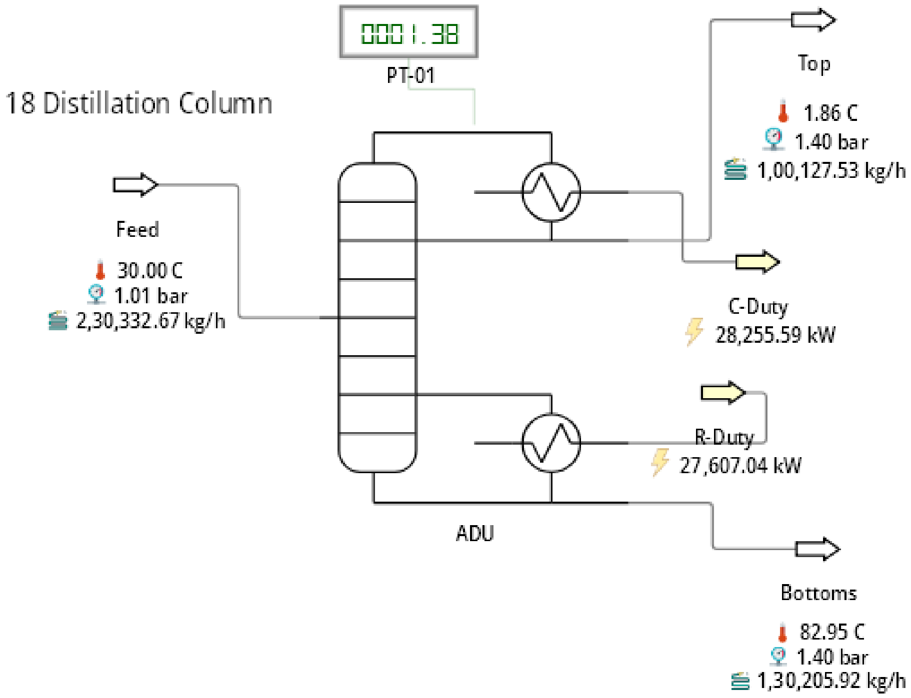


Figure 8 Flow sheet

3 CHEMSEP RIGOROUS SEPARATION COLUMN (CAPE-OPEN)

DWSIM Blocks Used

- Chemsep Rigorous Separation Column
- Material Stream

Procedure

1. Make a copy of all the blocks present in the flowsheet.
2. Now replace the shortcut column with the CHEMSEP Rigorous Separation Column form the columns unit operation tab

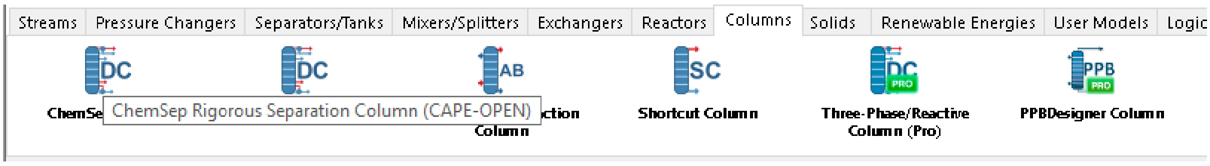


Figure 9 CHEMSEP Column

3. Connect feed stream and tops and bottom and remove the C-Duty and R-Duty Streams.
4. Now Click on "Open-CAPE-OPEN object editior". A new window will open as shown

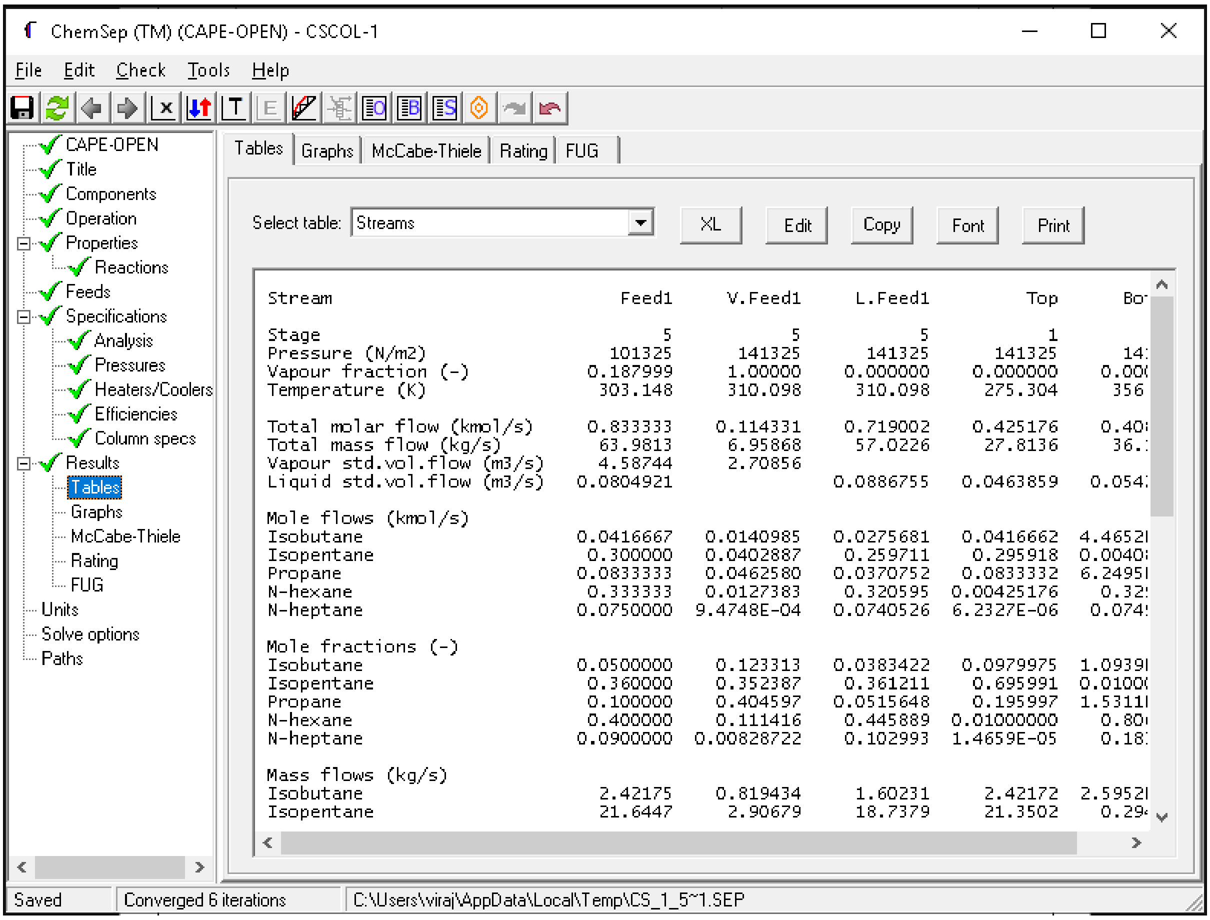


Figure 10 Cape open object editor

5. Click on operations tab and add the specifications shown

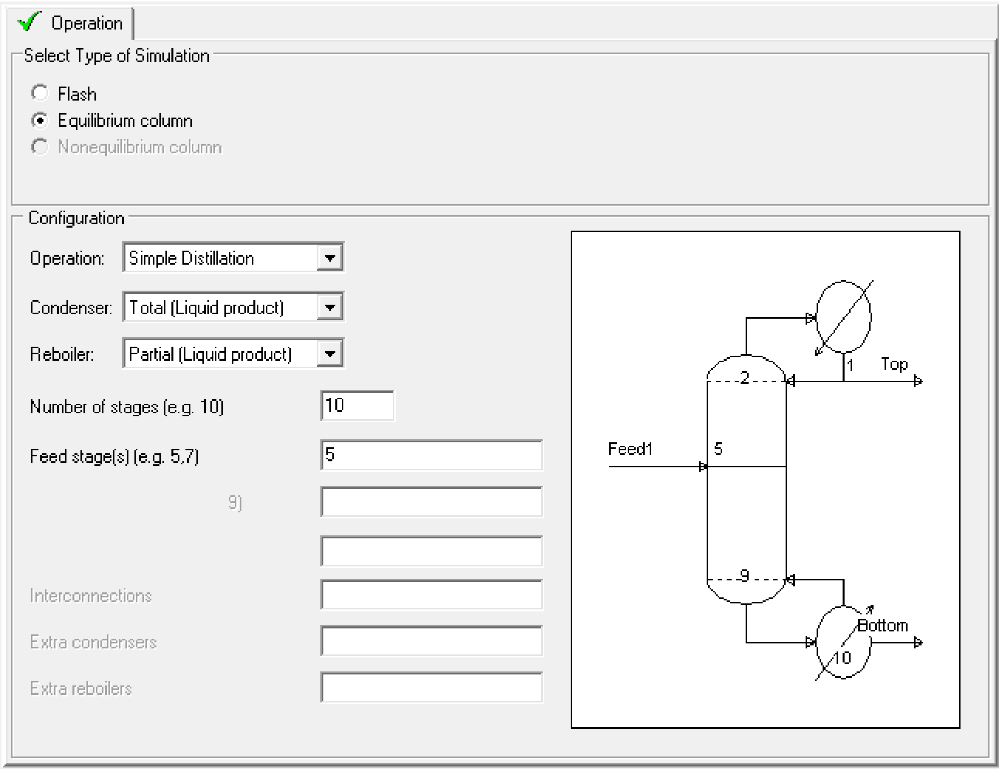


Figure 11 Operation tab of cape open

6. In Speifications tab click on Pressures, and specify condensor and reboiler pressures.

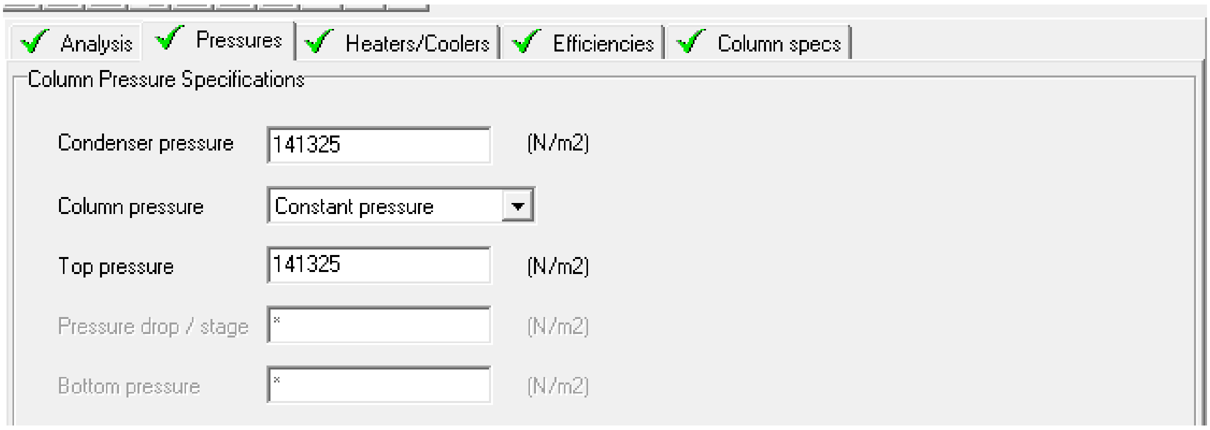


Figure 12 Pressures tab in specifications

7. Click on column specs and specify the details as shown

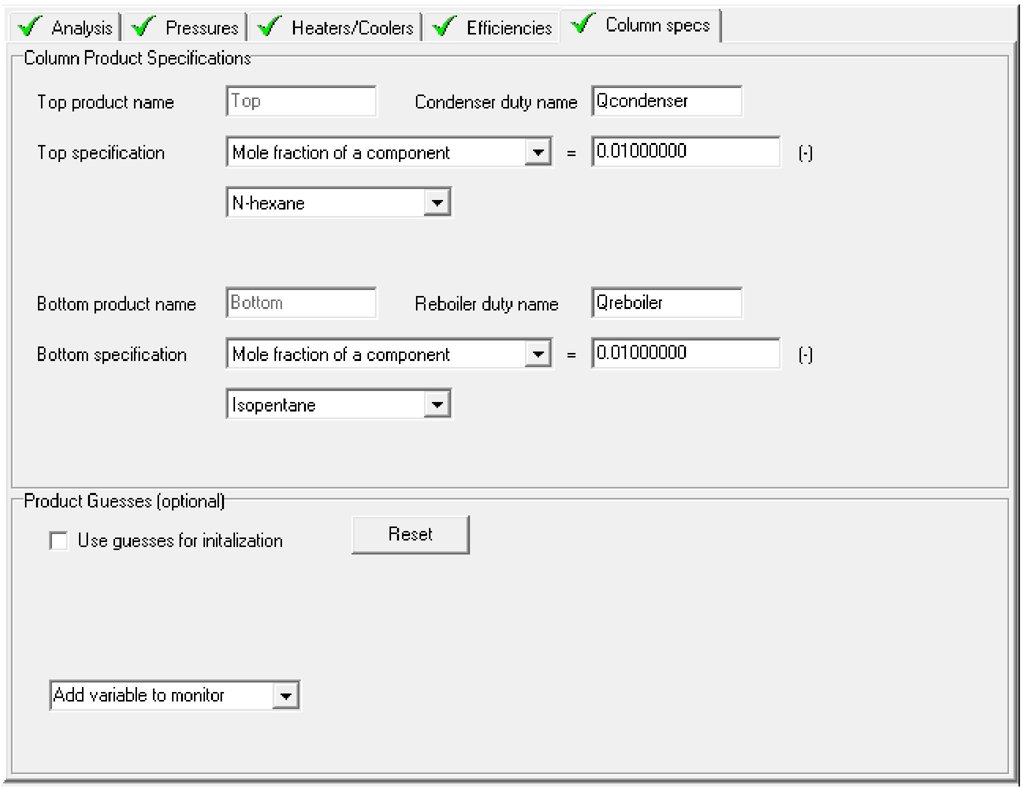


Figure 13 Column Specifications in Cape open

8. Once done by speifying all the variables. Run the simulation by pressing "Solve flow sheet" button on the top corner of the screen.

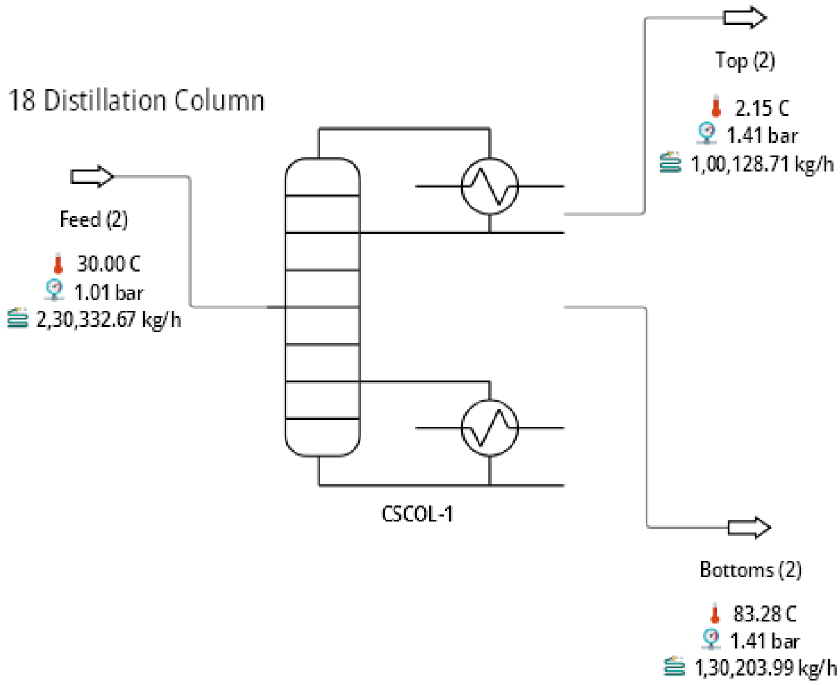
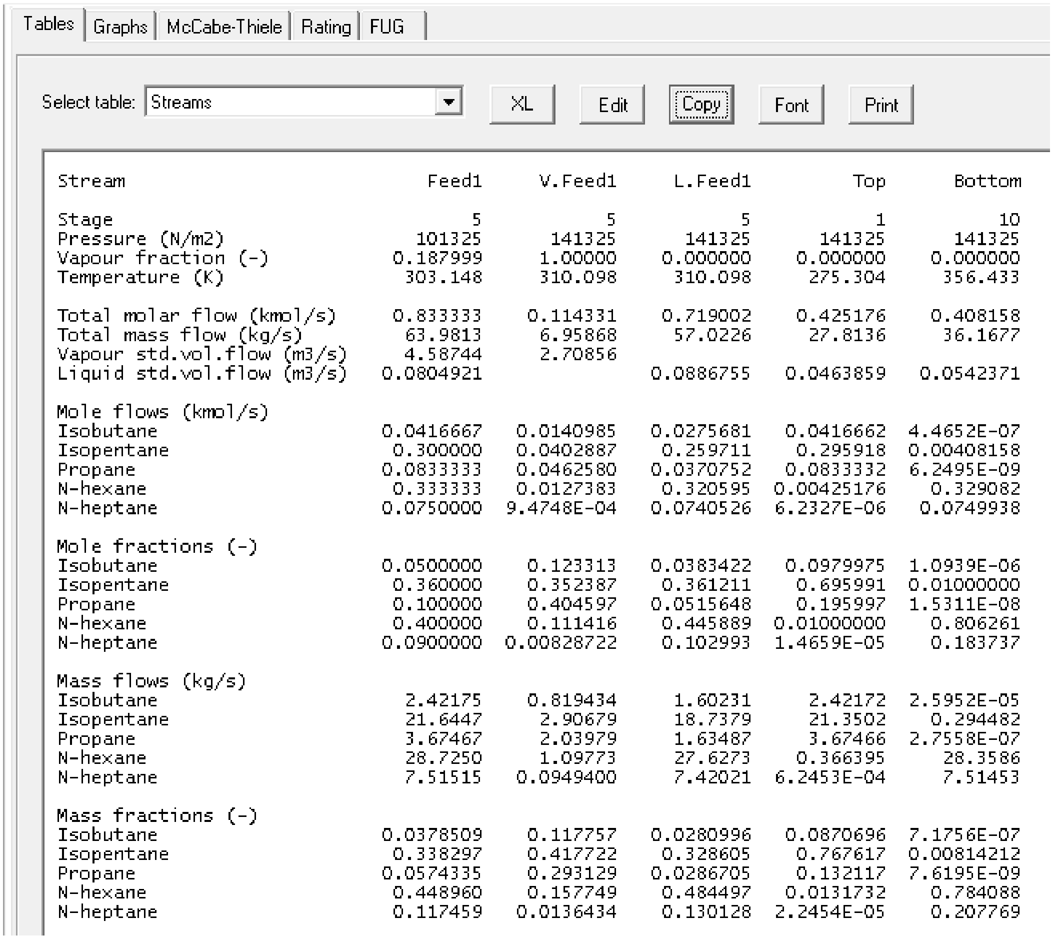


Figure 14 Flow sheet of CHEMSEP Column

9. After the flowsheet is solved succesfully click on the “Open-CAPE-OPEN object editior” to view the results.
10. Stream Results



Stream	Feed1	V.Feed1	L.Feed1	Top	Bottom
Stage	5	5	5	1	10
Pressure (N/m2)	101325	141325	141325	141325	141325
Vapour fraction (-)	0.187999	1.00000	0.000000	0.000000	0.000000
Temperature (K)	303.148	310.098	310.098	275.304	356.433
Total molar flow (kmol/s)	0.833333	0.114331	0.719002	0.425176	0.408158
Total mass flow (kg/s)	63.9813	6.95868	57.0226	27.8136	36.1677
Vapour std.vol.flow (m3/s)	4.58744	2.70856			
Liquid std.vol.flow (m3/s)	0.0804921		0.0886755	0.0463859	0.0542371
Mole flows (kmol/s)					
Isobutane	0.0416667	0.0140985	0.0275681	0.0416662	4.4652E-07
Isopentane	0.300000	0.0402887	0.259711	0.295918	0.00408158
Propane	0.0833333	0.0462580	0.0370752	0.0833332	6.2495E-09
N-hexane	0.333333	0.0127383	0.320595	0.00425176	0.329082
N-heptane	0.0750000	9.4748E-04	0.0740526	6.2327E-06	0.0749938
Mole fractions (-)					
Isobutane	0.0500000	0.123313	0.0383422	0.0979975	1.0939E-06
Isopentane	0.360000	0.352387	0.361211	0.695991	0.01000000
Propane	0.100000	0.404597	0.0515648	0.195997	1.5311E-08
N-hexane	0.400000	0.111416	0.445889	0.01000000	0.806261
N-heptane	0.0900000	0.00828722	0.102993	1.4659E-05	0.183737
Mass flows (kg/s)					
Isobutane	2.42175	0.819434	1.60231	2.42172	2.5952E-05
Isopentane	21.6447	2.90679	18.7379	21.3502	0.294482
Propane	3.67467	2.03979	1.63487	3.67466	2.7558E-07
N-hexane	28.7250	1.09773	27.6273	0.366395	28.3586
N-heptane	7.51515	0.0949400	7.42021	6.2453E-04	7.51453
Mass fractions (-)					
Isobutane	0.0378509	0.117757	0.0280996	0.0870696	7.1756E-07
Isopentane	0.338297	0.417722	0.328605	0.767617	0.00814212
Propane	0.0574335	0.293129	0.0286705	0.132117	7.6195E-09
N-hexane	0.448960	0.157749	0.484497	0.0131732	0.784088
N-heptane	0.117459	0.0136434	0.130128	2.2454E-05	0.207769

Figure 15 Stream Results

11. Mc-Cabe Thiele Graph

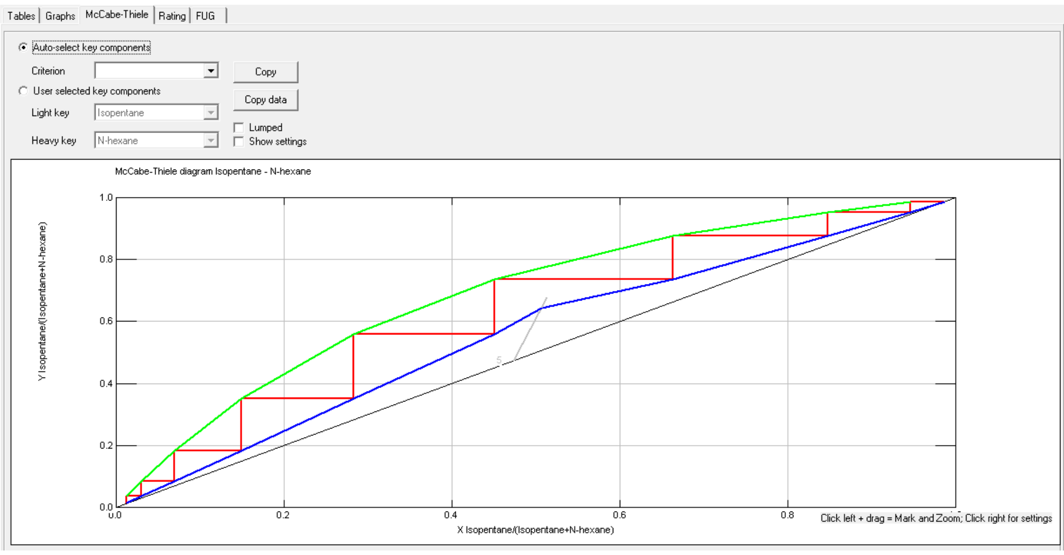


Figure 16 Mc-Cabe Thiele Graph

4 Results

Shortcut Column Properties	Feed	Top	Bottoms
Temperature (C)	30	1.8557	82.9526
Pressure (bar)	1.01325	1.4	1.4
Mass Flow (kg/h)	230333	100128	130206
Molar Flow (kmol/h)	3000	1530.61	1469.4
Volumetric Flow (m3/h)	13930.2	165.339	239.495
Density (Mixture) (kg/m3)	16.5348	605.589	543.669
Molecular Weight (Mixture) (kg/kmol)	76.7776	65.4166	88.6117
Specific Enthalpy (Mixture) (kJ/kg)	-293.547	-402.473	-227.714
Specific Entropy (Mixture) (kJ/[kg.K])	-0.75532	-1.28371	-0.58512
Molar Enthalpy (Mixture) (kJ/kmol)	-22537.8	-26328.4	-20178.1
Molar Entropy (Mixture) (kJ/[kmol.K])	-57.9916	-83.9756	-51.8485
Thermal Conductivity (Mixture) (W/[m.K])	0.0956115	0.114681	0.101067

ChemSep Column Properties	Feed (2)	Top (2)	Bottoms (2)
Temperature (C)	30	2.15354	83.2826
Pressure (bar)	1.01325	1.41325	1.41325
Mass Flow (kg/h)	230333	100129	130204
Molar Flow (kmol/h)	3000	1530.63	1469.37
Volumetric Flow (m3/h)	13930.2	164.508	215.093
Density (Mixture) (kg/m3)	16.5348	608.654	605.339
Molecular Weight (Mixture) (kg/kmol)	76.7776	65.4166	88.6123
Specific Enthalpy (Mixture) (kJ/kg)	-293.547	-401.848	-227.159
Specific Entropy (Mixture) (kJ/[kg.K])	-0.75532	-1.28142	-0.58357
Molar Enthalpy (Mixture) (kJ/kmol)	-22537.8	-26287.5	-20129
Molar Entropy (Mixture) (kJ/[kmol.K])	-57.9916	-83.8262	-51.7115
Thermal Conductivity (Mixture) (W/[m.K])	0.0956115	0.114569	0.101026

5 REFERENCES

1. Distillation Overview
2. Simulation File
3. Simulation Results