SuperFractionate User Manual
Version 1.0

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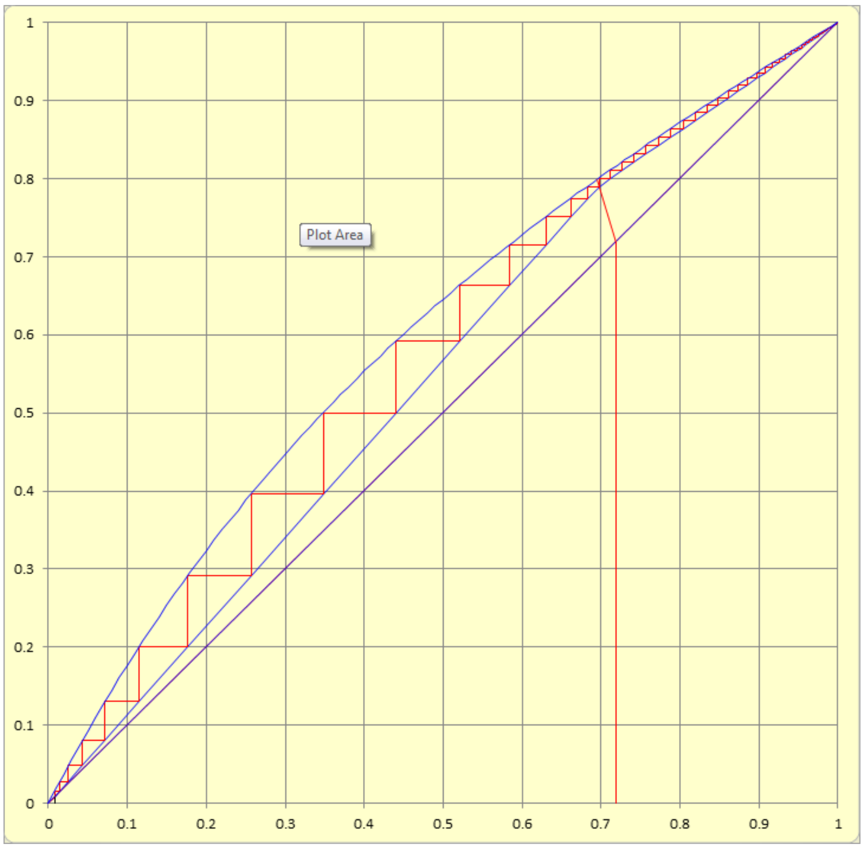

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Introduction

SuperFractionate, referred to hereafter as SF 1.0 uses the Ponchon-Savarit distillation method which was originally proposed as a graphical method. It required K-data as well as enthalpy data. If graphical inaccuracies are ignored it is actually a rigorous distillation method. However, due to the requirement of enthalpy data, the method was not as popular as the McCabe-Thiele shortcut distillation method which does not use enthalpy which in turn results in straight operating lines.

The emergence of fast computers and good programming languages enabled writing this program which will hopefully revive the Ponchon-Savarit distillation method.

This version of SF 1.0 contains very accurate VLE correlation for the ethylene/ethane and the propylene/propane systems. The ethylene/ethane data is a result of correlating the experimental data of Barclay & Manley using a 15-parameter BWR equation of state developed by Haddad.

Program Input

Title and Case

SF 1.0 allows for the entry of one Title and one Case. These entries are optional but their use is encouraged as a reference. They appear in the report and are saved with the input, thus making it easier to identify the project and case for which the input file was created.

System

Select C2 Splitter for the separation of ethylene from ethane or C3 Splitter for the separation of propylene form propane. Select other for other systems and select the desired Light & heavy components from the drop down boxes below.

Feeds

SF 1.0 allows up to for feeds. The thermodynamic entries are Pressure, vapor fraction are temperature. Two and only two of these entries are required. Do not specify all three, but if you do SF 1.0 will prompt you with an error. The light key and heavy key flowrates must also be specified.

Distillate & Bottoms

The distillate and bottoms light key mole fraction are required entries. Mole fractions must be greater than zero and less than one. If you make an invalid mole fraction entry, SF 1.0 will prompt an error. The default distillate phase is Liquid but you can change it via the drop down box.

The distillate & bottoms pressure are also a required entries. This distillate pressure is exactly what you want the distillate pressure to be. However, unless you are solving an academic problem with no pressure drop per stage, *the bottoms pressure is an estimate only. Once you run the problem once, check the results for the bottoms pressure, reenter it in the input form and run the problem again.*

Enter all pressures carefully, unlike mole fraction, SF 1.0 has no way to verify a pressure entry.

Condenser and stage pressure drop

The next two entries are for the condenser pressure drop and pressure drop per stage, both are required. The pressure is per stage is per ideal stage, not actual tray.

Side Exchangers

Side exchangers are optional. To install a side exchanger specify the temperature and the heat duty of the side exchanger. Note that every side exchanger has a maximum HEAT duty. SF 1.0 will calculate the maximum side reboiler duty and prompt an error if your entry is above the maximum.

Side Draws

Side draw are optional. To install a side draw, specify the light key mole fraction and the molar flow rate of the side draw. SF 1.0 has the default phase as liquid but can be changed to vapor in the drop down box.

Mode of Operation

At this time, SF 1.0 only allows the Design mode operation for which the ratio of actual reflux to minimum reflux (R/Rmin) is a required entry.

In the future, we hope to have a Rating mode where the user specifies the number of stages and SF 1.0 calculates the reflux needed.

Program Output

The output will start by a re-echo of the input data. This way,any person looking at the report will know what values where entered.

Physical Constants

SF 1.0 will print several physical constants of the light and heavy key components. At this time, these constants cannot be changed and are printed for information only.

Overall Material Balance

SF 1.0 will solve for the distillate and bottoms flow rate and will print out the overall and components flow rate for all inlet & outlets streams.

SF 1.0 will check the balance as there should not be any negative flow rates. Note that a large side draw flow rate will result in a negative flow rate.

Feed Initialization

Only two of the three thermodynamic conditions (Pressure, vapor fraction & temperature) were entered. In the Feed Initialization step, SF 1.0 will perform the necessary flash calculations to determine the third condition as well as compressibility factors and enthalpies ALL at the given feed pressure.

The same is then done for the distillate, reflux, overhead and bottoms streams.

Flashing of Feeds and Side Draws at Column Pressure

The thermodynamic conditions of the side draws have not been determined and the thermodynamic conditions of the feeds have only been determined at the feed pressure. SF 1.0 will estimate a feed stage pressure and perform isenthalpic flash calculations for each feed. This calculation is necessary to determine the actual state of the feed (vapor fraction) and the liquid and vapor mole fractions which will determine the q-line for a correct determination of the feed state.

SF 1.0 will also estimate a pressure for the side draws and (depending on the phase of the side draw) perform the necessary bubble point or dew point temperature calculation then determine the compressibility factors and enthalpy.

Sorting of Feeds and Side Draws

The order in which feeds are entered on the input form is not necessarily the order in which they feed the distillation column. Most people sort the feeds by the overall mole fraction of the light key and that is fine most of the time.

However, a saturated vapor feed with a light key overall mole fraction of 0.50 will probably have to enter the column at a lower feed state than a saturated liquid feed (vertical q-line) with a light key mole fraction of 0.49.

Until the flashes are performed, you have no way of knowing that, but not to worry, SF 1.0 will sort the feed for you and prompt you to let you know that the feeds have been sorted. At this point, you may want to resort your feeds even though the results are identical, but the prompts from SF 1.0 alerting you to the resorting might become annoying.

Minimum Conditions

Now that all flashes have been performed, SF 1.0 calculated the minimum conditions. The minimum conditions table might actually be confusing. SF 1.0 will go through every section feed and side draw and assume that a pinch will take place in that section. It calculates the minimum condenser duty, reboiler duty, reflux and boilup ratio assuming for that section and output a table of the results.

The actual minimum conditions are the LARGEST ones in the list.

SF 1.0 will output the controlling section (usually the feed with the highest flow rate), the pinch point temperature and the minimum reflux ratio, condenser and reboiler duty.

The column pinch point temperature is the temperature above which only a side reboiler can be added and below which only a side condenser can be added. SF 1.0 will check the side exchanger conditions and prompt an error if there is a violation.

Actual Conditions

The ratio of actual reflux to minimum reflux is a user input. SF 1.0 will use this entry to determine and output the actual reflux ratio and the actual condenser and reboiler duties.

At the actual conditions, SF 1.0 computed a column grand composite curve and computes the maximum side reboiler duty at its temperature.

For each side reboiler, SF 1.0 outputs the user supplied side exchanger duty and the maximum allowable side reboiler duty.

SF 1.0 will then compute the operating line, stage by stage from top to bottom taking into account the pressure drop entered by the user. In this process, SF 1.0 determines feed stages, draw stages and side exchanger stages and will output the results in sections, followed by the total number of stages.

A table representing the column profile is printed next followed by the minimum number of stages.