Flowsheet Analysis

One of the most useful functions of process simulators is the ability to manipulate and analyze the different design variables to determine the required value or study its effect on the process. In addition, calculations of certain values, such as conversion and yield, might sometimes be necessary although the results are not included in the simulation output. Another feature that is usually necessary is to optimize a process based on certain criteria.

The above features are available in Aspen Plus under the **Flowsheeting Options** and **Model Analysis Tools**. The following sections will discuss some of these features.

Sensitivity Analysis

Consider a simple mixing process in which methanol, ethanol, and water are mixed together in a mixer. The amount of methanol and water are known and fixed at 100 kmol/hr. However, the amount of ethanol must be manipulated to obtain a mole fraction of 0.50 moles of ethanol in the output stream, as shown in the diagram in Figure 56. Since Aspen Plus requires the definition of all input streams, it is not possible to know the outlet composition unless we either perform the calculations by hand in advance, or calculate do a trial and error until the desired specification is

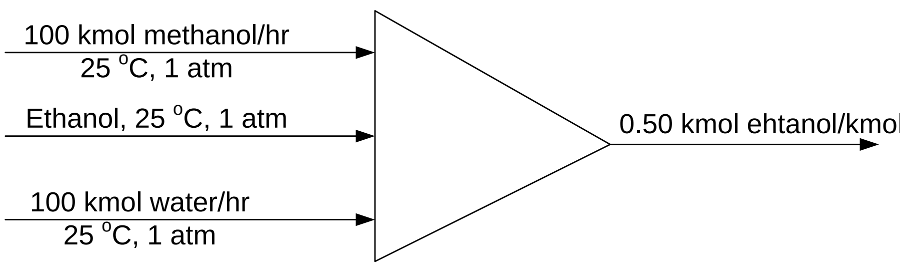


Figure 56. Simple mixing process with process specification for the outlet stream.

obtained. Obviously, these are not practical solutions especially if the mixer is part of a process.

The required design specification can be achieved via Aspen Plus Design Spec functionality available under **Flowsheeting Options | Design Spec**. To see how this functionality work, go the Design Spec folder and click the New… button. When asked for the ID, input XETOH. A new form is created than contains several tabs, as shown in Figure 57. In order to achieve the required specification, variables must be defined in the **Define** tab. The variable defined here can be the variable to which a design specification is desired or can be a part of an expression used to achieve the design specification (*e.g.*, reaction conversion). To create a new variable click on the New… button, input a name (XETOH), and select the ethanol composition of the output stream as Figure 58. By defining a variable, we make this property available to make the specification in the **Spec** tab. In this tab, we have three inputs:

1. Spec: used to input the variable or expression (in FORTRAN) the value of which is the design specification. The variables can be typed in directly or input through the variable list available by right-clicking on the field.

2. Target: a constant or expression which the Spec needs to match. If variables are used, the

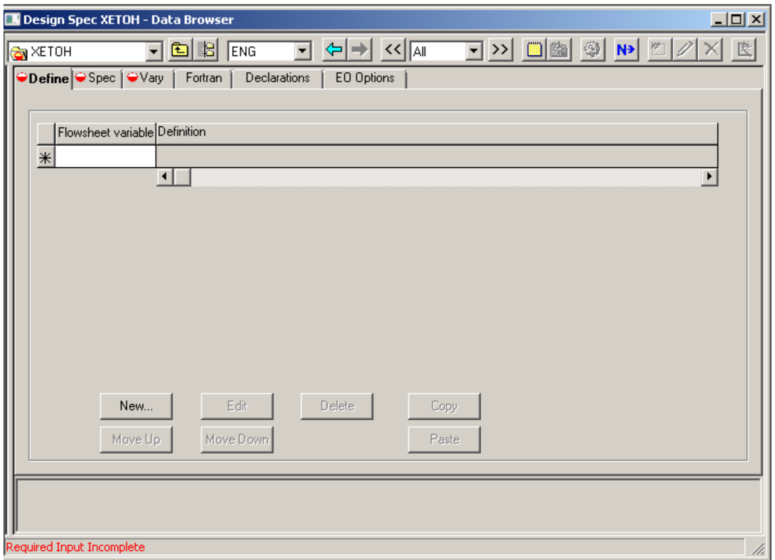


Figure 57. Design Spec form.

same input method in the Spec field can be followed.

3. Tolerance: the maximum absolute acceptable difference between the Spec and Target.

In this example, we need to set the ethanol fraction to 0.50. Therefore, our Spec variable is the XETOH, the Target is 0.50, and the tolerance can set to 0.01. In effect, these settings can be translated as:

$$XETOH = 0.50 \pm 0.01$$

The last thing to be defined is the manipulated variable, or the variable to be varied to achieve the design specification. This can be defined under the **Vary** tab. Here, a variable needs to be defined in a similar manner it was defined in the **Define** tab. In this example, we will vary the molar flow rate of the ethanol feed stream. A flow rate between 0 and 300 lbmol/hr is expected

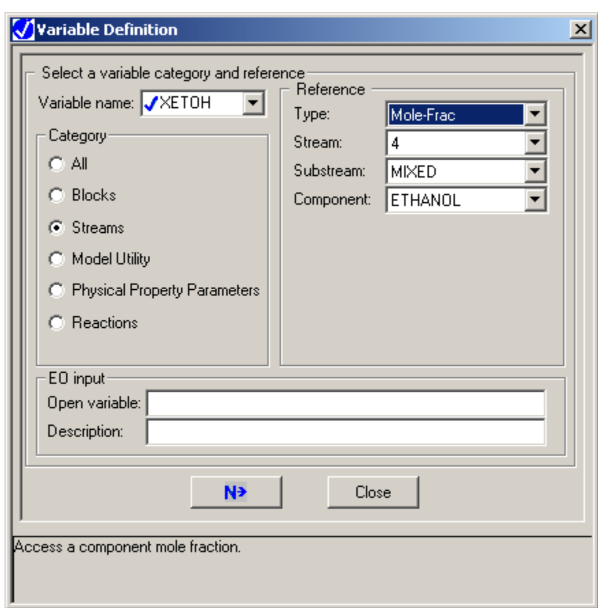


Figure 58. Defining variables for Design Spec.

to give the desired composition. The input form is show in Figure 59.

Once all the required information is input, the simulation can be run. The results for the Design Spec case are presented under the **Results** page of the XETOH form. The results show that the required ethanol flow rate is 203 kmol/hr which gives a composition of 0.504 mole ethanol/mol

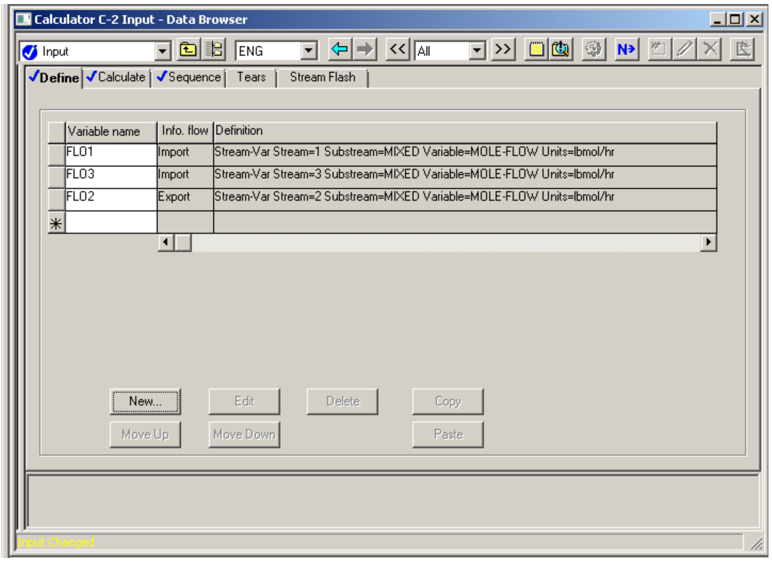


Figure 59. Defining the manipulated variable.

(within the 0.01 tolerance; the correct value is 200 kmol/hr). Also notice that this flow rate is copied to the stream and the flow rate is now changed to this new value.

> **NOTE:** If a design-spec does not converge:
>
> 1. Check to see that the manipulated variable is not at its lower or upper bound.
> 2. Verify that a solution exists within the bounds specified for the manipulated variable, perhaps by performing a sensitivity analysis.
> 3. Check to ensure that the manipulated variable does indeed affect the value of the sampled variables.
> 4. Try providing a better starting estimate for the value of the manipulated variable.

Calculators

In Aspen Plus, a calculator is used to insert FORTRAN code (or Excel sheet calculations) into the simulation. In the Calculator, variables are defined based similarly to that in the **Design Spec | Define** form. Here, however, the variables type need to be defined as either Import or Export variable. An import variable is one that is read from the simulation while an export variable is one that is written to the simulation.

The previous example can be repeated using the calculator block. In order to obtain a 0.50 fraction of ethanol we must have:

$$0.50 = \frac{\dot{m}_2}{\dot{m}_1 + \dot{m}_2 + \dot{m}_3} \qquad \longrightarrow \qquad \dot{m}_2 = \dot{m}_1 + \dot{m}_3$$

Thus, we need to find the value to $\dot{m}_2$ based on the above equation. To calculate this value, we

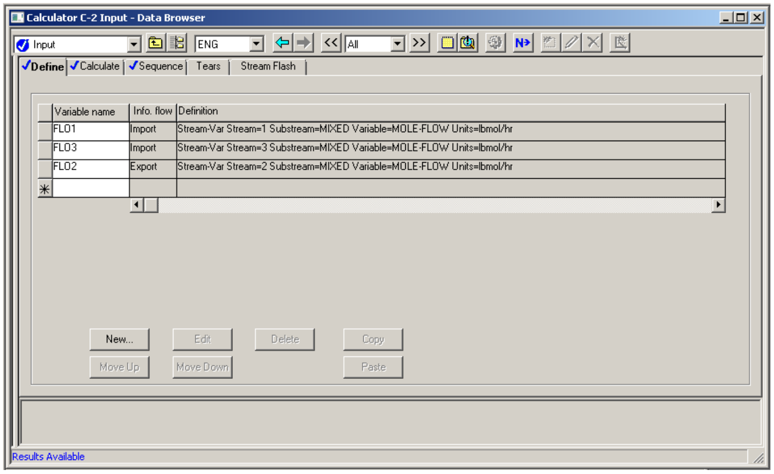


Figure 61. Calculator block variables definition.

need to read the flow rates of the two input streams (methanol and water) and output the new flow value for the ethanol stream. To do so, go to the **Flowsheeting Options | Calculator** and click the New... button. Then, go the **Input | Define** form and add the above variables as shown

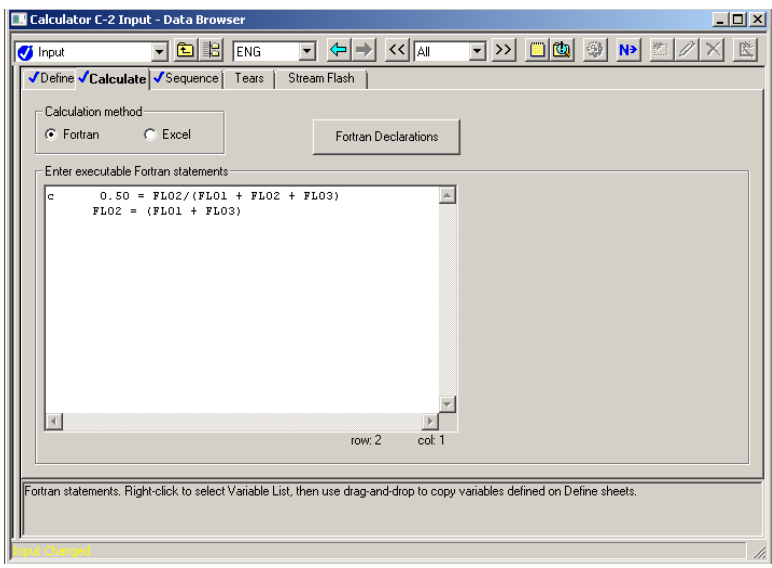


Figure 60. FORTRAN code for calculating the flow rate of ethanol.

in Figure 61.

Next, the specification, as put in the equation above is entered a FORTRAN code in the **Input | Calculate** form. FORTRAN is a programming language widely used for scientific calculations. In general, the syntax for FORTRAN is similar to other programming languages. To input a code in Aspen Plus, you need to leave 6 spaces, before you the first character (the first space is left for the letter "C" which indicates a comment line, and the next 5 is used to give the line an identifying number). For this example, the input code is shown in Figure 61.

The **Input | Sequence** tab is used to control the flow of information. By default, the use import/export variables is selected, which allows Aspen Plus to execute the calculator in the sequence of simulation.

Sensitivity Analysis

Usually the effect of one manipulated variable on a certain design variable is important to study. For example, we might be interested in studying the effect of the reactor temperature on the conversion, or the effect of reboiler heat duty on the product composition. In such situations a case study tool becomes handy. In Aspen Plus, this tool is called the **Sensitivity** tool and is available under the **Model Analysis Tool** folder.

To illustrate the use of the Sensitivity tool, the previous example will be repeated to find the flow rate of ethanol that will give the desired composition. To do so, go to the **Model Analysis Tool | Sensitivity** and click on the New… button. The input for this form is similar to that of Design Spec. Here, however, there is no Specification tab. Instead, a **Tabulate** tab is used to customize the way the output is presented. The input for this tab is shown in Figure 63. By default, the manipulated variable is presented in the first column of the table. The second row, as shown in the figure, will contain the ethanol mole fraction in the output stream (defined here as XETOH in the "Tabulated variable or expression" field). We can input here a FORTRAN expression. For example, we can type XETOH – 0.50 and determine where this value is zero. The result for the Sensitivity analysis is presented as table in the **Results** folder and can be plotted using the Plot menu. An example plot for the above result is shown in Figure 63.

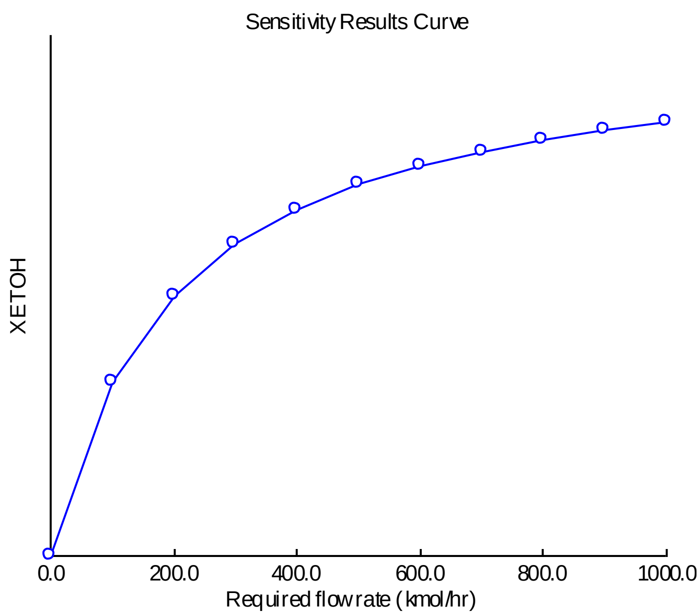


Figure 62. Sensitivity results plot.

Optimization

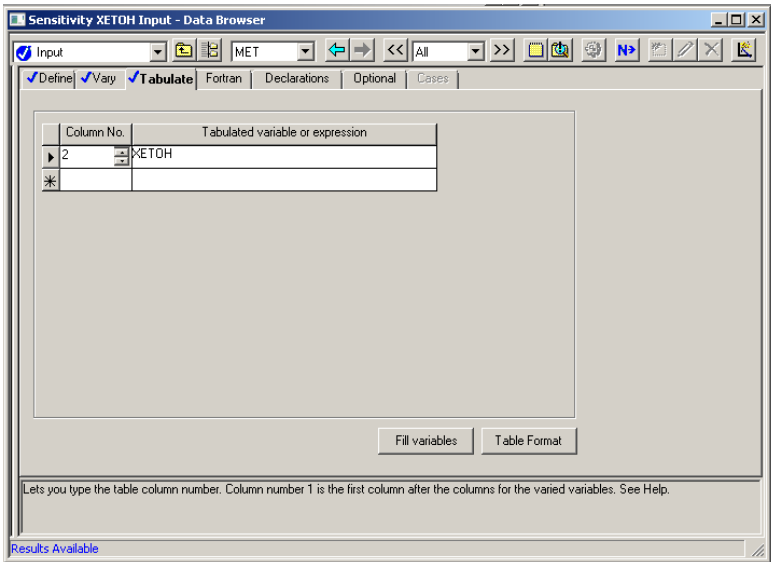


Figure 63. Setting up the way the sensitivity results are presented.

In optimization we try to find the "best" solution to a system. For example, the temperature which gives the highest conversion while minimizing the heat duty for the reactor. In this case, the optimization algorithm will try to find the best temperature within certain constraints (*e.g.*, the heat duty must be greater than zero; the conversion must be within certain range, etc).

In general the optimization problem is formulated as follows:

(24) $$\Phi = \Phi(x_1, x_2, x_3, \ldots, x_i)$$

Where Φ is the quantity to be optimized and is a function of the variables $(x_1 \ldots x_i)$ with any of the variables can take a continuous or discrete values. The variables can be subjected to constraints in the form of equalities, *e.g.*:

(25) $$f_1 = f_1(x_1, x_2, x_3, \ldots, x_i) = 0$$

or inequalities, *e.g.*:

(26) $$f_2 = f_2(x_1, x_2, x_3, \ldots, x_i) \leq 0$$

Consider, for example[*], a case where we want to find the minimum operating cost by controlling the reflux ratio of a distillation column while achieving a certain target composition. The total operating cost for the distillation column is divided as follows (for an assumed service life of L years):

1. Capital cost: this is obtained by multiplying the number of stages (N) by the cost per stage (C_N).
2. Annual maintainable cost (C_M).

[*] Taken from: Ralph Schefflan, *Teach Yourself the Basics of Aspen Plus* (Jonh Wiley & Sons, Inc, 2011), http://www.amazon.com/Teach-Yourself-Basics-Aspen-Plus/dp/0470567953.

3. Annual cost for heating in the reboiler: found by multiplying the annual heating load (R) by the cost of heating (C_R).
4. Annual cost for cooling the condenser: found by multiplying the annual cooling load (C) by the cost of cooling (C_C).
5. Annual operating cost (C_O).

Then, the objective function for this system will be the total operating cost over the service life of the distillation column:

$$\Phi = N \times C_N + (C_M + R \times C_R + C \times C_C + C_O) \times L \quad (27)$$

We can apply this optimization to process of separating a stream of equi-molar ethylbenzene/styrene at a pressure of 780 mmHg and 0.0001 vapor fraction. A DSTWU column with 95% ethylebenzene recovery, 5% styrene recovery, 760 mmHg condenser pressure, 7800 mmHg reboiler pressure, and total condenser will be used for this purpose. For the optimization, a new case can be setup from the **Optimization** folder. To define the case, variables, objectives and constraints, and manipulated variable(s) need to be defined. The variables needed for this example are the number of stages, the reboiler duty, and the condensers duty in the **Input | Define** form, as shown in Figure 65.

The objective function is defined in the **Input | Objectives & Constraints** form. The objective function can be entered directly as a variable or it can be defined in the **Input | Fortran** form. In this case, we will define a variable, PHI, to be minimized. In this form, constraints may be added, if necessary. The constraints are added in the **Model Analysis Tools | Constraint**. An example of constraint setup is shown in Figure 65.

The manipulated variable is setup in the **Input | Vary** variable. For this example, the reflux ratio will be selected with a range from 8 to 13. The definition for the objective function is input in the **Input | Fortran** as shown in Figure 66. The code defines the constants in Eq. (27) such as the service life of the column (10 years), the utilities costs, the operating cost, and the maintenance cost (5% of capital cost). In the given code, the operating cost is calculated for the entire service life.

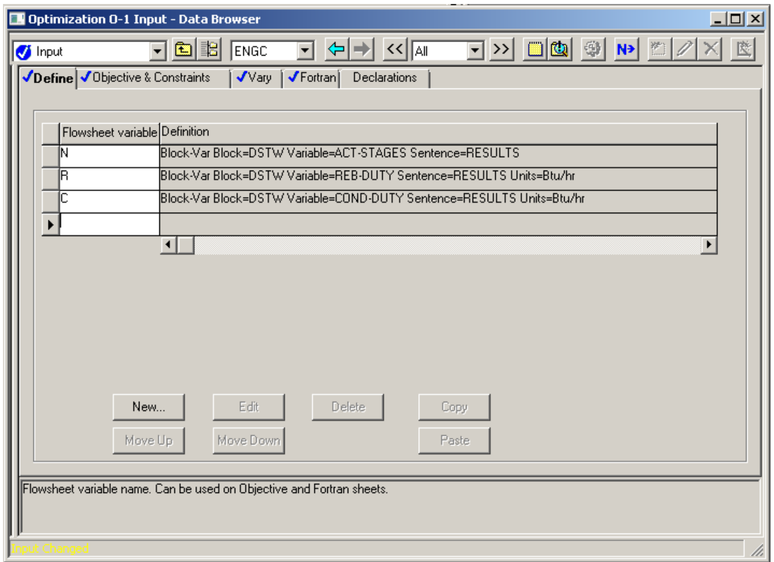


Figure 64. Defining variables for optimization cases.

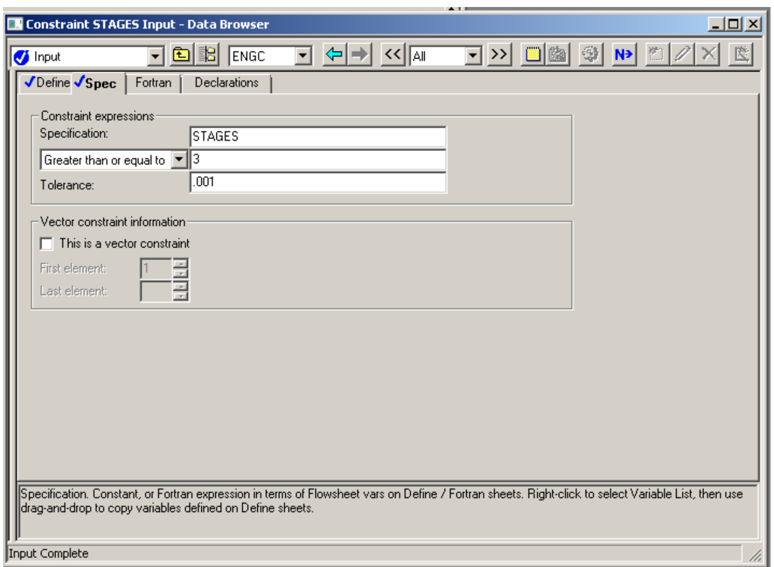


Figure 65. Setting constraints for the objective function.

The results for the optimization are presented under the **Results** page. In addition, the results for the reflux are shown in the **Convergence | Convergence | $OLVER01** page. For this column, a tall column with law reflux ratio is needed to obtain the desired separation.

NOTE:

Consider the following points given by Aspen Tech regarding optimization:

1. The convergence of the optimization can be sensitive to the initial values of the manipulated variables.

2. It is best if the objective, the constraints, and the manipulated variables are in the range of 1 to 100. This can be accomplished by simply multiplying or dividing the function.

3. The optimization algorithm only finds local maxima and minima in the objective function. It is theoretically possible to obtain a different maximum/minimum in the objective function, in some cases, by starting at a different point in the solution space.

4. Equality constraints within an optimization are similar to design specifications.

5. If an optimization does not converge, run sensitivity studies with the same manipulated variables as the optimization, to ensure that the objective function is not discontinuous with respect to any of the manipulated variables.

6. Optimization blocks also have convergence blocks associated with them. Any general techniques used with convergence blocks can be used if the optimization does not converge.

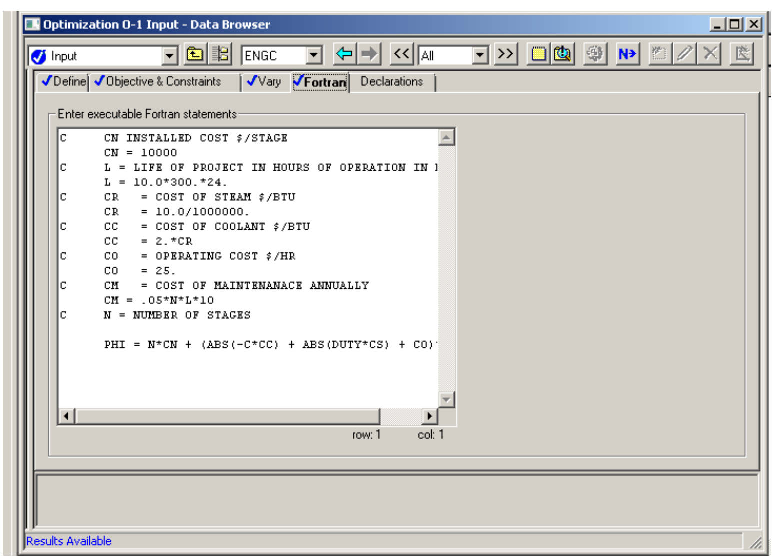
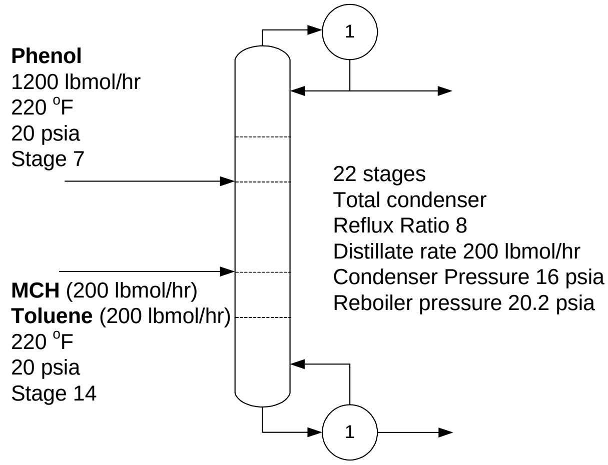


Figure 66. FORTRAN code for minimization of distillation column operating cost.

Exercise 1: Methylcyclohexane Separation

Methycyclohexane (MCH) and toluene are a difficult mixture to separate; as you can see from the equilibrium data presented in the figure below, where the vapor composition of MCH is very similar to that of liquid). Therefore, phenol is used to extract toluene and produce MCH with high concentrations. The extraction process is done in a distillation column as shown in the process diagram.



Questions: Part 1

Setup a sensitivity analysis tool to manipulate phenol flowrate and tabulate the mole fraction of MCH in distillate, reboiler duty, and condenser duty.

1. Prepare a plot showing the change in mole fraction of MCH in the distillate as a function of phenol flowrate.

2. Prepare a plot showing the change in reboiler duty as a function of phenol flowrate.

3. Prepare a plot showing the change in condenser duty as a function of phenol flowrate.

Questions: Part 2

Setup a design specification to determine the design specifications based on MCH purity in distillate by manipulating the flowrate of phenol. Setup the above design spec to give 98 mol% MCH.

1. What was the mol% MCH before setting up the design spec analysis?

....

2. What will be the required phenol flowrate to obtain the 98 mol% MCH?

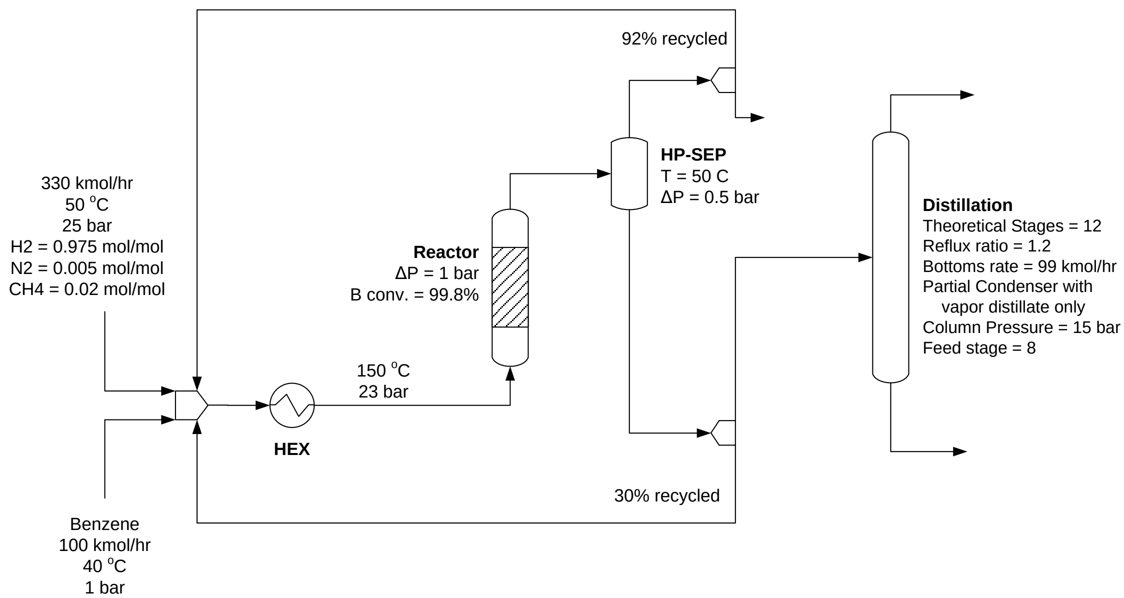
....

Exercise 2: Cyclohexane Production

In this exercise we will build our first process. The process is the cyclohexane production by hydrogenation of benzene according to the following reaction:

$$C_6H_6 + 3H_2 \leftrightarrow C_6H_{12}$$

This reaction is shown in the flowsheet below. Setup the simulation according to the given data.



Use the RK-SOAVE property method

Questions:

1. What is the CH recovery from the distillation column?

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2. What is the heat duty of the reactor in Btu/hr?

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3. Adjust the bottoms rate to obtain 99.99% CH recovery in the distillation column. What is the required bottoms rate?

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4. Perform a sensitivity analysis and plot the change in reactor duty as the liquid recycle split is varies from 10 to 40%.

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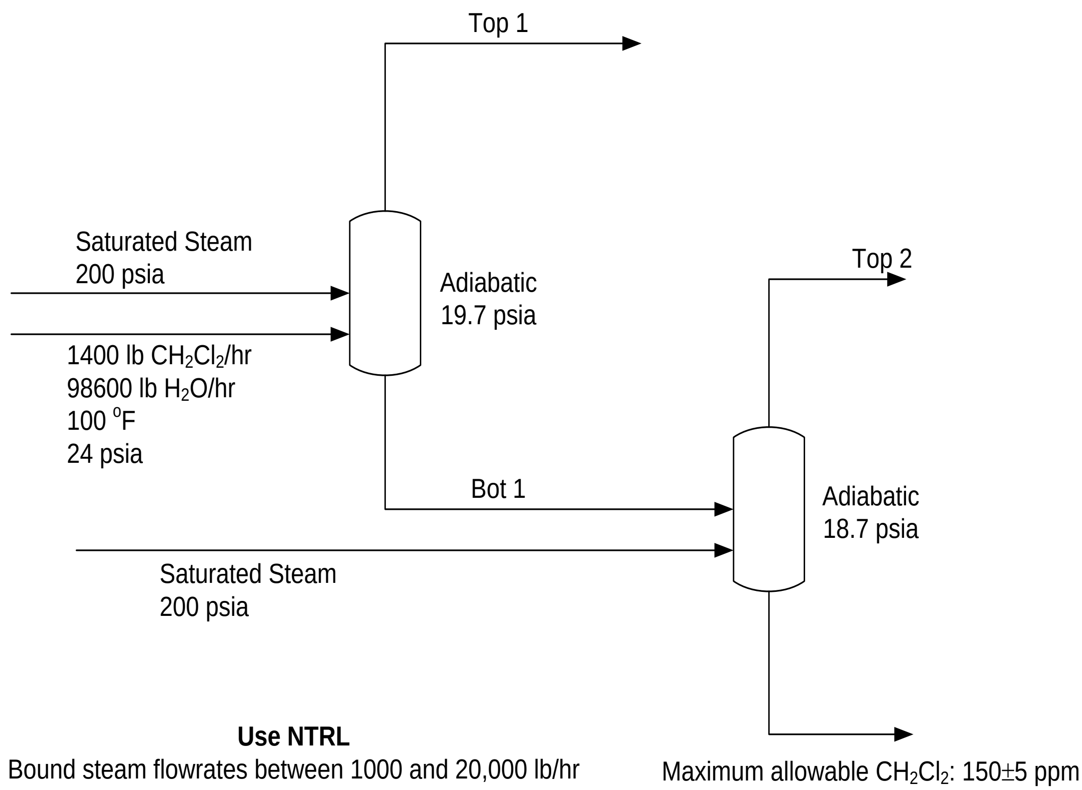
5. Add another variable to the sensitivity analysis in the previous part to study the effect of changing the conversion of the reaction. Prepare a plot with multiple graphs showing the change in reactor duty with split fraction at different conversions.

6. The cooling system around the reactor can handle a maximum operating load of 4.7 MMkcal/hr. Determine the amount of cyclohexane recycle necessary to keep the cooling load on the reactor to this amount. Pay attention to the sign convention used in Aspen Plus (input to block positive, removed from block negative).

Exercise 3: Optimization

Optimize the process shown below to minimize the amount of steam needed in each tower.



Questions:

1. What are the required streams flowrate?
