Chapter 4. Problem SM.4 – Toluene/Ethylbenzene Column

Background

In Problem SM.4 of the HYSYS manual, an organic stream leaving the decanter (S14) contains mostly methanol (ME), toluene (TL), ethylbenzene (EB), and styrene monomer (SM), and trace amounts (< 0.01 mol%) of hydrogen (H2) and water (WA), as shown in the table below for each reactor inlet temperature:

<table>
<thead>
<tr>
<th>Reactor R1 Inlet Temperatures</th>
<th>State</th>
<th>465°C</th>
<th>480°C</th>
<th>495°C</th>
<th>500°C</th>
<th>505°C</th>
</tr>
</thead>
<tbody>
<tr>
<td>H2 mol. frac.</td>
<td>0.593327</td>
<td>0.593929</td>
<td>0.591770</td>
<td>0.580471</td>
<td>0.570819</td>
<td>0.563603</td>
</tr>
<tr>
<td>ME mol. frac.</td>
<td>0.091082</td>
<td>0.12420</td>
<td>0.17182</td>
<td>0.23539</td>
<td>0.305690</td>
<td>0.390107</td>
</tr>
<tr>
<td>WA mol. frac.</td>
<td>0.283063</td>
<td>0.256658</td>
<td>0.21247</td>
<td>0.15930</td>
<td>0.1061</td>
<td>0.030569</td>
</tr>
<tr>
<td>TL mol. frac.</td>
<td>1.18099</td>
<td>1.14582</td>
<td>1.22223</td>
<td>1.11858</td>
<td>1.10645</td>
<td>1.04769</td>
</tr>
<tr>
<td>SM mol. frac.</td>
<td>0.53617</td>
<td>0.54123</td>
<td>0.55595</td>
<td>0.565165</td>
<td>0.565778</td>
<td>0.565778</td>
</tr>
</tbody>
</table>

In this above table, the components are listed in order of decreasing volatility (i.e., increasing boiling points) as pure chemical compounds at a pressure of 310 kPa. For this organic stream (S14), the light-key (LK) component is toluene and the heavy-key component (HK) is ethylbenzene. The purpose of the separation by distillation is to recycle the methanol and toluene in the liquid distillate stream and to recover the ethylbenzene and styrene monomer in the liquid bottoms stream.

In the “Flowsheet Design Specifications” section of Chapter 1 of the HYSYS manual, no specified limits exists on the hydrogen, methanol, and water in the liquid distillate stream; however, a maximum composition of ethylbenzene is set at 4 wt% and a maximum composition of combined ethylbenzene and styrene monomer is set at 5 wt% in the liquid distillate stream. The temperature of the bottoms stream cannot exceed 145°C with more than 50 mass% styrene monomer in that stream, in order to minimize polymerization of the styrene monomer (i.e., solid formation of a polymer).

Based on heuristic rules [Woods, 2007, pp. 91-94], distillation is the first choice to separate toluene from ethylbenzene in a liquid feed with composition between 15 to 80 wt% for the toluene. The ethylbenzene composition in the liquid distillate is set as a design specification at 4 wt%. The toluene composition in the liquid bottoms is chosen to be 0.01 mol% to maximize the amount of the toluene that is recycled back to the reactor. Distillation exploits the boiling-point differences of the chemical compounds by heating the liquid in the reboiler and cooling the vapor in the condenser. At 1 atm, toluene boils at 110.65°C, while ethylbenzene boils at 136.20°C. The more volatile toluene wants to concentrate in the condenser, while the less volatile ethylbenzene wants to concentrate in the reboiler.

Based on heuristics [Woods, 2007, p. 94], the column pressure is selected so that cooling water is used as the coolant and steam is used as the heating source, since these two are usually the cheapest of available utilities. Usually, a distillation column operates with a total condenser; that is, the saturated vapor coming off the top tray of the column is totally condensed to a saturated liquid using cooling water. When hydrogen is present in the liquid feed with a composition greater than 1 ppm, totally condensing the
Chapter 4. Problem SM.4 – Toluene/Ethylbenzene Column

vapor is not economically feasible because the bubble-point temperature would be around -252.6°C, the boiling point of hydrogen at 1 atm. Because of this fact, a more costly cooling medium would be required for the condenser, since the vapor could only be cooled close to 31°C with cooling water. Whenever a non-condensable like hydrogen is present in the feed, a partial condenser is a better choice, because the non-condensable can then leave the condenser in a vapor stream, instead of being condensed.

The distillation column operator ( ) in Aspen HYSYS rigorously solves the material and energy balances to separate a feed stream (F) into a non-condensable vent stream (V), a liquid distillate stream (D), and a liquid bottoms stream (B). The mathematical algorithm for a distillation column with a partial condenser (PC) is as follows:

\[
\begin{bmatrix}
\Psi_V, \Psi_D, \Psi_B, \dot{Q}_{PC}, \dot{Q}_R
\end{bmatrix} = \text{rcolumnHK}\left[\begin{bmatrix}
\Psi_F, P_{PC}, \Delta P_{PC}, P_R, \Delta P_R, N_S, N_{FS}, R, z_{D,HK}, VR_{PC}
\end{bmatrix}\right]
\]

- \(\Psi_i\) is a short notation for the process state—\(T_i, P_i, \dot{n}_i, and \bar{Z}_i\)—of Stream \(i\).
- \(T_i\) is the temperature of process stream \(i\), °C.
- \(P_i\) is the pressure of process stream \(i\), kPa.
- \(\dot{n}_i\) is the molar flow rate of process stream \(i\), kgmol/h.
- \(nc\) is the number of chemical components or compounds in the mixture.
- \(z_{i,j}\) is the bulk mole fraction of component \(j\) in process stream \(i\);
  vector \(\bar{Z}_i\) means all elements \(z_{i,1}, z_{i,2}, \ldots, z_{i,nc}\) for stream \(i\).
- \(\dot{Q}_u\) is the heat duty of the partial condenser (PC) or reboiler (R) unit \(u\), kJ/h.
- \(P_u\) is the exit pressure of the partial condenser or reboiler unit \(u\), kPa.
- \(\Delta P_u\) is the pressure drop thru the partial condenser or reboiler unit \(u\), kPa.
- \(N_S\) is the number of equilibrium stages or trays in the distillation column.
- \(N_{FS}\) is the feed-stage location, counting stages from the top of the column.
- \(R\) is the reflux ratio for the molar liquid flow back to the column over the distillate flow.
- \(z_{D,HK}\) is the mole fraction of the heavy key (HK) in the distillate stream.
- \(VR_{PC}\) is the vent ratio for the total molar flow of the vapor stream (V) leaving the partial condenser (PC) over the total molar flow of the feed (F) stream to the column.

The process states of the distillate and bottoms stream and the heat duties of the partial condenser and reboiler are determined by Algorithm “rcolumnHK”, knowing the process state of the feed stream, the exit pressures and pressure drops of the partial condenser and reboiler, the number of equilibrium stages, the feed-stage location, the reflux ratio, the mole fraction of the heavy key in the distillate stream, and the vent ratio for the vapor stream leaving the partial condenser. If you specify the mole fraction of the light key in the bottoms stream (\(z_{B,LK}\)) instead of the heavy key in the distillate stream (\(z_{D,HK}\)), then a second mathematical algorithm, named “rcolumnLK”, could also determine the material and energy requirements for the distillation column.

In order to apply these two mathematical algorithms in HYSYS, you need to have values for \(N_S, N_{FS}, R, \) and \(VR_{PC}\). Variable \(VR_{PC}\) can be approximated by taking the molar flow rates of any non-condensable components in the feed stream and dividing their sum by the total flow rate of the feed stream. How do you approximate the other three variables? Aspen HYSYS provides the “Shortcut Distillation” operator ( ) to approximate values for these three variables for a simple distillation column (one feed, one product, one bottoms, no column side streams, a total condenser, and a reboiler). Four shortcut techniques are implemented in
Chapter 4. Problem SM.4 – Toluene/Ethylbenzene Column

this HYSYS operator—the Fenske Equation for the minimum number of equilibrium stages, the Underwood Equations for the minimum reflux, the Gilliland Correlation for the number of theoretical equilibrium stages, and the Kirkbride Equation for the feed-stage location [Seader and Henley, 1998, pp. 497-512]. Based on economic heuristics, the actual reflux ratio \( R \) is 1.1 to 1.5 times the minimum reflux, with 1.1 used for a difficult separation (e.g., \( \alpha = 1.2 \)), 1.3 used for a moderate separation (e.g., \( \alpha = 2 \) to 3), and 1.5 used for an easy separation (e.g., \( \alpha = 5 \)) [ibid., pp.384], where alpha \( (\alpha) \) is the relative volatility—the ratio of the K-value (equilibrium distribution coefficient) of the light-key component to the K-value of the heavy-key component. As a first approximation, the number of theoretical equilibrium stages is about two times the minimum number of stages [Woods, 2007, p.95]. A better estimate is the one from the Gilliland Correlation. To allow for improved operability, about 10% more trays are added to the theoretical number from the Gilliland Correlation or at least two trays [ibid., p. 98]. In summary, these shortcut techniques and heuristic rules provide initial estimates for the number of stages, feed-stage location, and reflux ratio that can then be used to apply Algorithm "rcolumnHK" or "rcolumnLK" using the rigorous distillation column operator in Aspen HYSYS.

Shortcut Column Analysis

With this background information on the shortcut methods for distillation, we can now begin to simulate the separation of toluene from ethylbenzene in Stream S14 that leaves the decanter (F3), as depicted in the HYSYS process flow diagram (PFD) below.

Based on economic heuristic rules, the feed stream (S22) to the distillation column (C1) should be partially vaporized and not be a subcooled liquid (i.e., below its bubble-point temperature) or a superheated vapor (i.e., above its dew-point temperature) [Seader and Henley, 1998, p. 382]. The temperature for the feed stream should be close in value (about \( \pm 5^\circ \text{C} \)) to the temperature of the tray that it enters, in order to minimize the thermal effect on the column. Adjusting its vapor fraction \( 0.0 \leq V_f \leq 1.0 \) sets the temperature of the feed stream. The pressure for the column feed stream must be slightly greater than the pressure of the tray that it enters, in order to allow the feed material to flow into the column. How do you determine the temperature and pressure of the feed stream to the distillation column and use the HYSYS shortcut column operator to find the number of trays, feed-tray location, and reflux ratio? Proceed as follows:

1. Set the compositions for the light-key component in the bottoms stream as a saturated liquid and the heavy-key component in the distillate stream as a saturated liquid.
Chapter 4. Problem SM.4 – Toluene/Ethylbenzene Column

Based on the decanter organic stream (S14), toluene is the light key, while ethylbenzene is the heavy key. The design specification for the composition of ethylbenzene in the distillate stream is ≤ 4 wt%. The composition of toluene in the bottoms is set arbitrarily to 0.01 mol%, a reasonable value to increase the amount of toluene that will be recycled back to the reactor.

2. Pick the condenser pressure so that cooling water can be used to extract energy out of the vapor passing thru the condenser, or pick the reboiler pressure to minimize thermal degradation of any heavy-key (HK) or non-heavy-key (non-HK) components in the bottoms stream.

For the separation on the organic stream (S14), setting the reboiler pressure takes precedence because the temperature of the liquid bottoms stream cannot exceed 145°C with more than 50 mass% styrene monomer in that stream. If the ethylbenzene and styrene monomer from the decanter organic stream (S14) appeared only in the bottoms stream (S24) as a saturated liquid, then the pressure of the bottoms stream can be calculated at 145°C and \( V_f = 0 \). The mass ratio of styrene monomer (SM) to ethylbenzene (EB) is 58/31, based on the mass fraction of these two components in the decanter organic stream (S14). Using the 145°C, \( V_f = 0 \), and SM/EB mass ratio of 58/31 in the above HYSYS process flow diagram (PFD), Stream “SM 50wt%” predicts the pressure to be about 109 kPa. For 143°C, Stream “SM 50wt%” predicts 104 kPa. Thus, a pressure of 100 kPa for the bottoms stream is a reasonable starting value, and the separation will be done in a vacuum distillation column.

Under the “Flowsheet Design Variables” section in Chapter 1 of the HYSYS manual, nominal (i.e., near) atmospheric distillations will operate at 135 kPa top tray pressure and 125 kPa condenser outlet pressure. Avoid column operating pressures above nominal atmospheric. Allow 5 kPa pressure drop between the top of the column and the condenser outlet for a vacuum distillation column. For a distillation column, the feed, distillate, and bottoms streams are to be saturated liquids.

3. Set the pressure drop in the distillation column initially to 35 kPa for an easy separation and 50 kPa for a difficult separate. When the difference in the boiling temperatures at 1 atm between the heavy key and light key is ≤ 10°C, the separation by distillation is considered difficult. Have a 10 kPa pressure drop across the reboiler. After the shortcut methods have been applied, re-adjust the pressure drop using 1 kPa per stage in a nominal atmospheric column or 0.5 kPa per stage in a vacuum column, as suggested in Chapter 1 of the HYSYS manual.

At 1 atm, toluene boils at 110.65°C, and ethylbenzene boils at 136.20°C. Thus, the distillation separation of toluene from ethylbenzene is not a difficult one.

Toluene/Ethylbenzene Vacuum Distillation Column C1

<table>
<thead>
<tr>
<th>Stream</th>
<th>Pressure (kPa)</th>
<th>Pressure Drop (kPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Distillate Stream leaving the Condenser</td>
<td>70</td>
<td>ΔP = 5 kPa</td>
</tr>
<tr>
<td>Top Tray of the Distillation Column</td>
<td>75</td>
<td>ΔP = 30 kPa</td>
</tr>
<tr>
<td>Bottom Tray of the Distillation Column</td>
<td>90</td>
<td>ΔP = 10 kPa</td>
</tr>
<tr>
<td>Bottoms Stream leaving the Reboiler</td>
<td>100</td>
<td></td>
</tr>
</tbody>
</table>

4. Set the feed-stage location initially to 10 or 15 trays from the top of a distillation column for an easy separation and to 50 trays for a difficult separation. Using a pressure drop of 1 kPa.
Chapter 4. Problem SM.4 – Toluene/Ethylbenzene Column

per stage for nominal atmospheric column or 0.5 kPa per stage for a vacuum column, to
calculate the initial pressure for the feed stream. Using this calculated pressure, determine
the partially-vaporized state (0.0 ≤ \( V_f \) ≤ 1.0) of the feed stream that will enter the distillation
column, preferably as a saturated liquid (\( V_f = 0 \)). When non-condensable components are
present in the feed at greater than 1 ppm by weight, the feed vapor fraction must be greater
than zero, so that the non-condensable component can exist in the vapor phase and the feed
stream can enter the column at a temperature between the temperatures of the condenser and
reboiler. After the shortcut methods have been applied, re-adjust the pressure of the feed
stream, and re-determine its partially-vaporized state.

In the above PFD, the pressure of Stream S14 is dropped through a valve to 90 kPa, since the
pressure drop across the heater unit (EC1) is specified at 10 kPa. With this pressure drop, the
pressure of the feed stream (S22) to the column as a saturated liquid will be 80 kPa. If
HYSYS produces the error “A temperature in stream S22 is not found at the requested
conditions,” reset the \( V_f \) ≥ 0.01 to account for non-condensable components in the feed.

5. Place the HYSYS shortcut column operator on the PFD and define its Design/Connections
page. For example, as follows:

![HYSYS Shortcut Column](image)

To access the above HYSYS process flow diagram (minus the rigorous Column C1), click
one of the following web links to download the shortcut HYSYS file for a particular reactor
inlet temperature and then save it with your initials in its name to a folder:

SM4_shortcut_465,  SM4_shortcut_480,  SM4_shortcut_495,
SM4_shortcut_510,  SM4_shortcut_525,  SM4_shortcut_540.

6. Open the inlet stream to the shortcut distillation operator and define its process state by
copying the process state of the feed to the distillation column created in Step 4. Use the
Define from Other Stream… button to accomplish this task.

For the shortcut column operator, the cooling of the vapor at the top of the shortcut column is
assumed to occur in a total condenser, in order to produce only a saturated liquid leaving the
condenser. If non-condensable components (like hydrogen, oxygen, and nitrogen) are present in
small amounts within the feed stream to the shortcut column, set the mole fractions of the non-
condensable components to zero in that feed stream. Also, delete the temperature value in that
feed stream, so that HYSYS can calculate the bubble-point temperature for a specified vapor
fraction of zero.
Chapter 4. Problem SM.4 – Toluene/Ethylbenzene Column

For the toluene/ethylbenzene separation, Stream 22 is copied into Stream 22sc and the temperature of Stream 22sc is then deleted, its mole fraction for hydrogen is set to zero, and its new composition is normalized, in order to have the bubble-point temperature calculated.

7. Calculate the relative volatility ($\alpha$) of the light-key to heavy-key component, in order to determine the difficulty of the separation. Use the Worksheet/K value page of the Material Stream window for the inlet stream to the shortcut distillation operator, to complete the equation “$\alpha = \frac{K_{NL}}{K_{EB}}$”.

For Stream S22sc in the above HYSYS process flow diagram, $\alpha = \frac{1.451}{0.7118} = 2.0385$, which is a moderate distillation separation for a reactor inlet temperature of 540°C.

8. Complete the Design/Parameters page for the shortcut distillation operator by specifying the light-key component and its mole fraction in the bottoms, the heavy-key component and its mole fraction in the distillate, the exit pressure of the condenser (i.e., the pressure of the distillate stream), and the exit pressure of the reboiler (i.e., the pressure of the bottoms stream).

For the toluene/ethylbenzene separation, the C1sc Shortcut Column/Design/Parameters page is as follows:

The design specification for the light key of toluene in the bottoms stream is 0.01 mol%, while that for the heavy key of ethylbenzene in the distillate stream is 4 wt% with a maximum composition of combined ethylbenzene and styrene monomer at 5 wt%. To account for the styrene monomer contribution, the initial mass fraction of ethylbenzene in the distillate stream is set at 3.5 wt%.

Using Stream “EB 3.5 wt%” in the HYSYS process flow diagram, 3.5 wt% for ethylbenzene in the distillate stream was converted to its mole fraction equivalent of 0.0305174. After this mole fraction value has been entered into the “Heavy Key in Distillate” on the C1sc Shortcut Column/Design/Parameters page, HYSYS displays it as “0.0305”. To confirm that 0.0305174 was entered, copy the value in the light key “Mole Fraction” area and paste it into a newly-opened Word document.

Once the mole fraction of the light key in the bottoms, the mole fraction of the heavy key in the distillate, the exit pressure of the condenser, and the exit pressure of the reboiler are specified, the HYSYS shortcut column operator automatically calculates the minimum reflux ratio ($R_{min}$) using the Fenske equation. For the toluene/ethylbenzene column, its $R_{min}$ equals 4.430, for a Reactor R1 inlet temperature of 540°C.
Chapter 4. Problem SM.4 – Toluene/Ethylbenzene Column

9. Specify the external reflux ratio on the **Design/Parameters** page to be 1.1 to 1.5 times the minimum reflux ratio ($R_{\text{min}}$). Use $1.1 \times R_{\text{min}}$ for a difficult separation (e.g., $\alpha = 1.2$), $1.3 \times R_{\text{m}}$ for a moderate separation (e.g., $\alpha = 2$ to $3$), and $1.5 \times R_{\text{m}}$ for an easy separation (e.g., $\alpha = 5$)

For the toluene/ethylbenzene separation, the **C1sc Shortcut Column/Design/Parameters** page shows a specified value of 5.759 for the reflux ratio (i.e., $1.3 \times R_{\text{m}}$), as follows:

10. Examine the actual number of trays (predicted by the Gilliland Correlation) and the feed-stage location (predicted by the Kirkbride Equation) on the **C1sc Shortcut Column/Performance** page. Also, view the condenser and reboiler temperatures.

For the toluene/ethylbenzene separation, the number of stages is 29.7, the feed-stage location is 4.2, the condenser temperature is 72°C, and the reboiler temperature is 142°C, as follows:

Based on the heuristic rule for improving operability, round up the values for the number of stages and the feed-stage location, so that their one’s digit ends in five or zero. Thus, 29.7 becomes 30, and 4.2 becomes 5. If a value was 38.9, then it would be rounded up to 40. The values of 30, 5, around 72°C, and around 142°C are to be used in the rigorous distillation column operator for a reactor inlet temperature of 540°C.

11. Re-adjust the pressure of the feed stream and re-determine its partially-vaporized state, if the rounded-up feed-stage location is different than the initial value for the feed tray. Also, re-adjust the pressure drop in the column using 1 kPa per stage, if the rounded-up number of column trays is different than the initial value of trays for nominal atmospheric column. For
Chapter 4. Problem SM.4 – Toluene/Ethylbenzene Column

a vacuum column, use 0.5 kPa per stage. Redo the shortcut column calculations based on these re-adjusted values.

For the toluene/ethylbenzene separation, the pressure of the exit stream (S14B) for the valve operation (V1) would be reset based on the re-adjusted value for the pressure of the feed stream. Also, the pressure in Stream S22sc would be reset to the re-adjusted value that appears in Stream S22.

Using this 11-step procedure, the shortcut column results for each reactor inlet temperature can be determined, as shown in the table below:

<table>
<thead>
<tr>
<th>Quantity</th>
<th>465°C</th>
<th>480°C</th>
<th>495°C</th>
<th>510°C</th>
<th>525°C</th>
<th>540°C</th>
</tr>
</thead>
<tbody>
<tr>
<td>Condenser Temperature</td>
<td>73°C</td>
<td>73°C</td>
<td>73°C</td>
<td>72°C</td>
<td>74°C</td>
<td>72°C</td>
</tr>
<tr>
<td>Condenser Pressure</td>
<td>70 kPa</td>
<td>70 kPa</td>
<td>70 kPa</td>
<td>70 kPa</td>
<td>70 kPa</td>
<td>70 kPa</td>
</tr>
<tr>
<td>EB in Distillate, wt%</td>
<td>1.5</td>
<td>2.0</td>
<td>2.5</td>
<td>3.0</td>
<td>3.0</td>
<td>3.5</td>
</tr>
<tr>
<td>EB in Distillate, mol%</td>
<td>1.3043</td>
<td>1.74039</td>
<td>2.17692</td>
<td>2.61404</td>
<td>2.61404</td>
<td>3.05174</td>
</tr>
<tr>
<td>Reflux Ratio</td>
<td>2</td>
<td>2</td>
<td>2</td>
<td>3</td>
<td>4</td>
<td>6</td>
</tr>
<tr>
<td>Number of Trays</td>
<td>30</td>
<td>30</td>
<td>30</td>
<td>30</td>
<td>30</td>
<td>30</td>
</tr>
<tr>
<td>Feed Tray Number</td>
<td>5</td>
<td>5</td>
<td>5</td>
<td>5</td>
<td>5</td>
<td>5</td>
</tr>
<tr>
<td>Feed Temperature</td>
<td>98°C</td>
<td>100°C</td>
<td>103°C</td>
<td>107°C</td>
<td>110°C</td>
<td>118°C</td>
</tr>
<tr>
<td>Feed Pressure</td>
<td>80 kPa</td>
<td>80 kPa</td>
<td>80 kPa</td>
<td>80 kPa</td>
<td>80 kPa</td>
<td>80 kPa</td>
</tr>
<tr>
<td>Bottoms Temperature</td>
<td>144°C</td>
<td>144°C</td>
<td>144°C</td>
<td>143°C</td>
<td>144°C</td>
<td>142°C</td>
</tr>
<tr>
<td>Bottoms Pressure</td>
<td>100 kPa</td>
<td>100 kPa</td>
<td>100 kPa</td>
<td>100 kPa</td>
<td>100 kPa</td>
<td>100 kPa</td>
</tr>
<tr>
<td>TL in Bottoms, mol%</td>
<td>0.01</td>
<td>0.01</td>
<td>0.01</td>
<td>0.01</td>
<td>0.01</td>
<td>0.01</td>
</tr>
</tbody>
</table>

In summary, the Fenske-Underwood-Gilliland-Kirkbride shortcut techniques predict the reflux ratio, the number of equilibrium stages or trays, and the location of the feed tray for each reactor inlet temperature. Once a distillation column is built, the number of trays and feed-tray location are physically fixed. During steady-state operation of this column, the reflux ratio will be varied to satisfy the design specification for a distillation column. For a fair comparison of the net profits of the flowsheet at different reactor inlet temperatures, the number of trays should remain constant during the calculations; however, several feed location can physically exist on a constructed distillation column.

For the toluene/ethylbenzene separation, the number of trays is set to 30, and the feed location is 5 for all reactor inlet temperatures. The initial value for the reflux ratio is 4. The initial temperatures for the distillate and bottoms stream are chosen as 74 and 143°C.

These shortcut-determined values are approximations that allow you to begin a rigorous simulation of a distillation column using Algorithm “rcolumnHK” or “rcolumnLK” in Aspen HYSYS. In the rigorous distillation column operator, you will manually adjust the value of the reflux ratio, in order to meet the design specifications that have been set for the process flowsheet.

Rigorous Column Analysis

With the shortcut methods for distillation completed, the Design/Connections page for the rigorous distillation column operator can be defined for the toluene/ethylbenzene separation, as follows:
When the feed to a distillation column contains one or more non-condensable components like hydrogen and that column is part of a recycle loop in the flowsheet, a partial condenser should always be used to create a vapor or vent stream for those non-condensable components. What flow rate should you specify for this vapor stream? A better specification is the vent ratio—the molar flow of the vapor stream leaving the partial condenser over the feed molar flow to the column. The vent ratio for the partial condenser ($VR_{PC}$) can be determined by taking the molar flow rates of any non-condensable components in the feed stream and dividing their sum by the total molar flow rate of the feed stream. For feed Stream S22 in the toluene/ethylbenzene separation, $VR_{PC} = 0.2184 \text{ kmol/h of H2} / 511.3 \text{ kmol/h of feed} = 5 \times 10^{-4}$. A value ten or hundred times greater like $1 \times 10^{-2}$ should be used for the vent ratio of the condenser vapor stream, because this value is less likely to constrain the iterative process that converges the material and energy balances of the distillation column. A stricter vent ratio like $1 \times 10^{-3}$ will lead to an iteration error of “two liquid phases were found on the condenser stage.” Using $1 \times 10^{-2}$ eliminates this error.

In the Parameters/Profile page, the initial estimates for the temperatures of the condenser and reboiler can be set to 74 and 143°C, respectively, as predicted by the shortcut column operator. Thus,

The Design/Monitor page contains the design specifications that must be set for the distillation column. The initial view for this page is as follows:
where the reflux ratio and four flow rates are listed under the “Specifications” section. In the separation of toluene from ethylbenzene, the design specifications are 4 wt% for the ethylbenzene in the distillate stream with a maximum composition of combined ethylbenzene and styrene monomer at 5 wt% and 0.01 mol% for the toluene in the bottoms stream. Thus, we want to delete the four flow rates and then add three compositions—one for the light key, one for the heavy key, and one for a non-heavy key—as new specifications. We also want to add a vent ratio (aka, a feed ratio in HYSYS) for the vapor stream leaving the partial condenser and the temperature of the bottoms stream.

Each of the four flow rates under the “Specifications” section are deleted through the View… button. The Add Spec… button is used to include each of the five new specifications, as follows:

After defining the new specifications, the Design/Monitor page with the new specifications and their values for a reactor inlet temperature of 540°C is as follows:
Once three of the four specifications are checked under the “Active” column, HYSYS does the iterative calculations to find the material and energy requirements for the distillation column. HYSYS will only do the calculation once the “Degrees of Freedom” area reads zero. You can reset the iterative calculations and then restart them by using the **Reset** and **Run** buttons, respectively. The currently-checked three specifications are for Algorithm “rcolumnHK”. If the second specification for the light key is checked and the third specification for the heavy key is unchecked, then the HYSYS column operator would be solving Algorithm “rcolumnLK”.

In the above Design/Monitor page, the “Specified Value” and “Current Value” columns display the supplied and converged values for the six specifications, respectively. The current values for the three checked specifications have converged to within set tolerances for the iterative calculations. Note that the current value for the unchecked specification of the light key may be far from its specified value. By changing the specified value for the reflux ratio, you can manually iterate (i.e., do trial and error) on the reflux ratio until the desired value for the unchecked specification is matched by rounding its “Current Value” expressed in scientific notation to a value of 10.00e-5. For example, a value of 9.83e-5 rounds to 10.0e-5 or 1.00e-4, and it would be an acceptable match to a “Specified Value” of 1.00e-4.

When you supply a change in value for the reflux ratio, sometimes the iteration appears not to converge after 10 to 20 iterations. When this situation occurs, you should click the **Stop** button to re-initialize the iteration process, and then click the **Run** button to restart the iteration. If convergence still does not occur after 10 to 20 iterations, you should stop the iteration process, increase or decrease the value for the reflux ratio, reset the iteration process, and then run the iteration process again.

How do you know that you have converged to a correct solution? By unchecking the heavy-key specification and then checking the light-key specification, you can see if HYSYS converges to the same solution. If so, then you can feel confident that you have a correct solution.

**References**
