Chapter 4. Problem SM.7 – Ethylbenzene/Styrene Column

Background

In Problem SM.6 of the HYSYS manual, a modified form of successive substitution, called the Wegstein method, was used to close the material and energy balances of the recycle loop. The design parameters as specified in Chapter 1 of the HYSYS manual for this recycle loop were all met except for one. Based on pilot-plant studies, equimolar amounts of toluene and methanol are to enter Reactor R1 through Stream 10. However, the recycle loop convergence in Problem SM.6 was based on equimolar amounts of toluene and methanol entering the flowsheet by way of Streams S1 and S4. After re-converging the recycle loop for equimolar amounts of toluene and methanol entering the reactor and a production rate of 288.5022 kgmol/h (i.e., 250,000 mt/yr) of styrene monomer in Stream 24, a finishing distillation column (C2) will be needed to produce two purified streams—ethylbenzene in its distillate and styrene in its bottoms.

After this re-convergence, the bottoms stream (S24) from the toluene/ethylbenzene column (C1) leaves the recycle loop. Stream S24 contains mostly ethylbenzene (EB) and styrene monomer (SM), and trace amounts (< 0.01 mol%) of hydrogen (H2), methanol (ME), water (WA), and toluene (TL), as shown in the table below for each reactor inlet temperature:

Process State of Stream S24 for Different Reactor R1 Inlet Temperatures

State	465°C	480°C	495°C	510°C	525°C	540°C
Vapor Fraction	0.00	0.00	0.00	0.00	0.00	0.00
Temperature, °C	144.22	143.79	143.36	142.84	142.22	141.62
Pressure, kPa	100.00	100.00	100.00	100.00	100.00	100.00
Flow, kgmol/h	317.38	331.92	347.92	370.22	401.08	437.56
H2 mol. frac.	1.39665e-057	9.99998e-031	9.99538e-031	2.33608e-034	1.00000e-030	9.96235e-031
ME mol. frac.	4.32665e-024	3.63646e-024	2.86867e-024	2.18396e-024	1.51687e-024	8.40406e-025
WA mol. frac.	9.92075e-031	9.98192e-031	9.99418e-031	1.00000e-030	9.99999e-031	9.99838e-031
TL mol. frac.	9.90157e-005	9.84912e-005	9.74657e-005	9.51272e-005	9.97872e-005	9.74816e-005
EB mol. frac.	0.090890	0.130700	0.170676	0.220628	0.280584	0.340556
SM mol. frac.	0.909011	0.869202	0.829227	0.779277	0.719316	0.659346
Flow, kg/h	33113.52	34656.74	36355.45	38722.98	41999.27	45872.16
H2 mass frac.	2.69870e-059	1.93077e-032	1.92840e-032	4.50264e-036	1.92521e-032	1.91575e-032
ME mass frac.	1.32876e-024	1.11593e-024	8.79642e-025	6.69037e-025	4.64145e-025	2.56859e-025
WA mass frac.	1.71299e-031	1.72223e-031	1.72302e-031	1.72236e-031	1.72038e-031	1.71812e-031
TL mass frac.	8.74442e-005	8.69142e-005	8.59429e-005	8.38002e-005	8.78040e-005	8.56764e-005
EB mass frac.	0.092486	0.132893	0.173406	0.223941	0.284469	0.344875
SM mass frac.	0.907427	0.867020	0.826508	0.775975	0.715443	0.655040

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 100 kPa. For this process stream (S24), the light-key (LK) component is ethylbenzene and the heavy-key component (HK) is styrene monomer. The purpose of the separation by distillation in finishing Column C2 is to recover nearly-pure ethylbenzene in the liquid distillate stream and nearly-pure styrene monomer in the liquid bottoms stream.

In the "Flowsheet Design Specifications" section of Chapter 1 of the HYSYS manual, a maximum composition of toluene and styrene monomer is set at 0.8 wt% and 3 wt% in the liquid distillate stream, respectively. A maximum of 300 ppm by weight of ethylbenzene is to appear in the bottoms 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 ethylbenzene from styrene monomer in a liquid feed with composition between 15 to 80 wt% for the ethylbenzene. The styrene monomer composition in the liquid distillate is set as a design specification at 3 wt%, while that of ethylbenzene is set at 300 ppm (by weight) in the liquid bottoms. 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, ethylbenzene boils at 136.20°C, while styrene monomer boils at 145.16°C. The more volatile ethylbenzene wants to concentrate in the condenser, while the less volatile styrene monomer 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 vapor is not economically feasible because the bubble-point temperature would be around -252.6°C, the boiling point of hydrogen at 1 atm. Since the composition of hydrogen in the Stream S24 is much less the 1 ppm, a total condenser can be used in the finishing column.

The distillation column operator () in Aspen HYSYS rigorously solves the material and energy balances to separate a feed stream (F) into a liquid distillate stream (D) and a liquid bottoms stream (B). The mathematical algorithm for a distillation column with a total condenser (TC) is as follows:

$$\left[\overline{\Psi}_D, \overline{\Psi}_B, \dot{Q}_{TC}, \dot{Q}_R\right] = \text{rcolumnLK}\left[\overline{\Psi}_F,\ P_{TC}, \Delta P_{TC},\ P_R, \Delta P_R,\ N_S, N_{FS},\ R, z_{B,LK}\right]$$

$\overline{\Psi}_i$	is	a short notation for the process state— T_i, P_i, $\dot{n}_i$, and $\overline{Z}_i$ —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 $\overline{Z}_i$ 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 total condenser (TC) or reboiler (R) unit *u*, kJ/h.
P_u	is	the exit pressure of the total condenser or reboiler unit *u*, kPa.
ΔP_u	is	the pressure drop thru the total 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.
$z_{B,LK}$	is	the mole fractions of the light key (LK) in the bottoms stream.

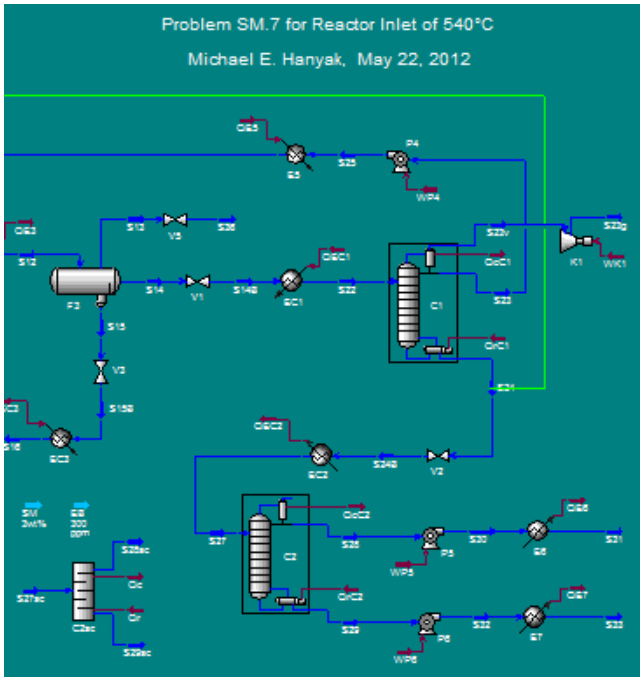
The process states of the distillate and bottoms stream and the heat duties of the total condenser and reboiler are determined by Algorithm "**rcolumnLK**", knowing the process state of the feed stream, the exit pressures and pressure drops of the total condenser and reboiler, the number of equilibrium stages, the feed-stage location, the reflux ratio, and the mole fraction of the light key in the bottoms stream. If you specify the mole fraction of the heavy key in the distillate stream ($z_{D,HK}$) instead of the light key in the bottoms stream ($z_{B,LK}$), then a second mathematical algorithm, named "**rcolumnHK**", 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}, and R. How do you approximate these 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 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 (α) 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 "**rcolumnLK**" or "**rcolumnHK**" 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 ethylbenzene from styrene monomer in Stream S24 that leaves the toluene/ethylbenzene column (C1), as depicted in the HYSYS process flow diagram (PFD) below.



Based on economic heuristic rules, the feed stream (S27) to the distillation column (C2) 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 ±5°C) to the temperature of the tray that it enters, in order to minimize the thermal effect on the column. Adjusting its vapor fraction ($0.0 \le V_f \le 1.0$) 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.

   Based on the liquid stream (S24) leaving Column C1, ethylbenzene is the light key, while styrene monomer is the heavy key. The design specification for the composition of **styrene monomer** in the distillate stream is ≤ **3 wt%**. The design specification for the composition of **ethylbenzene** in the bottoms is ≤ **300 ppm** by weight.

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 ethylbenzene-styrene stream (S24), 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 only ethylbenzene and styrene monomer from Stream S24 appeared in the bottoms stream (S29) 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 9997/3, based on the design specification of 300 ppm of ethylbenzene in the product styrene stream (S29). Using the 145°C, $V_f = 0$, and SM/EB mass ratio of 9997/3 in the above HYSYS process flow diagram (PFD), Stream "**EB 300 ppm**" predicts the pressure to be about 99.4 kPa. For 143°C, Stream "**EB 300 ppm**" predicts 94.23 kPa. Thus, a pressure of **95 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, ethylbenzene boils at 136.20°C, and styrene monomer boils at 145.16°C. Thus, the distillation separation of ethylbenzene from styrene monomer is a difficult one.

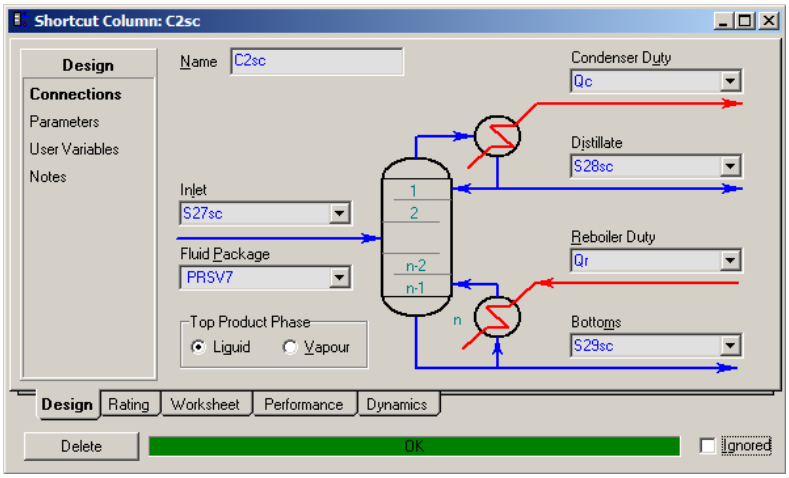
Ethylbenzene/Styrene Vacuum Distillation Column C2

Distillate Stream leaving the Condenser	30 kPa	
		ΔP = 5 kPa
Top Tray of the Distillation Column	35 kPa	
		ΔP = 50 kPa
Bottom Tray of the Distillation Column	85 kPa	
		ΔP = 10 kPa
Bottoms Stream leaving the Reboiler	95 kPa	

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 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 ($0.0 \le V_f \le 1.0$) 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 S24 is dropped through a valve to 70 kPa, since the pressure drop across the heater unit (EC2) is specified at 10 kPa. With this pressure drop, the pressure of the feed stream (S24) to the column as a saturated liquid will be 60 kPa. If HYSYS produces the error "**A temperature in stream S27 is not found at the requested conditions**," reset the $V_f \ge 0.01$ 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:



   To access the above HYSYS process flow diagram (minus the rigorous Column C2), 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:

   SM7_shortcut_465, SM7_shortcut_480, SM7_shortcut_495,

   SM7_shortcut_510, SM7_shortcut_525, SM7_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.

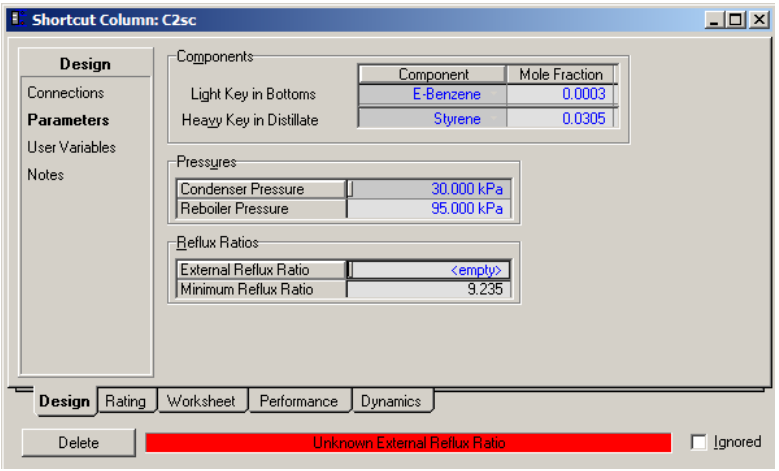
For the ethylbenzene/styrene separation, Stream 27 is copied into Stream 27sc and the temperature of Stream 27sc is then deleted, its mole fraction for hydrogen is set to zero, and its new composition is normalized, in order to have the bubble-point temperature calculated.

7. Calculate the relative volatility (α) 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 "$\alpha = K_{LK} / K_{HK}$".

   For Stream **S27sc** in the above HYSYS process flow diagram, $\alpha = \frac{K_{TL}}{K_{EB}} = \frac{1.181}{0.9066} = 1.3027$, which is a difficult 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 ethylbenzene/styrene separation, the **C2sc Shortcut Column/Design/Parameters** page is as follows:



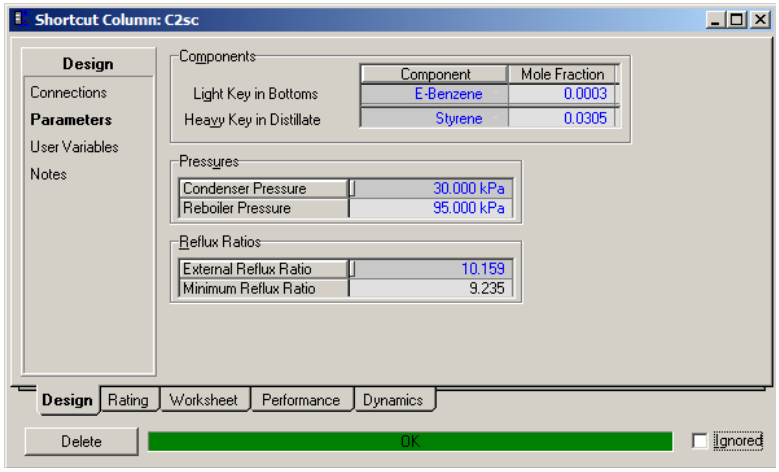
The design specification for the light key of ethylbenzene in the bottoms stream is 300 ppm by weight, while that for the heavy key of styrene monomer in the distillate stream is 3 wt%.

Using Stream "**EB 300 ppm**" in the HYSYS process flow diagram, 300 ppm by weight in the bottoms stream was converted to its mole fraction equivalent of 0.000294311. Also, Stream "**SM 3wt%**" was used to convert the 3 wt% for styrene monomer in the distillate stream to its mole fraction equivalent of 0.0305252.

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 ethylbenzene/styrene column, its R_{min} equals 9.123, for a Reactor **R1** inlet temperature of 540°C.

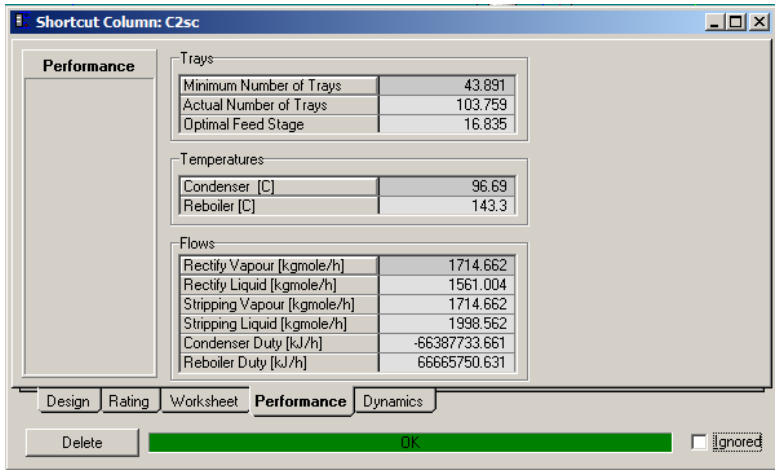
9. Specify the external reflux ratio on the **Design/Parameters** page to be 1.1 to 1.5 times the minimum reflux ratio (R_{min}). Use $1.1\times R_{min}$ for a difficult separation (e.g., $\alpha = 1.2$), $1.3\times R_m$ for a moderate separation (e.g., $\alpha = 2$ to 3), and $1.5\times R_m$ for an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

   For the ethylbenzene/styrene separation, the **C2sc Shortcut Column/Design/Parameters** page shows a specified value of 10.159 for the reflux ratio (i.e., $1.1\times R_m$), 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 **C2sc Shortcut Column/Performance** page. Also, view the condenser and reboiler temperatures.

    For the ethylbenzene/styrene separation, the number of stages is 103.8, the feed-stage location is 16.8, the condenser temperature is 97°C, and the reboiler temperature is 143°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, 103.8 becomes **105**, and 16.8 becomes **20**. The values of 105, 20, around 97°C, and around 143°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 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 number of column trays

is different than the initial value of trays for nominal atmospheric column. For a vacuum column, use 0.5 kPa per stage. Redo the shortcut column calculations based on these re-adjusted values.

For the ethylbenzene/styrene separation, the pressure of the exit stream (S24B) for the valve operation (V2) would be reset based on the re-adjusted value for the pressure of the feed stream. Also, the pressure in Stream S27sc would be reset to the re-adjusted value that appears in Stream S27.

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

Shortcut Column Results for Different Reactor R1 Inlet Temperatures

Quantity	465°C	480°C	495°C	510°C	525°C	540°C
Condenser Temperature	97°C	97°C	97°C	97°C	97°C	97°C
Condenser Pressure	30 kPa	30 kPa	30 kPa	30 kPa	30 kPa	30 kPa
SM in Distillate, wt%	3.00	3.00	3.00	3.00	3.00	3.00
SM in Distillate, mol%	3.05252	3.05252	3.05252	3.05252	3.05252	3.05252
Reflux Ratio	38.0	26.4	20.2	15.6	12.3	10.1
Number of Trays	100	100	100	100	100	100
Feed Tray Number	20	20	20	20	20	20
Feed Temperature	115°C	115°C	115°C	115°C	115°C	114°C
Feed Pressure	45 kPa	45 kPa	45 kPa	45 kPa	45 kPa	45 kPa
Bottoms Temperature	143°C	143°C	143°C	143°C	143°C	143°C
Bottoms Pressure	95 kPa	95 kPa	95 kPa	95 kPa	95 kPa	95 kPa
EB in Bottoms, ppm	300	300	300	300	300	300
EB in Bottoms, mol%	0.0294311	0.0294311	0.0294311	0.0294311	0.0294311	0.0294311

Because of the structural integrity of the height for a distillation column, the number of trays was selected to be the lower value of 100 instead of 105. Also, the feed tray is set at 20 for all reactor inlet conditions.

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 ethylbenzene/styrene separation, the number of trays is set to **100**, and the feed location is **20** for all reactor inlet temperatures. The initial value for the reflux ratio is **10**. The initial temperatures for the distillate and bottoms stream are chosen as **97** and **143°C**.

These shortcut-determined values are approximations that allow you to begin a rigorous simulation of a distillation column using Algorithm "**rcolumnLK**" or "**rcolumnHK**" 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 ethylbenzene/styrene separation, as follows:

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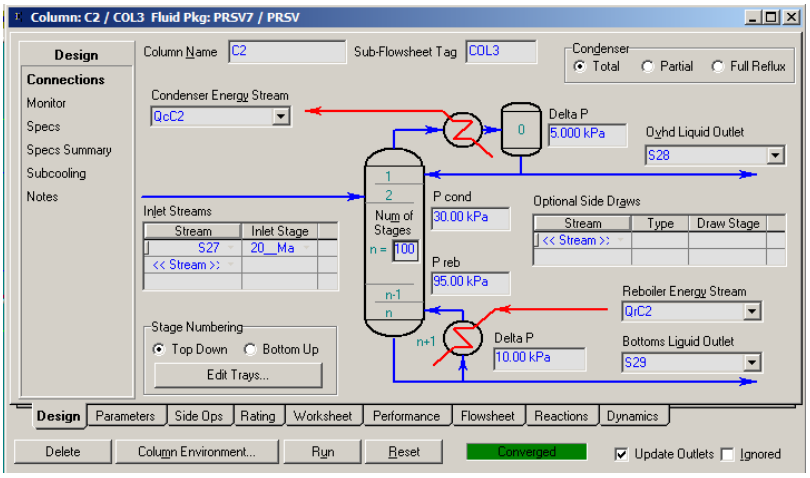
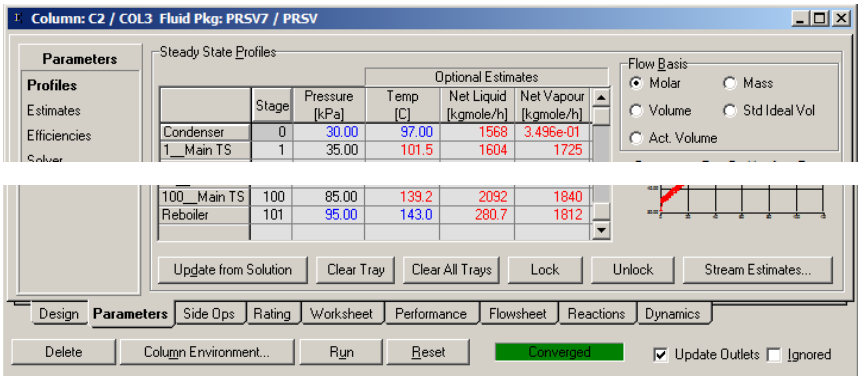
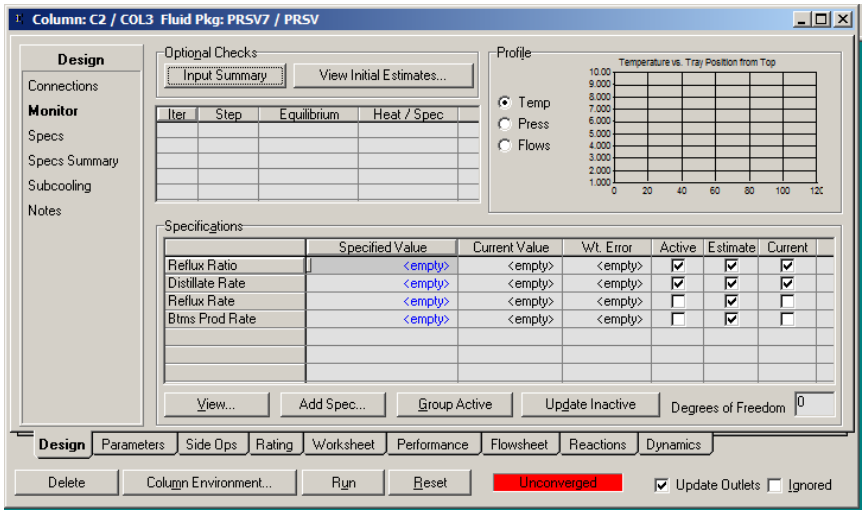


Since the composition of non-condensable components like hydrogen is ≤ 1 ppm by weight, a total condenser can be used instead of a partial condenser.

In the **Parameters/Profile** page, the initial estimates for the temperatures of the condenser and reboiler can be set to 97 and 143°C, respectively, as predicted by the shortcut column operator. Thus,

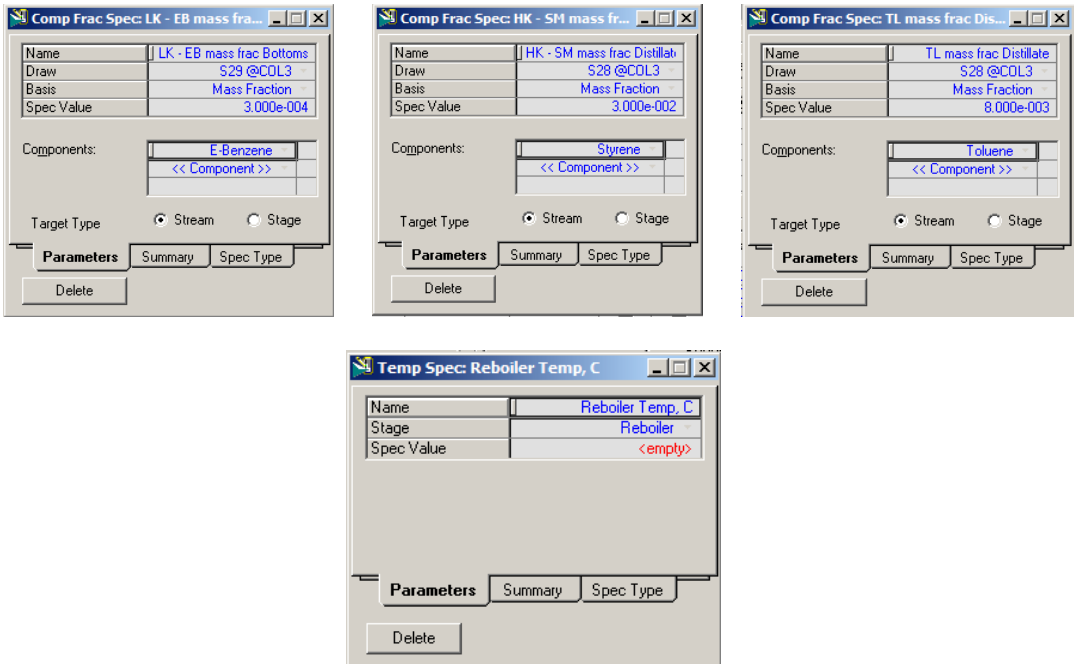


The **Design/Monitor** page contains the design specifications that must be set for the distillation column. The initial view for this page is as follows:

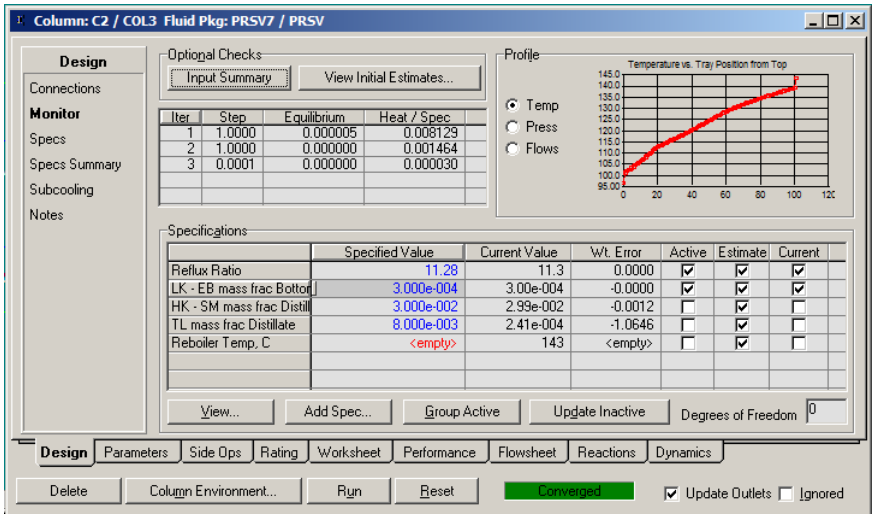


where the reflux ratio and three flow rates are listed under the "Specifications" section. In the separation of ethylbenzene from styrene monomer, the design specifications are 300 ppm by weight for the ethylbenzene in the bottoms stream and 3 wt% and 0.8 wt% for the styrene monomer and toluene, respectively, in the distillate stream. Thus, we want to delete the three flow rates and then add three compositions—one for the light key, one for the heavy key, and one for a non-light key—as new specifications. We also want to add the temperature of the bottoms stream.

Each of the three flow rates under the "Specifications" section are deleted through the **View…** button. The **Add Spec…** button is used to include each of the four 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 two 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 two specifications are for Algorithm "**rcolumnLK**". If the third specification for the heavy key is checked and the second specification for the light key is unchecked, then the HYSYS column operator would be solving Algorithm "**rcolumnHK**".

In the above **Design/Monitor** page, the "Specified Value" and "Current Value" columns display the supplied and converged values for the four specifications, respectively. The current values for the two checked specifications have converged to within set tolerances for the iterative calculations. Note that the current value for the unchecked specification of the heavy 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 3.00e-2. For example, a value of 2.99e-2 rounds to 3.00e-2, and it would be an acceptable match.

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, select the ***Reset*** 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 light-key specification and then checking the heavy-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

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