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THE UNIVERSITY OF BRITISH COLUMBIA

**Chemical & Biological Engineering**  
Faculty of Applied Science

**CHBE 376: Computer Flowsheeting & Unit  
Operation Design**

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## **CHBE 376**

Instructor: Jonathan Verrett

# **First, Second and Third Complex Block – Simulation**

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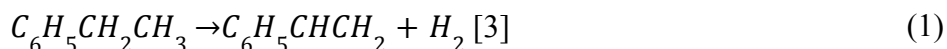
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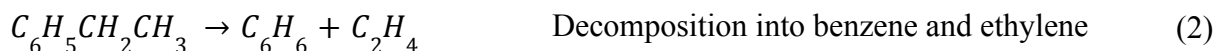
# 1. Process Type

My simulation will focus on the production of styrene via catalytic dehydrogenation of ethylbenzene. In 2019, the US produced over 4.5 million metric tons of styrene. [1] This process is widely used by ethylbenzene manufacturers where little ethylbenzene is sold commercially, rather the product is immediately made into styrene; the demand for ethylbenzene is heavily dependent on the demand for styrene production. [2]

The dehydrogenation reaction of ethylbenzene shown below:



The process occurs at above 600°C [4] and a low pressure (0.4-1.4 bar) [5] to favor the generation of products. The process utilizes a metal catalyst such as zinc or magnesium oxides on activated carbon to minimize side reactions, however since the process occurs at high temperatures the decomposition of ethylbenzene to benzene and ethylene occurs and is considered an undesirable side reaction. In addition, the hydrodealkylation of ethylbenzene forms methane and toluene. The side reactions are shown below:



# 2. Major Units

I anticipate the following units when designing the process and the arrangement of the units are shown in the block flow diagram.

- 2 Distillation Columns
- 1 Separator
- 1 Catalytic Reactor
- 4 Heat Exchangers

### 3. Block Flow Diagram

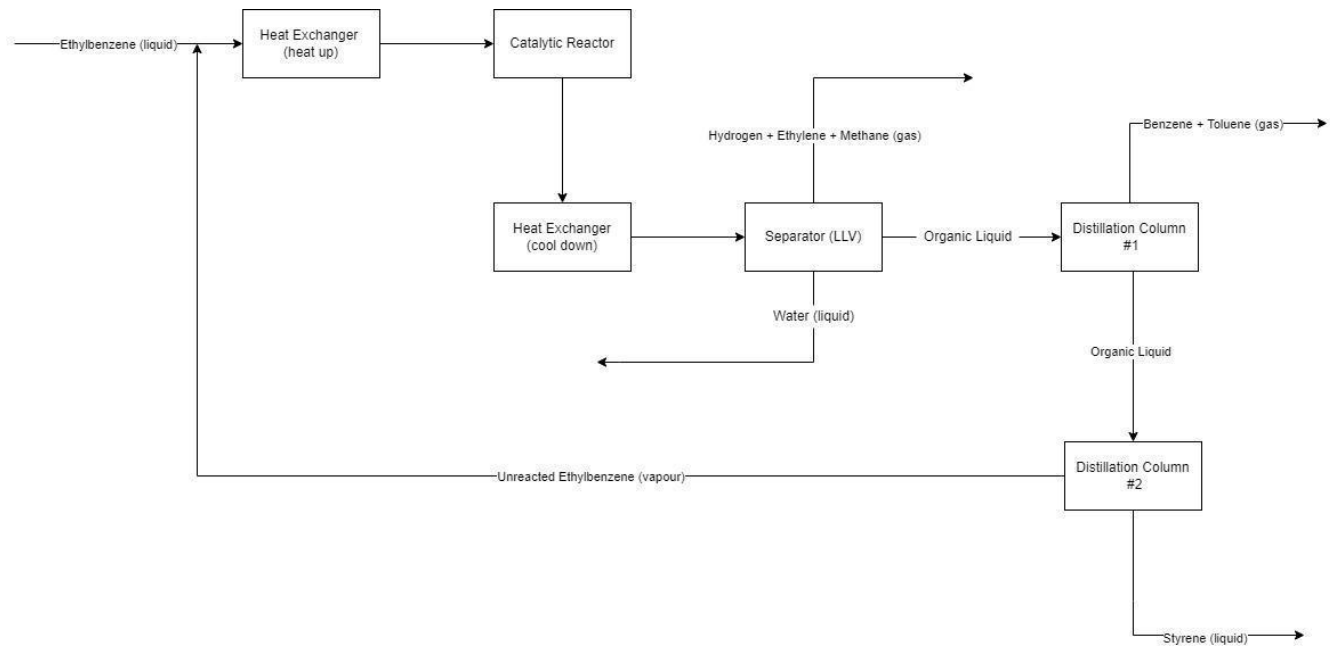
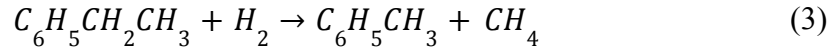
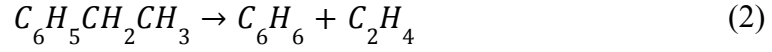
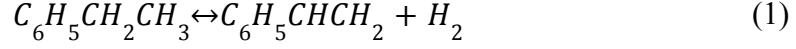


Figure 1: Block flow diagram of the production of styrene via the dehydrogenation of ethylbenzene

## 4. Components

The dehydrogenation of ethylbenzene to produce styrene process is comprised of three reactions (one main reaction and two side reactions carried out at varying conditions [6]:



The major components relevant to the simulation are listed in table 1 below.

Name	Formula
Ethylbenzene	$C_6H_5CH_2CH_3$
Styrene	$C_6H_5CHCH_2$
Hydrogen	$H_2$
Benzene	$C_6H_6$
Ethylene	$C_2H_4$
Toluene	$C_6H_5CH_3$
Methane	$CH_4$
Water	$H_2O$

## 5. Property Method

Conditions in the process vary at relatively low pressures from 0.4 to 1.4 bar and at temperatures above 600°C. There is one non-hydrocarbon component namely hydrogen gas. Every other component is a hydrocarbon. However, due to the significant presence of water in the feed stream, this nonpolar component may suggest property methods such as PENG-ROB are not appropriate in this case – especially in complex blocks that deal with LLV separation. Therefore, NTRL is an appropriate property method to use in this simulation.

## 6. Catalytic Reactor Setup

This reactor setup will focus on the dehydrogenation of ethylbenzene (EB) production step, which was reaction 1. This is typically produced using an iron catalyst [7]. Common side reactions for this system are the generation of benzene, and ethylene, and the production of toluene and methane shown in reaction 2 and 3 respectively. There also exist other reactions consisting of water and other side reaction products, however these further side reactions will not be considered in this complex block as they do not enhance or detriment the dehydrogenation of ethylbenzene.

In many processes, a mixture of fresh ethylbenzene and recycled styrene, benzene, and toluene is fed into the catalytic reactor. The latter of which comes from the distillate streams of distillation columns. The feed consists of the majority ethylbenzene (>95.0% wt.) relative to all reactive species (excluding water). For this simulation we will assume a molar feed consisting of 98.3% ethylbenzene, 0.988% styrene, 0.0407% benzene, and 0.691% toluene. This feed stream of 719 kmol/hr reactive species is mixed with 7777 kmol/hr of water. [7] The feed stream is typically preheated to temperatures ranging from 500 °C to 600 °C and fed into a fixed bed reactor at 1 bar; the larger limit of the range of temperatures will be used. The reaction is endothermic and typically reactor temperatures will range from 600°C to 620°C [8]. At higher temperatures, the thermal-decomposition of styrene begins to occur.

For this system, a plug flow reactor (RPLUG) will be used to simulate this reaction step. Kinetic data provided as an example by Lee *et al.* describes rates for 3 relevant reactions in this process [7]. The catalyst specifications will not be entered into ASPEN as they have been considered in the developed rate laws shown below.

Table 1 provides the rate laws and parameters for the kinetic coefficient to be derived from the Arrhenius equation [7]

Rate Law $\frac{kmol}{kg_{cat} sec}$	Frequency Factor $\frac{kmol}{kg_{cat} sec}$	Activation Energy $\frac{kJ}{kmol}$
$r_1 = \frac{k_1 K_{EB} \left[ P_{EB} - \left( \frac{P_{ST} P_{H_2}}{K_{eq}} \right) \right]}{\left( 1 + K_{EB} P_{EB} + K_{H_2} P_{H_2} + K_{ST} P_{ST} \right)^2}$	$7.57 \times 10^{-5}$	$E_{A_1} = 0.17538$
$r_2 = \frac{k_2 K_{EB} P_{EB}}{\left( 1 + K_{EB} P_{EB} + K_{H_2} P_{H_2} + K_{ST} P_{ST} \right)^2}$	$1.51 \times 10^{-6}$	$E_{A_2} = 0.29629$
$r_3 = \frac{k_3 K_{EB} P_{EB} K_{H_2} P_{H_2}}{\left( 1 + K_{EB} P_{EB} + K_{H_2} P_{H_2} + K_{ST} P_{ST} \right)^2}$	$5.11 \times 10^{-6}$	$E_{A_1} = 0.47476$

Table 2 provides the parameters for the driving, and absorption force in the LHHW kinetics setup.

Parameter	Value
$K_{EB}$	$8.47 \times 10^{-5} Pa^{-1}$
$K_{ST}$	$3.40 \times 10^{-4} Pa^{-1}$
$K_{H_2}$	$3.90 \times 10^{-5} Pa^{-1}$
$K_{eq}$	$8.58 \times 10^{11} Pa$

The frequency factors in Lee *et al.* has units of kmol/(kg<sub>cat</sub>h) while the rate concentration basis is the partial pressure (bar) of each component; the reaction takes place in the vapor phase. Appropriate unit conversions have been made for the values in table 1 and 2. The reactor is set up at 620°C and 1 bar. [7]

Given the nature of the rate laws shown in table 1, Langmuir-Hinshelwood-Hougen-Watson kinetics will be used to estimate the kinetics of the catalytic reactions. The coefficients of the LHHW kinetics in ASPEN are derived from the following:

$$\ln \ln K_i = A + \frac{B}{T} + C \ln T + D T$$

Since the parameters in table 1 are independent of temperature, we will only be concerned with the coefficient  $A$ . Since there is no second term in the driving force for reactions 2 and 3, the coefficient for  $A$  has been set to a large negative value to simulate  $K = 0$  without resulting in a math error. The

absorption force for each reaction is shown below, and is identical for each reaction as shown in table 1.

Prior to setting up the kinetic reactor, an equilibrium reactor has been set up to compare the conversions of ethylbenzene and styrene and selectivity of styrene to the catalytic reactor. Simulations show in an equilibrium reactor with identical operation conditions, the conversion of ethylbenzene is found to be 99.4%, the conversion of ethylbenzene to styrene is 42.2%, and the selectivity of ethylbenzene to styrene is 42.5%.

From Lee *et al.* the size of the reactor had an internal diameter of 3.50 meters and a length of 1.43 meters, and the catalyst weight was set to 78330 kg. The iron catalyst particle size was specified to be 0.25-0.42 mm; bed voidage is 0.4. [7]

For the RPLUG reactor specified above, the final ethylbenzene conversion is found to be 88.9% which is lower than the conversion simulated for REQUIL, due to the presence of a backward reaction i.e. the second term of the driving force. The conversion of ethylbenzene to styrene is 86.4%, and the selectivity of ethylbenzene to styrene is 97.2%, which are both significant increases compared to the equilibrium conversions/selectivities which emphasizes the importance of the catalyst in styrene production. The concentration profiles over the reactor are shown in figure 1 below:

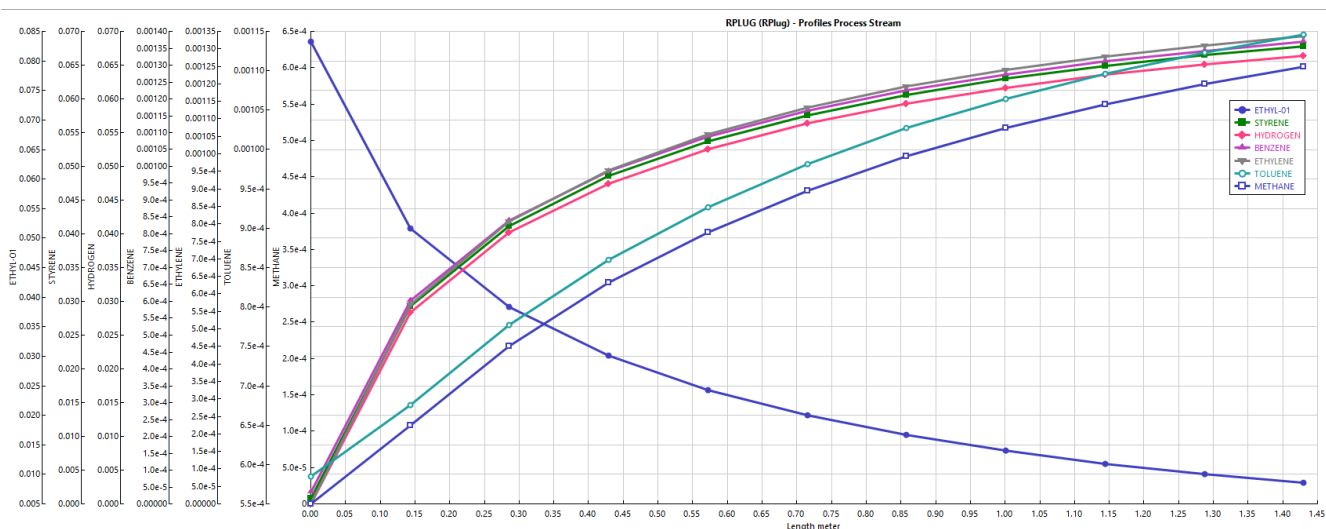


Figure 1 illustrates the concentration profile of each reactive component (excluding water) along the length of the catalytic reactor.



## 7. LLV Separator – Sensitivity Analysis

This complex block will primarily focus on the operating temperature required for optimal separation of the styrene and organic side products in the LLV separator. After exiting the catalytic reactor as described in the first complex block, the outlet stream cools down the 50°C [8]. This ensures the majority of liquid organic matter and water are in their liquid phases; this minimizes the amount of organic matter in the vapor stream. The organic matter and water should be easily separable due to their intrinsic immiscible properties.

To simulate this complex block, Flash3 will be used as it is desired to have 2 liquid outlet streams and 1 vapor outlet stream. The initial operating temperature and pressure is set to 50°C and 1 bar respectively. The limits of the operating conditions should ensure that all inclusive settings restrict the vaporization of styrene, benzene, and toluene. The primary goal of this sensitivity analysis is to understand the behavior of the separation between water and organic matter at different operating temperatures. This is done by varying the temperature of the flash drum. It can be seen in figure 2, the mole fractions of styrene and water in the second liquid stream (primarily water) increase with increasing flash temperature.

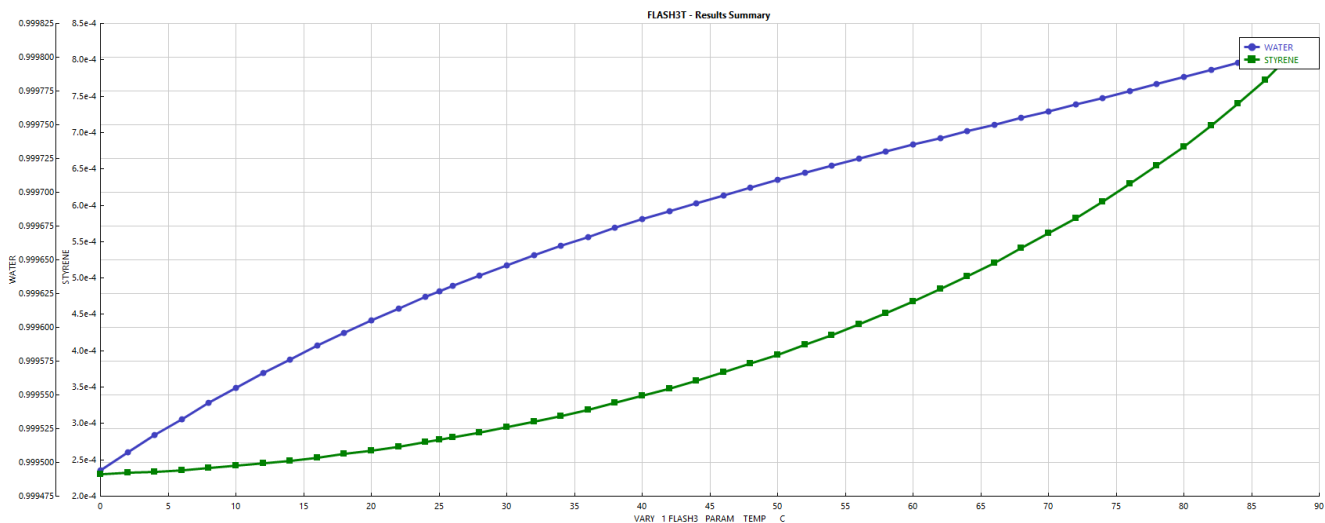


Figure 2 illustrates the mole fraction of styrene and water in the second liquid stream of the LLV separator

Figure 3 shows the behavior of the same variables but for the first liquid stream (primarily organic liquid). It can be seen that the mole fractions of water and styrene also ultimately increase as the flash temperature increases, however after a certain temperature, the mole fraction of styrene in this stream

reaches its maximum before decreasing rapidly to 0 at 90°C. This is possibly due to the sudden vaporization of the organic liquid stream. The absence of the organic liquid stream leaves water as the only liquid stream, causing the pure water composition and the switch in streams.

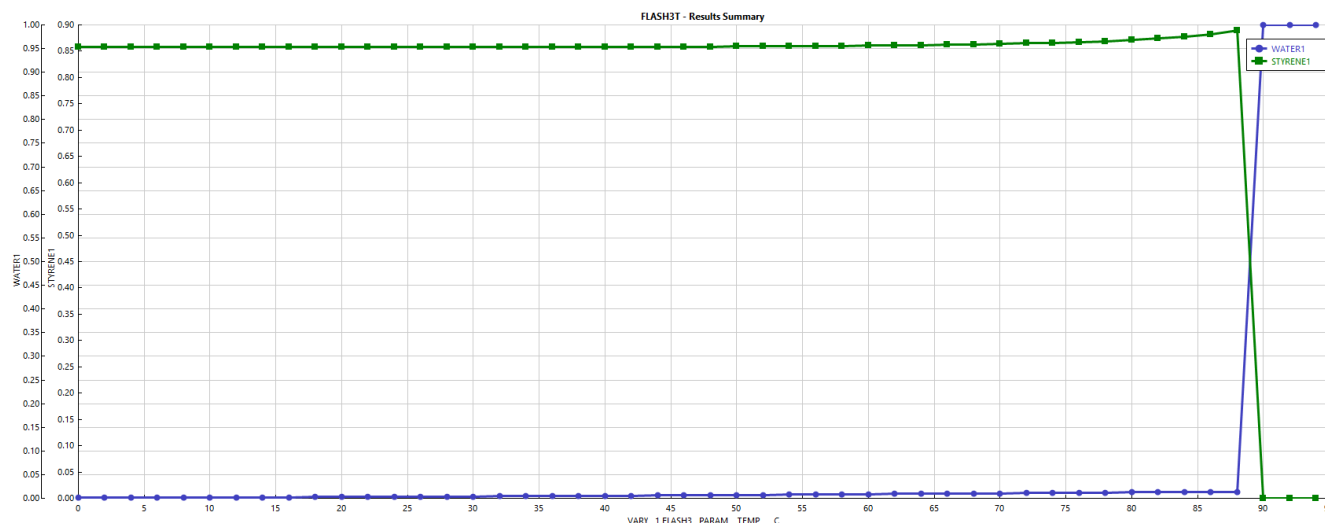


Figure 3 illustrates the mole fraction of styrene and water in the first liquid stream of the LLV separator

After careful analysis the maximum styrene composition shown in figure 3 does not indicate the maximum flow rate of styrene – which is not desired. Therefore, a sensitivity analysis of styrene flow rate is more appropriate. Figure 4 below illustrates the molar flow rate of styrene and water in the organic liquid dominant stream of the LLV separator. The sudden increase in water flow rate can be attributed to the complete vaporization of the organic liquid, causing water to appear in the first liquid stream of the LLV separator. This is quickly vaporized as well once temperatures approach 95°C.

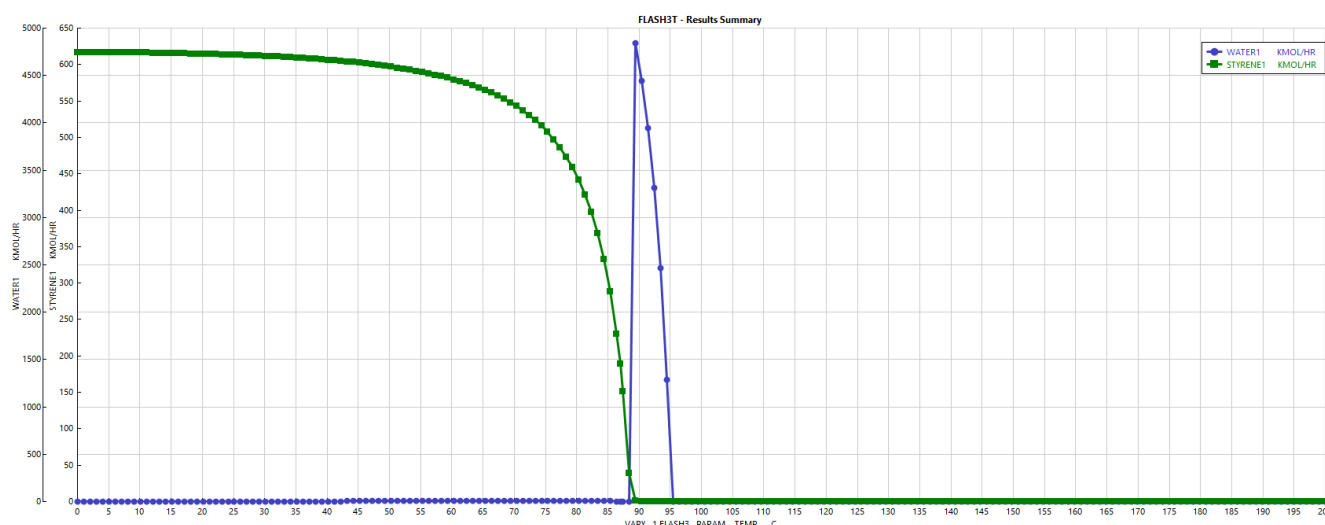


Figure 4 illustrates the molar flow of styrene and water in the first liquid stream of the LLV separator

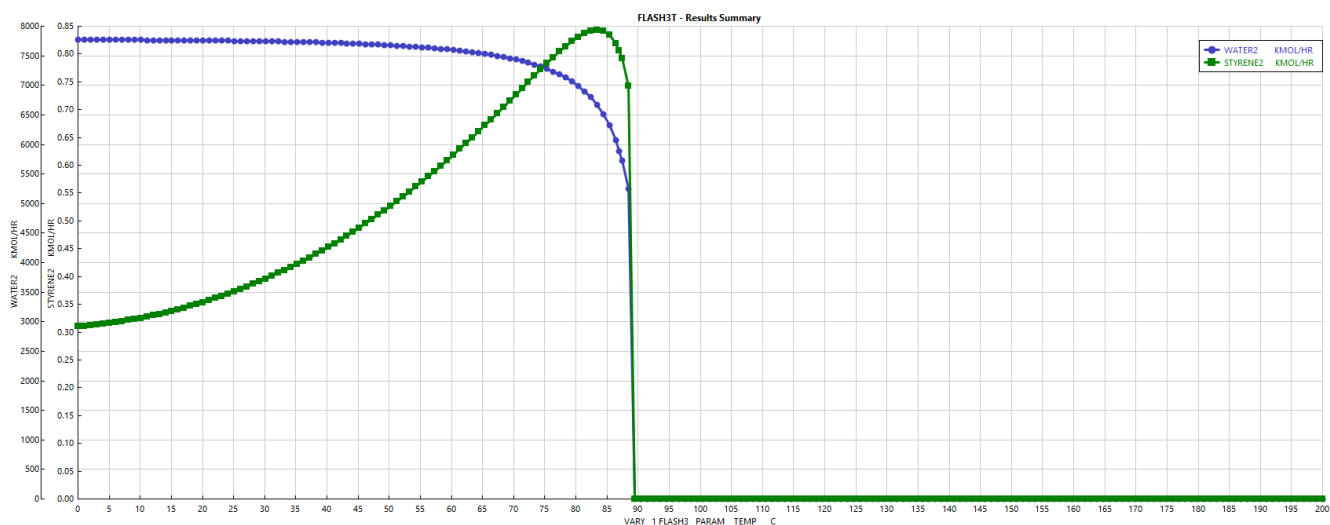


Figure 5 illustrates the molar flow rate of styrene and water in the second liquid stream of the LLV separator

Figure 5 above illustrates the molar flow rate of styrene and water in the water dominant stream of the LLV separator. The organic species completely vaporizes as the flash temperature approaches 90°C due to the vaporization of the organic mixture (methane, toluene, ethylene, and benzene) which agrees with the relationship found in figure 3. Note the water flow rate also reaches zero as the water is now only present in the first liquid stream.

From the sensitivity analysis conducted, it is clear a lower temperature achieves the optimal recovery of styrene. At the lower limits (below 0°C), solidification of streams can occur, which will cause equipment damage. Additionally, as seen from the trends described above in figure 4 and 5, the changes in styrene flow rate at lower temperatures are negligible. Moreover, operating at temperatures below room temperature can be costly as cooling utilities will be required. At the upper limits of temperature operating conditions, the vaporization of one or both liquid streams will occur, resulting in a redundant flash separator. Therefore, an intermediate temperature should be chosen to maximize net process revenue – ensuring operating/reliability/maintenance and utility costs can be covered by the revenue generated by the market value of the finished product.

## 8. Distillation Column Design

The last complex block will focus on the design of a pair of distillation columns to separate styrene (heavy key) from the rest of the organic liquid recovered from the LLV separator. The light key will be specified as ethyl-benzene. A pair of DSTWU models will be used to initially model and estimate the parameters of the column. This will provide accurate estimates for variables such as reflux ratio, number of stages, feed stage etc. in order to conduct more rigorous distillation calculations using RadFrac. The first DSTWU column have a feed entering at 50°C consisting of the following stream elements:

Table 3 provides corresponding molar flow rates and compositions of the entering feed stream.

Component	Molar Flow (kmol/hr)	Mole Fraction
ETHYL-01	74.5877	0.1073
STYRENE	597.0725	0.8590
HYDROGEN	0.0426	0.0001
BENZENE	9.0830	0.0131
ETHYLENE	0.1026	0.0001
TOLUENE	9.2403	0.0133
METHANE	0.0111	0.0000
WATER	4.9210	0.0071
Total	695.0608	1.0000

If we desire a 90%, and 1% recovery of the LK and HK component respectively in the distillate with a reflux ratio of 1.5 times the minimum reflux ratio, the following results give an approximation of necessary parameters for the distillation column:

Minimum reflux ratio	7.42198	
Actual reflux ratio	11.133	
Minimum number of stages	33.1946	
Number of actual stages	51.1852	
Feed stage	34.4627	
Number of actual stages above feed	33.4627	
Reboiler heating required	18434	kW
Condenser cooling required	14251.9	kW
Distillate temperature	-19.494	C
Bottom temperature	173.336	C
Distillate to feed fraction	0.138837	

From the DSTWU shortcut simulation conducted above, to obtain the specified fractional recoveries, a reflux ratio of 11.133 is required with a column consisting of 52 stages, the 34th stage being the feed

stage. The distillate to feed fraction is calculated to be 0.138837. The distillate feed of the shortcut simulation achieves a styrene purity of 98.75% with a molar flow of 591.102 kmol/hr (screenshot of flow rates are shown in the appendix).

Table 4 shows the results of the first RadFrac model simulation.

Parameter	Value
Condenser Heat Duty [kW]	-11084.7
Reboiler Heat Duty [kW]	15825.7
Number of Stages	52
Feed Stage	34
Distillate Stream Temperature [°C]	132.713
Bottom Stream Temperature [°C]	144.436

The column's bottom feed is planned to be sent to a second distillation column to increase the purity. After conducting the shortcut DSTWU method analysis similar to the first column, the predicted minimum reflux ratio was determined to be 60.159, and the actual ratio being 90.800 resulting in a bottoms styrene purity of 99.4%. The results of this shortcut simulation is shown below:

Minimum reflux ratio	60.5197	
Actual reflux ratio	90.7796	
Minimum number of stages	30.6334	
Number of actual stages	45.7133	
Feed stage	31.0801	
Number of actual stages above feed	30.0801	
Reboiler heating required	32005.4	kW
Condenser cooling required	32007.4	kW
Distillate temperature	136.726	C
Bottom temperature	144.897	C
Distillate to feed fraction	0.0584644	

Since the feed of the second distillation column is already quite pure, there is significantly less distillate flow as shown by the distillate to feed fraction. Similarly to the first column, a rigorous RadFrac model will be used to simulate the distillation process using the estimated parameters obtained above. The results of the second RadFrac simulation are shown in the table below:

Table 4 shows the results of the second RadFrac model simulation.

Parameter	Value
Condenser Heat Duty [kW]	-31752.7
Reboiler Heat Duty [kW]	32099.9
Number of Stages	46
Feed Stage	32
Distillate Stream Temperature [°C]	137.257
Bottom Stream Temperature [°C]	144.882

The temperature and composition profiles shown in the appendices agree with the physical phenomena concerning the distillation column. Temperature at upper stages will have a lower temperature due to the substantially higher concentration of the less volatile component compared to the lower stages of the column. Ultimately, this dual column configuration is able to achieve a 99.4% styrene pure stream in the bottom stream.

## 9. References

- [1] Published by Lucía Fernández and O. 19, “Styrene production U.S. 2019,” *Statista*, 19-Oct-2021. [Online]. Available: <https://www.statista.com/statistics/974845/us-styrene-production-volume/>. [Accessed: 26-Jan-2022].
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- [3] W. L. Luyben, “Design and control of the Styrene process,” *Principles and Case Studies of Simultaneous Design*, pp. 291–317, 2011.
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- [6] A. Streitwieser, and C.H. Heathcock. “Introduction to Organic Chemistry,” 1992. MacMillan.
- [7] W. Jae Lee and G. F. Froment, “Ethylbenzene dehydrogenation into styrene: Kinetic modeling and reactor simulation,” *Industrial & Engineering Chemistry Research*, vol. 47, no. 23, pp. 9183–9194, 2008.
- [8] A. Pérez Sánchez, E. J. Pérez Sánchez, and R. M. Segura Silva, “Simulation of the styrene production process via catalytic dehydrogenation of ethylbenzene using CHEMCAD® process simulator,” *Tecnura*, vol. 21, no. 53, pp. 15–31, 2017.

## 10. Appendices

### Results from RPLUG Simulation:

Material	Heat	Load	Vol.% Curves	Wt. % Curves	Petroleum	Polymers	Solids
					Units	FEED	OUTLET
Molar Vapor Fraction						1	1
Molar Liquid Fraction						0	0
Molar Solid Fraction						0	0
Mass Vapor Fraction						1	1
Mass Liquid Fraction						0	0
Mass Solid Fraction						0	0
Molar Enthalpy				cal/mol		-45058.9	-39691.4
Mass Enthalpy				cal/gm		-1769.23	-1672.8
Molar Entropy				cal/mol-K		-2.93412	0.273637
Mass Entropy				cal/gm-K		-0.115208	0.0115324
Molar Density				mol/cc		1.37748e-05	1.34663e-05
Mass Density				gm/cc		0.000350816	0.000319523
Enthalpy Flow				cal/sec		-1.06344e+08	-1.00547e+08
Average MW						25.468	23.7276
<b>- Mole Flows</b>				<b>kmol/hr</b>		<b>8496.37</b>	<b>9119.59</b>
ETHYL-01				kmol/hr		707	78.29
STYRENE				kmol/hr		7.104	618.143
HYDROGEN				kmol/hr		0	605.557
BENZENE				kmol/hr		0.293	12.4813
ETHYLENE				kmol/hr		0	12.1883
TOLUENE				kmol/hr		4.968	10.4506
METHANE				kmol/hr		0	5.48257
WATER				kmol/hr		7777	7777

### Results from REQUIL Simulation:

Material	Heat	Load	Vol.% Curves	Wt. % Curves	Petroleum	Polymers	Solids			
					Units	EQ-FEED		EQ-LIQ		EQ-VAP
						1				1
						0				0
						0				0
						1				1
						0				0
						0				0
					cal/mol	-45058.9				-41596.7
					cal/gm	-1769.23				-1719.04
					cal/mol-K	-2.93412				-0.345982
					cal/gm-K	-0.115208				-0.0142982
					mol/cc	1.37748e-05				1.34663e-05
					gm/cc	0.000350816				0.000325853
					cal/sec	-1.06344e+08				-1.03327e+08
						25.468				24.1976
					<b>kmol/hr</b>	<b>8496.37</b>		<b>0</b>		<b>8942.44</b>
					kmol/hr	707		0		1.27137
					kmol/hr	7.104		0		280.027
					kmol/hr	0		0		13.2656
					kmol/hr	0.293		0		173.441
					kmol/hr	0		0		173.148
					kmol/hr	4.968		0		264.625
					kmol/hr	0		0		259.657
					kmol/hr	7777		0		7777



## Kinetic Parameters for RPLUG: Reaction 1

RPLUG (RPlug) - Stream Results (Boundary) × Main Flowsheet × R-1 (LHHW) × +

☒ Stoichiometry ☒ Kinetic ☐ Equilibrium ☐ Activity ☐ Comments

1) ETHYL-01 --> STYRENE(MIXED) + HYDROGEN(MIXED)

Reacting phase: **Vapor** Rate basis: **Cat (wt)**

LHHW kinetic expression

$$r = \frac{[\text{Kinetic factor}][\text{Driving force expression}]}{[\text{Adsorption expression}]}$$

Kinetic factor

If To is specified: Kinetic factor =  $k(T/T_o)^n e^{-(E/R)(1/T-1/T_o)}$

If To is not specified: Kinetic factor =  $kT^n e^{-E/RT}$

k: **7.57e-05**

n: **0**

E: **0.17538 kJ/kmol**

To: **C**

☒ Driving Force Expression

Reacting phase: **Vapor**

[Ci] basis: **Partial pressure**

Enter term: **Term 1**

Term 1

Concentration exponents for reactants		Concentration exponents for products	
Component	Exponent	Component	Exponent
ETHYL-01	1	STYRENE	0
		HYDROGEN	0

Coefficients for driving force constant

A: **-9.37687** B: **0** C: **0** D: **0**

☒ Adsorption Expression

Reacting phase: **Vapor**

[Ci] basis: **Partial pressure**

Adsorption expression exponent: **2**

Concentration exponents

Component	Term no. 1	Term no. 2	Term no. 3	Term no. 4	Term no. 5
HYDROGEN	0	0	1	0	
STYRENE	0	0	0	1	

Adsorption constants

Term no.	1	2	3	4
Coefficient A	0	-9.37687	-10.1517	-7.98656
Coefficient B	0	0	0	0
Coefficient C	0	0	0	0
Coefficient D	0	0	0	0

## Reaction 2

RPLUG (RPlug) - Stream Results (Boundary) × Main Flowsheet × R-1 (LHHW) × +

Stoichiometry Kinetic Equilibrium Activity Comments

2) ETHYL-01 --> BENZENE(MIXED) + ETHYLENE(MIXED)

Reacting phase **Vapor** Rate basis **Cat (wt)**

LHHW kinetic expression

$$r = \frac{[\text{Kinetic factor}][\text{Driving force expression}]}{[\text{Adsorption expression}]}$$

Kinetic factor

If To is specified Kinetic factor =  $k(T/T_o)^n e^{-(E/R)[1/T-1/T_o]}$

If To is not specified Kinetic factor =  $kT^n e^{-E/RT}$

k **1.51e-06**

n **0**

E **0.29629 kJ/kmol**

To **C**

Solids

Driving Force

Adsorption

Driving Force Expression

Reacting phase **Vapor**

[Ci] basis **Partial pressure**

Enter term **Term 1**

Term 1

Concentration exponents for reactants

Component	Exponent
ETHYL-01	1

Concentration exponents for products

Component	Exponent
BENZENE	0
ETHYLENE	0

Coefficients for driving force constant

A: **-9.37687** B: **0** C: **0** D: **0**

Adsorption Expression

Reacting phase **Vapor**

[Ci] basis **Partial pressure**

Adsorption expression exponent **2**

Concentration exponents

Component	Term no. 1	Term no. 2	Term no. 3	Term no. 4	Term no. 5
ETHYL-01	0	1	0	0	
HYDROGEN	0	0	1	0	
STYRENE	0	0	0	1	

Adsorption constants

Term no.	1	2	3	4
Coefficient A	0	-9.37687	-10.1517	-7.98656
Coefficient B	0	0	0	0
Coefficient C	0	0	0	0
Coefficient D	0	0	0	0

## Reaction 3

RPLUG (RPlug) - Stream Results (Boundary) × Main Flowsheet × R-1 (LHHW) × +

Stoichiometry Kinetic Equilibrium Activity Comments

3) ETHYL-01 + HYDROGEN --> TOLUENE(MIXED) + METHANE(MIXED)

Reacting phase: Vapor Rate basis: Cat (wt)

LHHW kinetic expression

$r = \frac{[\text{Kinetic factor}][\text{Driving force expression}]}{[\text{Adsorption expression}]}$

Kinetic factor

If  $T_0$  is specified Kinetic factor =  $k(T/T_0)^n e^{-(E/R)[1/T-1/T_0]}$

If  $T_0$  is not specified Kinetic factor =  $kT^n e^{-E/RT}$

k: 5.11e-06

n: 0

E: 0.47476 kJ/kmol

$T_0$ : C

Solids

Driving Force

Adsorption

Driving Force Expression

Reacting phase: Vapor

[Ci] basis: Partial pressure

Enter term: Term 1

Term 1

Concentration exponents for reactants

Component	Exponent
ETHYL-01	1
HYDROGEN	1

Concentration exponents for products

Component	Exponent
TOLUENE	0
METHANE	0

Coefficients for driving force constant

A: -19.5286 B: 0 C: 0 D: 0

Close

Adsorption Expression

Reacting phase: Vapor

[Ci] basis: Partial pressure

Adsorption expression exponent: 2

Concentration exponents

Component	Term no. 1	Term no. 2	Term no. 3	Term no. 4	Term no. 5
ETHYL-01	0	1	0	0	0
HYDROGEN	0	0	1	0	0
STYRENE	0	0	0	0	1

Adsorption constants

Term no.	1	2	3	4
Coefficient A	0	-9.37687	-10.1517	-7.98656
Coefficient B	0	0	0	0
Coefficient C	0	0	0	0
Coefficient D	0	0	0	0

Close

## Sensitivity Analysis:

Main Flowsheet x FLASH3 (Flash3) - Stream Results (Boundary) x **FLASH3T** x FLASH3T - Results Summary - Plot

☒ Vary ☒ Define ☒ Tabulate Options Cases Fortran Declarations Comments

^ Sampled variables (drag and drop variables from form to the grid below)

Variable	Definition
▶ <b>WATER2</b>	Mole-Flow Stream=L2 Substream=MIXED Component=WATER Units=kmol/hr
▶ <b>STYRENE2</b>	Mole-Flow Stream=L2 Substream=MIXED Component=STYRENE Units=kmol/hr
▶ <b>WATER1</b>	Mole-Flow Stream=L1 Substream=MIXED Component=WATER Units=kmol/hr
▶ <b>STYRENE1</b>	Mole-Flow Stream=L1 Substream=MIXED Component=STYRENE Units=kmol/hr
*	

☒ Vary ☒ Define ☒ Tabulate Options Cases Fortran Declarations Comments

☒ Active ☐ Case study

^ Manipulated variables (drag and drop variables from form to the grid below)

Variable	Active	Manipulated variable	Units
▶ 1	<input checked="" type="checkbox"/>	Block-Var Block=FLASH3 Variable=TEMP Sentence=...	C

New Delete Copy Paste Send to Aspen Multi-Case

^ Edit selected variable

Manipulated variable

Variable: 1

Type: Block-Var

Block: FLASH3

Variable: TEMP

Sentence: PARAM

Units: C

Manipulated variable limits

☒ Equidistant ☐ Logarithmic ☐ List of values

Start point: 0 C

End point: 200 C

☒ Number of points: 200

☐ Increment: 1.005025 C

Report labels

Main Flowsheet x FLASH3 (Flash3) - Stream Results (Boundary) x **FLASH3T** x FLASH3T

☒ Vary  
 ☒ Define  
 ☒ **Tabulate**  
 Options  
 Cases  
 Fortran  
 Declarations  
 Comments

	Column No.	Tabulated variable or expression
▶	<b>1</b>	<b>WATER2</b>
▶	<b>2</b>	<b>STYRENE2</b>
▶	<b>3</b>	<b>WATER1</b>
▶	<b>4</b>	<b>STYRENE1</b>
*		

DSTWU Simulation Flowrates

	Units	L1	COL1-BOT	COL1-DIS
Pressure	bar	1	1	1
Molar Vapor Fraction		0	0	0
Molar Liquid Fraction		1	1	1
Molar Solid Fraction		0	0	0
Mass Vapor Fraction		0	0	0
Mass Liquid Fraction		1	1	1
Mass Solid Fraction		0	0	0
Molar Enthalpy	cal/mol	21648.1	30219.2	-5531.85
Mass Enthalpy	cal/gm	209.689	290.076	-56.7809
Molar Entropy	cal/mol-K	-77.0533	-62.8856	-103.992
Mass Entropy	cal/gm-K	-0.746358	-0.603644	-1.06741
Molar Density	mol/cc	0.00845081	0.00755064	0.00957236
Mass Density	gm/cc	0.872454	0.7866	0.932581
Enthalpy Flow	cal/sec	4.17965e+06	5.02444e+06	-148285
Average MW		103.239	104.177	97.4244
<b>— Mole Flows</b>	<b>kmol/hr</b>	<b>695.061</b>	<b>598.561</b>	<b>96.5002</b>
ETHYL-01	kmol/hr	74.5877	7.45877	67.1289
STYRENE	kmol/hr	597.073	591.102	5.97073
HYDROGEN	kmol/hr	0.042566	2.64026e-11	0.042566
BENZENE	kmol/hr	9.08299	7.22859e-22	9.08299
ETHYLENE	kmol/hr	0.10262	6.36526e-11	0.10262
TOLUENE	kmol/hr	9.24035	1.27682e-09	9.24035
METHANE	kmol/hr	0.0111189	6.89679e-12	0.0111189
WATER	kmol/hr	4.92095	3.05233e-09	4.92095

RADFRAC

Configuration

Streams

Pressure

Condenser

Reboiler

3-Phase

Comments

Setup options

Calculation type

Equilibrium

Number of stages

52

Stage Wizard

Condenser

Partial-Vapor

Reboiler

Kettle

Valid phases

Vapor-Liquid

Convergence

Standard

Operating specifications

Reflux ratio

Mole

11.133

Distillate to feed ratio

Mole

0.138837

Free water reflux ratio

0

Feed Basis

Design and specify column internals

Configuration

Streams

Pressure

Condenser

Reboiler

3-Phase

Comments

Feed streams

	Name	Stage	Convention
▶	L1	34	Above-Stage

Product streams

	Name	Stage	Phase	Basis	Flow	Units
▶	COL1-BOT	52	Liquid	Mole		kmol/hr
▶	COL1-DIS	1	Vapor	Mole		kmol/hr

Pseudo streams

	Name	Pseudo Stream Type	Stage	Internal Phase	Reboiler Phase	Reboiler Conditions	Pumparot ID
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## RADFRAC RESULTS

Summary

Balance

Split Fraction

Reboiler

Utilities

Stage Utilities

Status

Basis

Mole

Condenser / Top stage performance

	Name	Value	Units
▶	Temperature	132.713	C
▶	Subcooled temperature		
▶	Heat duty	-11084.7	kW
▶	Subcooled duty		
▶	Distillate rate	96.5002	kmol/hr
▶	Reflux rate	1074.34	kmol/hr
▶	Reflux ratio	11.133	
▶	Free water distillate rate		
▶	Free water reflux ratio		

Reboiler / Bottom stage performance

	Name	Value	Units
▶	Temperature	144.436	C
▶	Heat duty	15825.7	kW
▶	Bottoms rate	598.561	kmol/hr
▶	Boilup rate	1553.34	kmol/hr
▶	Boilup ratio	2.59512	
▶	Bottoms to feed ratio	0.861163	



☒ Configuration
 ☒ Streams
 ☒ Pressure
 ☒ Condenser
 ☒ Reboiler
 3-Phase
 Comments

View
 

Top / Bottom

Top stage / Condenser pressure
 

Stage 1 / Condenser pressure
 

1 bar

Stage 2 pressure (optional)
 

☒ Stage 2 pressure
 
 bar

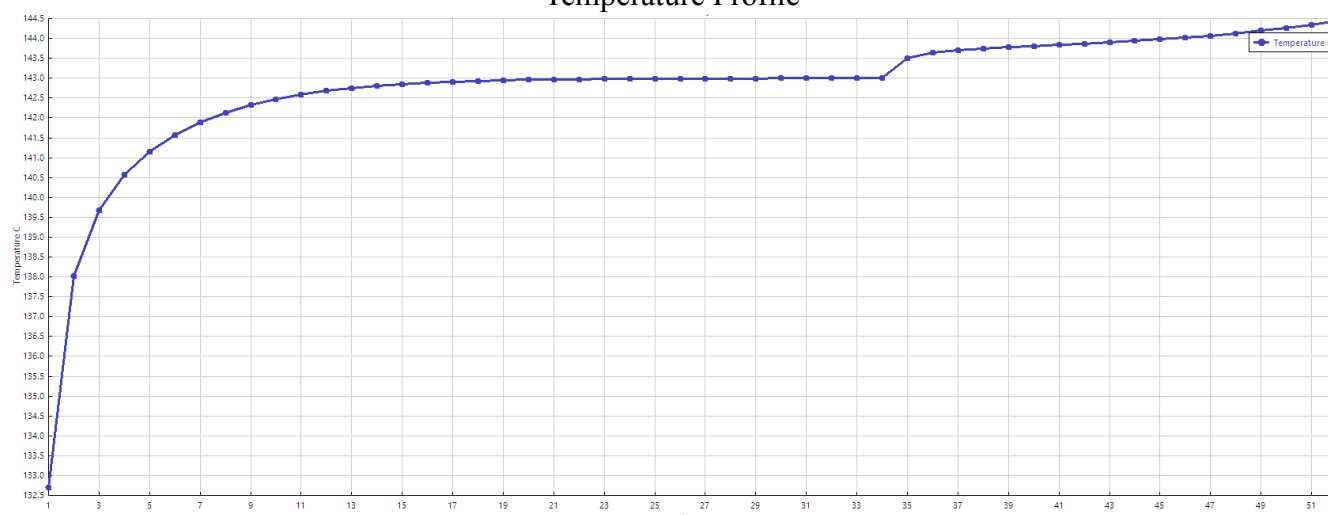
☐ Condenser pressure drop
 
 bar

Pressure drop for rest of column (optional)
 

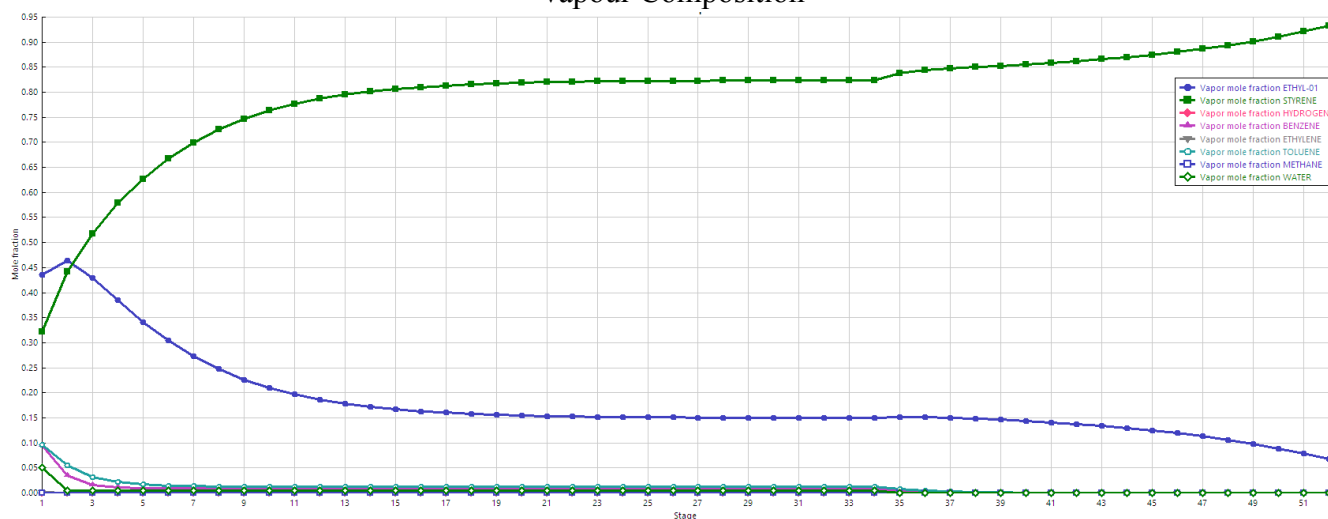
☒ Stage pressure drop
 
 bar

☐ Column pressure drop
 
 bar

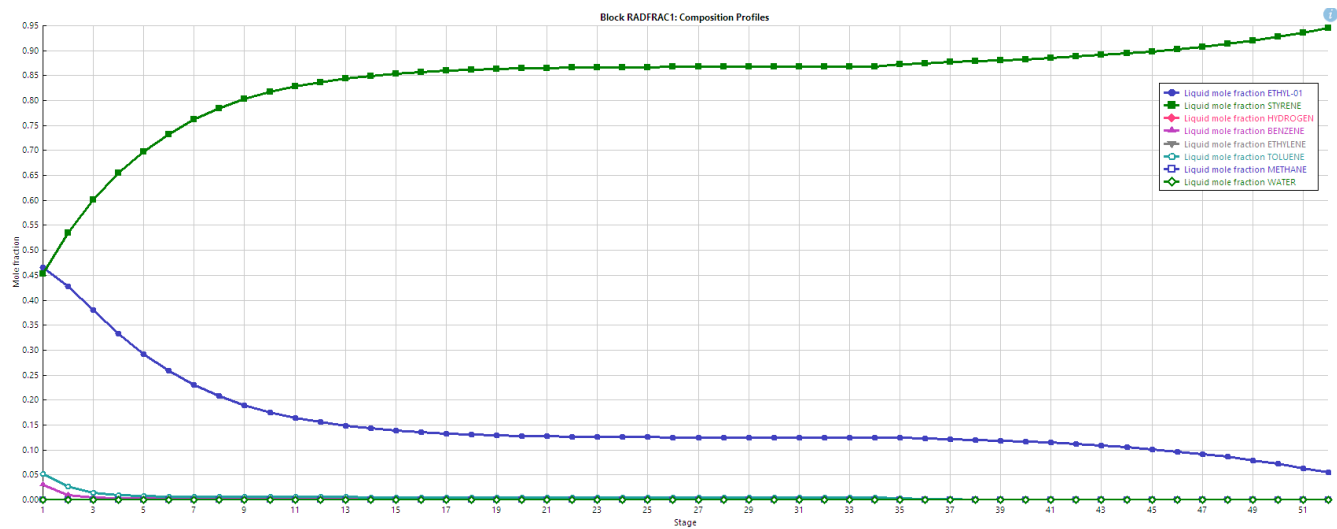
Temperature Profile



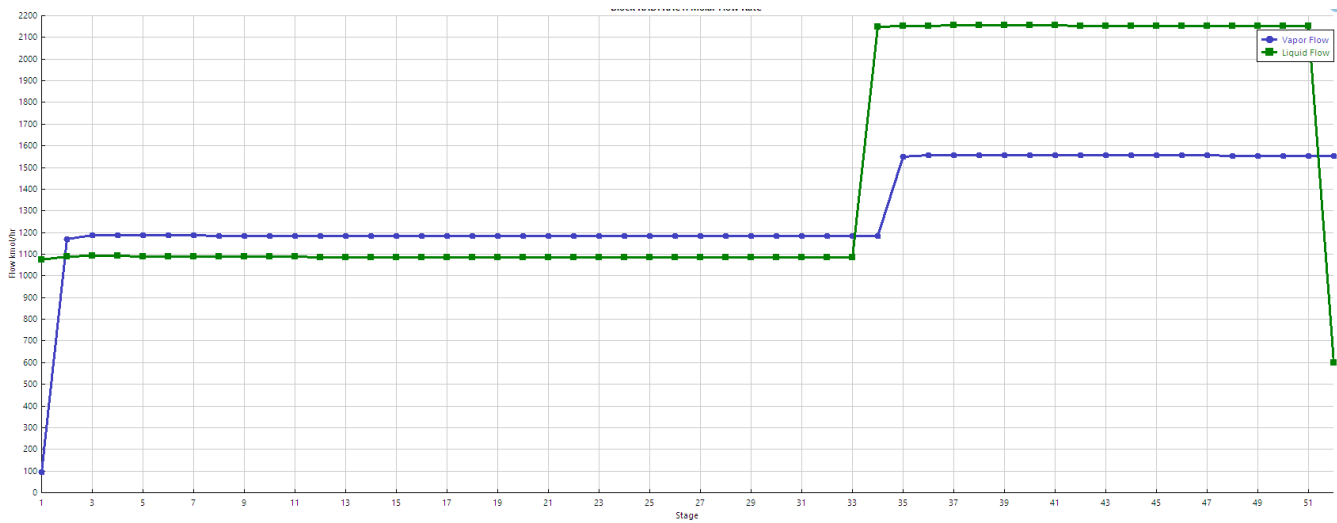
Vapour Composition



Liquid Composition



Flowrate Profile



DSTWU 2 Flow Rates

	Units	COL1-BOT ▾	COL2-BOT ▾	COL2-DIS ▾
Pressure	bar	1	1	1
Molar Vapor Fraction		0	0	0
Molar Liquid Fraction		1	1	1
Molar Solid Fraction		0	0	0
Mass Vapor Fraction		0	0	0
Mass Liquid Fraction		1	1	1
Mass Solid Fraction		0	0	0
Molar Enthalpy	cal/mol	29047.7	30405.4	7133.15
Mass Enthalpy	cal/gm	278.604	291.901	67.3948
Molar Entropy	cal/mol-K	-63.7505	-62.7651	-84.9606
Mass Entropy	cal/gm-K	-0.61145	-0.602566	-0.802717
Molar Density	mol/cc	0.00753334	0.00755341	0.00722865
Mass Density	gm/cc	0.785436	0.786787	0.76509
Enthalpy Flow	cal/sec	4.82966e+06	4.75984e+06	69339.2
Average MW		104.261	104.163	105.841
<b>— Mole Flows</b>	<b>kmol/hr</b>	<b>598.561</b>	<b>563.566</b>	<b>34.9945</b>
ETHYL-01	kmol/hr	32.5941	3.25941	29.3347
STYRENE	kmol/hr	565.966	560.307	5.65966
HYDROGEN	kmol/hr	1.02566e-78	0	0
BENZENE	kmol/hr	1.6856e-11	2.1994e-32	1.6856e-11
ETHYLENE	kmol/hr	5.56803e-48	0	0
TOLUENE	kmol/hr	0.000120765	7.58626e-15	0.000120765
METHANE	kmol/hr	1.09066e-57	0	0
WATER	kmol/hr	3.40491e-42	0	0

### RadFrac2 Setup

Configuration

Streams

Pressure

Condenser

Reboiler

3-Phase

Comments

Setup options

Calculation type

Equilibrium

Number of stages

46

Stage Wizard

Condenser

Partial-Vapor

Reboiler

Kettle

Valid phases

Vapor-Liquid

Convergence

Standard

Operating specifications

Distillate to feed ratio

Mole

0.0584644

Reflux ratio

Mole

90.7796

Free water reflux ratio

0

Feed Basis

Design and specify column internals

Configuration

Streams

Pressure

Condenser

Reboiler

3-Phase

Comments

Feed streams

	Name	Stage	Convention
▶	COL1-BOT	32	Above-Stage

Product streams

	Name	Stage	Phase	Basis	Flow	Units	Flow Ra
▶	COL2-DIS	1	Vapor	Mole		kmol/hr	
▶	COL2-BOT	46	Liquid	Mole		kmol/hr	

Pseudo streams

	Name	Pseudo Stream Type	Stage	Internal Phase	Reboiler Phase	Reboiler Conditions	Pumparound ID	P
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<input checked="" type="checkbox"/> Configuration	<input checked="" type="checkbox"/> Streams	<input checked="" type="checkbox"/> Pressure	<input checked="" type="checkbox"/> Condenser	<input checked="" type="checkbox"/> Reboiler	3-Phase	Comments
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View Top / Bottom

Top stage / Condenser pressure

Stage 1 / Condenser pressure  bar

Stage 2 pressure (optional)

☒ Stage 2 pressure  bar

☐ Condenser pressure drop  bar

Pressure drop for rest of column (optional)

☒ Stage pressure drop  bar

☐ Column pressure drop  bar

#### Condenser / Top stage performance

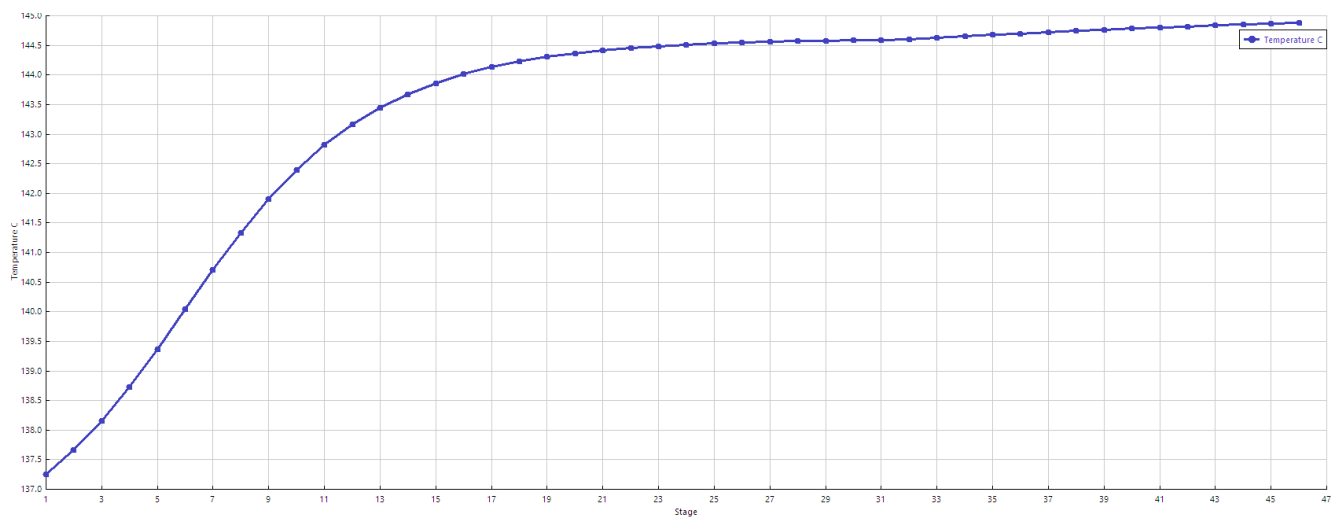
	Name	Value	Units
▶	Temperature	137.257	C
▶	Subcooled temperature		
▶	Heat duty	-31752.7	kW
▶	Subcooled duty		
▶	Distillate rate	34.9945	kmol/hr
▶	Reflux rate	3176.79	kmol/hr
▶	Reflux ratio	90.7796	
▶	Free water distillate rate		
▶	Free water reflux ratio		

#### Reboiler / Bottom stage performance

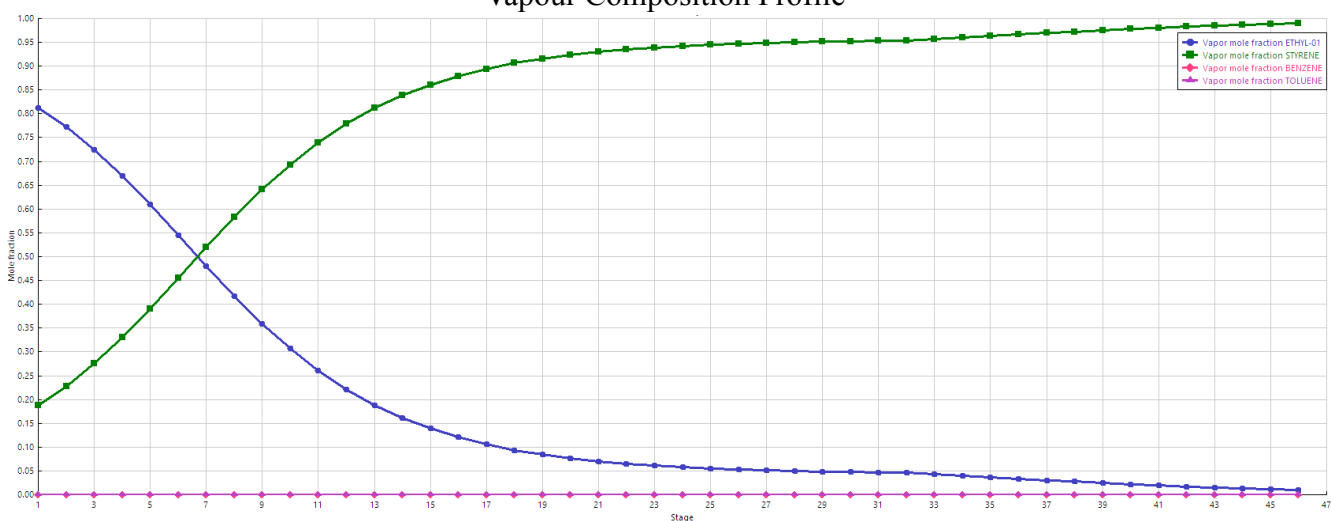
	Name	Value	Units
▶	Temperature	144.882	C
▶	Heat duty	32099.9	kW
▶	Bottoms rate	563.566	kmol/hr
▶	Boilup rate	3146.34	kmol/hr
▶	Boilup ratio	5.5829	
▶	Bottoms to feed ratio	0.941536	

	Units	COL1-BOT ▾	COL2-BOT ▾	COL2-DIS ▾
Pressure	bar	1	1	1
Molar Vapor Fraction		0	0	1
Molar Liquid Fraction		1	1	0
Molar Solid Fraction		0	0	0
Mass Vapor Fraction		0	0	1
Mass Liquid Fraction		1	1	0
Mass Solid Fraction		0	0	0
Molar Enthalpy	cal/mol	29047.7	30359.6	16452.1
Mass Enthalpy	cal/gm	278.604	291.452	155.52
Molar Entropy	cal/mol-K	-63.7505	-62.7938	-63.2354
Mass Entropy	cal/gm-K	-0.61145	-0.602821	-0.597756
Molar Density	mol/cc	0.00753334	0.00755273	2.93061e-05
Mass Density	gm/cc	0.785436	0.786741	0.00310023
Enthalpy Flow	cal/sec	4.82966e+06	4.75267e+06	159926
Average MW		104.261	104.166	105.788
<b>— Mole Flows</b>	<b>kmol/hr</b>	<b>598.561</b>	<b>563.566</b>	<b>34.9945</b>
ETHYL-01	kmol/hr	32.5941	4.18477	28.4093
STYRENE	kmol/hr	565.966	559.381	6.58503
HYDROGEN	kmol/hr	1.02566e-78	0	0
BENZENE	kmol/hr	1.6856e-11	5.1468e-23	1.6856e-11
ETHYLENE	kmol/hr	5.56803e-48	0	0
TOLUENE	kmol/hr	0.000120765	4.91371e-10	0.000120765
METHANE	kmol/hr	1.09066e-57	0	0
WATER	kmol/hr	3.40491e-42	0	0

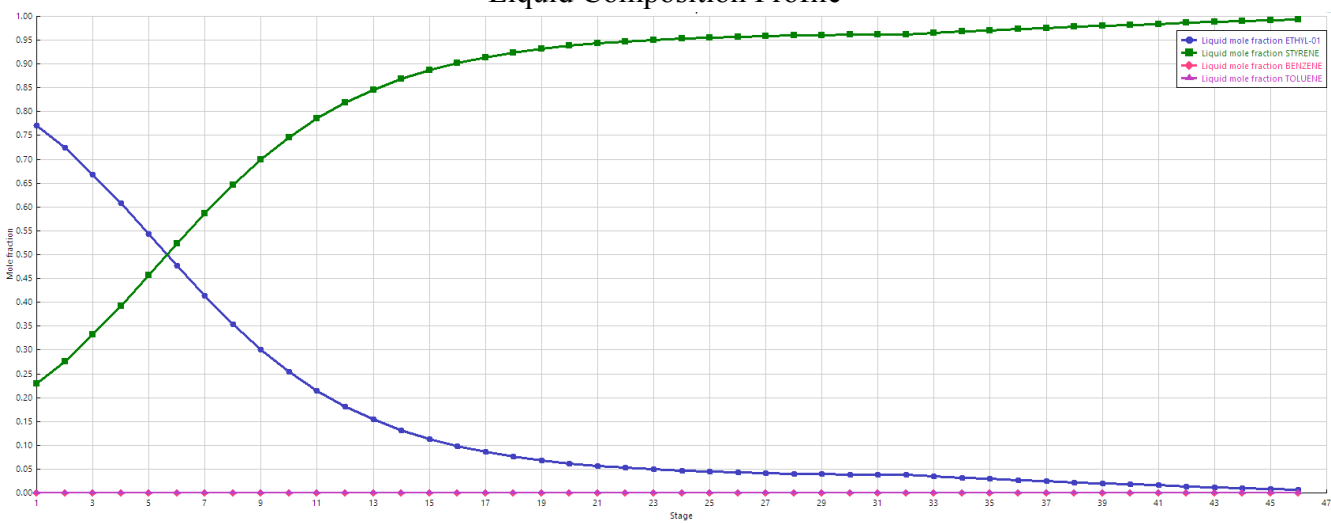
### Temperature Profile



Vapour Composition Profile



Liquid Composition Profile



Flowrate Profile



