P03 eLEAPS Problem Session Script

Problem Name: **P03 Distillation Column**
Problem Description: **Binary Vapor-Liquid Equilibrium using Raoult's Law**

Date: ________________ **Your Name:** ____

Problem Session Objectives

- To apply the five stages of the problem solving methodology.
- To apply material balances to solve a distillation column problem.

- To use the concept of vapor-liquid equilibrium (VLE) for a binary system.
- To characterize VLE using a temperature-composition (TXY) diagram.
- To characterize VLE using a pressure-composition (PXY) diagram.

Reference Readings

- Felder and Rousseau, 3rd Edition, Section 6.4, Multi-Component Gas-Liquid Systems. Specifically, the material on binary vapor-liquid equilibrium using Raoult's law.
- Felder and Rousseau, 3rd Edition, Section 6.1, Single-Component Phase Equilibrium. Specifically, the Antoine equation for vapor pressure and boiling temperature of a pure chemical compound.

- Distillation Column - "Visual Encyclopedia of Chemical Engineering Equipment"
  On the CD-ROM in the textbook by Felder and Rousseau

Review Materials

- Hanyak's "Rigorous Model for Multi-Component VLE," CinChE Manual, Chapter 6.
- Hanyak's "Raoult's Law Model for Multi-Component VLE," CinChE Manual, Chapter 6.
- Hanyak's "Pure-Component Phase Equilibrium," CinChE Manual, Chapter 6.

Interaction 1:

Topic: Distillation Column

Background: Welcome to the eLEAPS problem session about a distillation column. Save this script document to the desktop. Click here to open and save the solution template also to the desktop. Close all internet browser windows. Open the two saved documents with **Adobe Reader**.

In the solution template document, right click and select **Print**, choose "**Document and Markups**" under **Comments and Forms**, and print it to get a PAPER COPY. Print to a color printer for the best effect. You will fill-in this paper copy as you do the problem session. Close the template document and then delete it, since it is no longer needed.

P03 eLEAPS Problem Solution Template

Coaching Script and Solution Template

This coaching script contains two kinds of pages—script and template. They are arranged similar to the left and right pages in a book. The left page is an interaction in the coaching script. The right page is the current focus in the solution template that is associated with the left coaching script page.

How you navigate through the coaching script depends up the type of computer that you are using—a personal computer with a mouse or an Apple iPad with a stylus pen. In either case, you have opened this coaching script using the Acrobat Reader program that is installed on your computer and not the Acrobat Reader plug-in found in a web browser.

Please complete the first interaction in the first coaching script page. Then, proceed to navigate through the coaching script based upon your computer type, as describe below.

Personal Computer with a Mouse

The Acrobat Reader program should have displayed this coaching script in its two-page view mode. If not, then select the **View/Page Display/Two Page Scrolling** option from the menu bar.

In the two-page view mode, the left column of pages will be the coaching script, while the right column of pages will be the current focus in the solution template. You can magnify the view (i.e., zoom in) so that the coaching script page is readable. Then, you can use the horizontal scroll bar to move between the left page (the coaching script) and its right page (the template solution).

After you manually complete a portion of your PAPER COPY of the problem solution template (as directed by its associated coaching script interaction), you can then delete the boxes in the right page to view the correct answers. You can also view the popup notes found in the right page.

You proceed to the next script **Interaction** by scrolling down to the next set of two pages in the Acrobat Reader program.

Apple iPad with a Rubber-Domed Stylus Pen

The Acrobat Reader app for the iPad (downloaded from the App Store) does not support the two-page view mode. To simulate this viewing mode, select the **Single Page** option under **Document Modes** in the menu bar.

In the **Single Page** mode, you will be able to horizontally swipe between the left page (the coaching script) and its right page (the template solution).

After you manually complete a portion of your PAPER COPY of the problem solution template (as directed by its associated coaching script interaction), you can then delete the boxes in the right page to view the correct answers. You can also view the popup notes found in the right page.

You proceed to the next script **Interaction** by swiping pass the current right page in the Acrobat Reader app.

If you quickly tap the **Home** button on the iPad twice, you can conveniently switch between the Adobe Reader and any other apps.

P03 eLEAPS Problem Session Script

Interaction 2:	
Topic:	Distillation Column
Background:	A distillation column problem is used to illustrate the application of vapor-liquid equilibrium for a benzene-styrene system. The first step in the problem-solving methodology (PSM) is to analyze the problem statement and create a conceptual model composed of a labeled Diagram, Other Givens, Finds, and initial Assumptions. Please examine the **Conceptual Model** on Page 1 in your PAPER COPY of the template document. As indicated by the yellow highlights to the right of this script page, you are to complete labeling the process state of Streams F, D, V, and B.
VLE Binary System Question:	The definition of vapor-liquid equilibrium (or any phase equilibrium) is based on a closed system. Click here to see the definition of multi-component phase equilibrium. Since the reboiler in the conceptual model is a continuous system, are its exiting vapor and liquid streams (V and B) actually in equilibrium?
Option 1:	○ yes.
Option 2:	○ maybe.
Option 3:	○ no.
Feedback 1:	Select the text of only ONE option and then highlight it. After selecting your option, click this yellow rectangle and then delete it to see the feedback for each option.
Feedback 2:	
Feedback 3:	

Before continuing, close ALL browser and other windows that you opened during this interaction.

Problem Statement

{ Problem 6.46 in Felder & Rousseau, 2nd Edition }

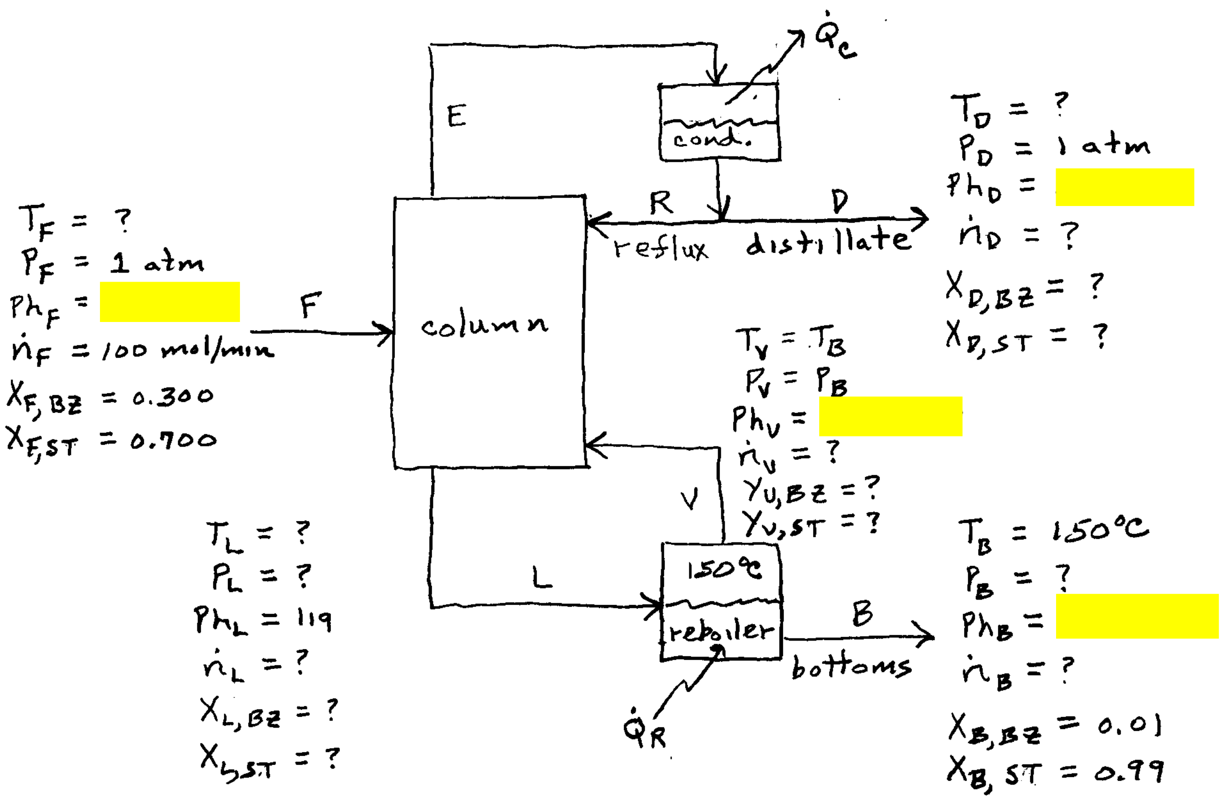
Similar to Problem 6.60 in F&R, 3rd Ed.

A saturated-liquid feed mixture containing 30.0 mole% benzene and 70.0 mole% styrene is to be separated in a distillation column. The column produces an overhead product (a saturated-liquid distillate) and a bottoms product. The bottoms product is 99 mole% styrene and contains 2.0% of the benzene fed to the column.

The liquid stream leaving the bottom of the column (not the bottoms product) goes to a partial reboiler, in which a portion of it is vaporized at 150°C and returned to the bottom of the column. The residual liquid from the reboiler is the bottoms product. The vapor and liquid streams exiting the rebolier are in equilibrium. The boilup ratio, or mole ratio of the vapor and liquid streams leaving the reboiler, is 2.5:1.

Calculate the compositions (component mole fractions) of the distillate product, the vapor returned to the column from the reboiler, and the liquid feed to the reboiler, and estimate the required operating pressure of the reboiler. Also, estimate the temperatures of the feed and distillate streams at a pressure of 1 atm.

Conceptual Model



Other Givens:

$\dot{n}_V / \dot{n}_B = 2.5$ boilup ratio

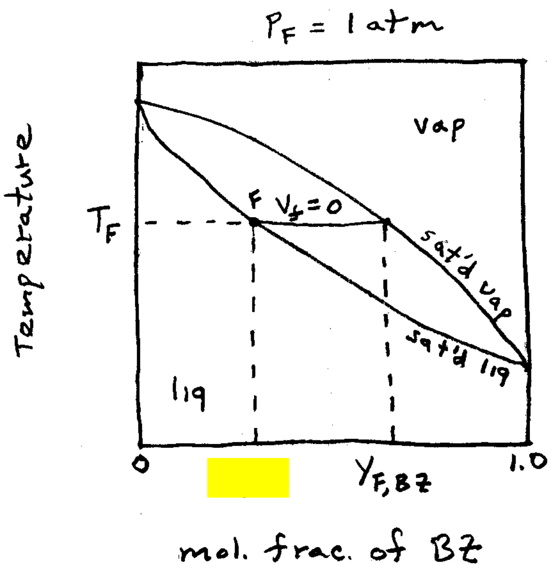
$0.01 \dot{n}_B = 0.02(0.30 \dot{n}_F)$

Finds:

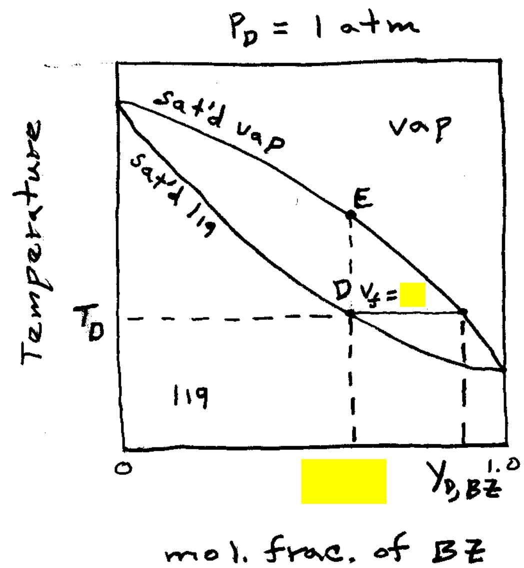
$x_{D,BZ}$ and $x_{D,ST}$	P_B in atm
$y_{V,BZ}$ and $y_{V,ST}$	T_F in °C
$x_{L,BZ}$ and $x_{L,ST}$	T_D in °C

Interaction 3:	
Topic:	Distillation Column
Background:	The vapor-liquid equilibrium (VLE) conditions of the feed and distillate streams can be represented on a Temperature-Composition (TXY) diagram, while the VLE condition of the bottoms stream can be represented on a Pressure-Composition (PXY) diagram. Click here to examine a general explanation of the Raoult's Law Model for multi-component vapor-liquid equilibrium. Please examine the **TXY** and **PXY diagrams** on Page 2 in your PAPER COPY of the template document. As indicated by the yellow highlights to the right of this script page, you are to complete the composition variables on the x-axis of the two TXY diagrams and the PXY diagram. Also, label the vapor fraction on the distillate TXY diagram.
VLE Binary System Question:	The condenser at the top of the column labeled as "cond." on Page 1 in your PAPER COPY of the template document operates how?
Option 1:	○ as a partial condenser.
Option 2:	○ as a total condenser.
Option 3:	○ as a sub-cooled condenser.
Feedback 1:	Select the text of only ONE option and then highlight it. After selecting your option, click this yellow rectangle and then delete it to see the feedback for each option.
Feedback 2:	
Feedback 3:	

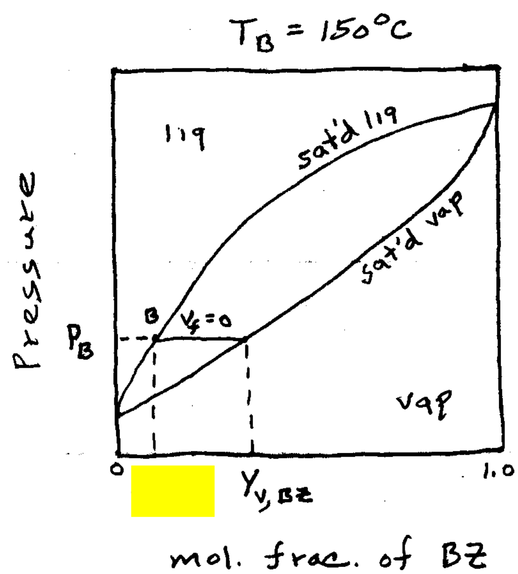
Feed Condition



Distillate Condition



Bottoms Condition



Assumptions

1. continuous process
2. steady state
3. no reaction
4. Raoult's Law for Vap-Liq Equilibrium

P03 eLEAPS Problem Session Script

Interaction 4:

Topic:	Distillation Column
Background:	The second step in the problem-solving methodology (PSM) is to review the conceptual model and create a mathematical model composed of first principle equations, additional equations, and a degrees-of-freedom analysis. Please examine **Mathematical Model A** for the entire distillation column on Page 3 in your PAPER COPY of the template document. As indicated by the yellow highlights to the right of this script page, you are to complete writing the first seven equations (Eqs. ① to ⑥ and the "check" equation) in the overall math model, and you are to complete the degrees of freedom for these equations.
Mathematical Model Question:	To solve this problem, imaginary system boundaries in the Conceptual Model on Page 1 can be drawn around the condenser, the column, the reboiler, and overall (i.e., all three process units). Which ONES of the following reasons explain why the overall balances are written FIRST?
Option 1:	☐ Because not enough information is directly given about Streams E, R, and D.
Option 2:	☐ Because not enough information is directly given about Streams L, V, and B.
Option 3:	☐ Because enough information is directly given about Streams F, D, and B.
Feedback 1:	Select the text of your first option and then highlight it. If necessary, select the text of additional options and highlight them. After selecting your option(s), click this yellow rectangle and then delete it to see the feedback for each option.
Feedback 2:	
Feedback 3:	

Mathematical Model A, Overall Balance

① Total: $\dot{n}_F - \dot{n}_D - \dot{n}_B = 0$

② benzene: $0.3\,\dot{n}_F - \dot{n}_{D,BZ} - \quad = 0$

③ styrene: $0.7\,\dot{n}_F - \dot{n}_{D,ST} - \quad = 0$

vars = 5
eqns = 3
dof =

(check) Mix D: $\dot{n}_D = \dot{n}_{D,BZ} + \dot{n}_{D,ST}$

④ $0.01\,\dot{n}_B = 0.02\,(0.3\,\dot{n}_F)$

⑤ Comp. D: $\dot{n}_{D,BZ} = \dot{n}_D\,X_{D,BZ}$

⑥ $\dot{n}_{D,ST} = \dot{n}_D\,X_{D,ST}$

vars =
eqns =
dof =

Interaction 5:	
Topic:	Distillation Column
Background:	The mole fractions for Stream D are calculated using Equations ① to ⑥ in the over material balances on Page 3 in your PAPER COPY of the template document. As indicated by the yellow highlight in Equations ⑦ and ⑧ to the right of this script page, complete the two functional forms to find the temperatures of Streams F and D. Click here to examine a general explanation of the Raoult's Law Model for multi-component vapor-liquid equilibrium.
VLE Binary System Question:	For the feed and distillate streams, what are their vapor fractions?
Option 1:	○ 1.0
Option 2:	○ 0.3
Option 3:	○ 0.0
Feedback 1:	Select the text of only ONE option and then highlight it. After selecting your option, click this yellow rectangle and then delete it to see the feedback for each option.
Feedback 2:	
Feedback 3:	

Mathematical Model A, Overall Balance

① Total: $\dot{n}_F - \dot{n}_D - \dot{n}_B = 0$

② benzene: $0.3\,\dot{n}_F - \dot{n}_{D,BZ} - 0.01\,\dot{n}_B = 0$

③ styrene: $0.7\,\dot{n}_F - \dot{n}_{D,ST} - 0.99\,\dot{n}_B = 0$

# vars = 5
# eqns = 3
dof = 2

(check) Mix D: $\dot{n}_D = \dot{n}_{D,BZ} + \dot{n}_{D,ST}$

④ $0.01\,\dot{n}_B = 0.02\,(0.3\,\dot{n}_F)$

⑤ Comp. D: $\dot{n}_{D,BZ} = \dot{n}_D\, X_{D,BZ}$

⑥ $\dot{n}_{D,ST} = \dot{n}_D\, X_{D,ST}$

# vars = 7
# eqns = 6
dof = 1

⑦ vle of F: $[T_F] = vlet[P_F, \;]$

⑧ vle of D: $[T_D] = vlet[P_D, \;]$

# vars = 13
# eqns = 8
dof = 5

Interaction 6:	
Topic:	Distillation Column
Background:	Once the overall math model is solved for the molar flow rate for Stream B, the reboiler balance can be used to calculate the remaining "Find" quantities listed in the conceptual model. Please examine **Mathematical Model B** for the reboiler on Page 3 in your PAPER COPY of the template document. As indicated by the yellow highlights to the right of this script page, you are to complete writing the functional form of "**vlep**" for the vapor-liquid equilibrium between Streams V and B. Click here to examine a general explanation of the Raoult's Law Model for multi-component vapor-liquid equilibrium s.
Mathematical Model Question:	In the reboiler math model, the "Mix V" equation is marked as NOT being linear independent. Is it really a dependent equation, and therefore not part of the math model?
Option 1:	○ yes.
Option 2:	○ no.
Feedback 1:	Select the text of only ONE option and then highlight it. After selecting your option, click this yellow rectangle and then delete it to see the feedback for each option.
Feedback 2:	

Mathematical Model A, Overall Balance

① Total: $\dot{n}_F - \dot{n}_D - \dot{n}_B = 0$

② benzene: $0.3\,\dot{n}_F - \dot{n}_{D,BZ} - 0.01\,\dot{n}_B = 0$

③ styrene: $0.7\,\dot{n}_F - \dot{n}_{D,ST} - 0.99\,\dot{n}_B = 0$

# vars = 5
# eqns = 3
dof = 2

(check) Mix D: $\dot{n}_D = \dot{n}_{D,BZ} + \dot{n}_{D,ST}$

④ $0.01\,\dot{n}_B = 0.02\,(0.3\,\dot{n}_F)$

⑤ Comp. D: $\dot{n}_{D,BZ} = \dot{n}_D\, X_{D,BZ}$

⑥ $\dot{n}_{D,ST} = \dot{n}_D\, X_{D,ST}$

# vars = 7
# eqns = 6
dof = 1

⑦ vle of F: $[T_F] = \text{vlet}[P_F,\ V_f = 0,\ \bar{X}_F]$

⑧ vle of D: $[T_D] = \text{vlet}[P_D,\ V_f = 0,\ \bar{X}_D]$

# vars = 13
# eqns = 8
dof = 5

Given: $\dot{n}_F,\ P_F,\ P_D,\ \bar{X}_F$

Mathematical Model B, Reboiler Balance

① Total: $\dot{n}_L - \dot{n}_V - \dot{n}_B = 0$

② benzene: $\dot{n}_{L,BZ} - \dot{n}_{V,BZ} - 0.01\,\dot{n}_B = 0$

③ styrene: $\dot{n}_{L,ST} - \dot{n}_{V,ST} - 0.99\,\dot{n}_B = 0$

# vars = 7
# eqns = 3
dof = 4

(dep) Mix V: $\dot{n}_V = \dot{n}_{V,BZ} + \dot{n}_{V,ST}$

(check) Mix L: $\dot{n}_L = \dot{n}_{L,BZ} + \dot{n}_{L,ST}$

④ Boilup: $\dot{n}_V = 2.5\,\dot{n}_B$

⑤-⑦ vle V & B: $[P_B,\ \bar{Y}_V] = \text{vlep}[\quad]$

⑧ Comp. V: $\dot{n}_{V,BZ} = \dot{n}_V\, Y_{V,BZ}$

⑨ $\dot{n}_{V,ST} = \dot{n}_V\, Y_{V,ST}$

⑩ Comp. L: $\dot{n}_{L,BZ} = \dot{n}_L\, X_{L,BZ}$

⑪ $\dot{n}_{L,ST} = \dot{n}_L\, X_{L,ST}$

# vars = 15
# eqns = 11
dof = 4

Given: $T_B,\ \dot{n}_B,\ \bar{X}_B$

Interaction 7:

Topic: Distillation Column

Background: The third step in the problem-solving methodology (PSM) is to transform the mathematical model into a mathematical algorithm. A mathematical algorithm does not tell you how to solve, but it identifies the order in which the equations are to be solved.

Please examine the two mathematical algorithms for the overall distillation process and the reboiler on Page 4 in your PAPER COPY of the template document and also as Page 4 to the right of this script page. Remember that each variable that appears in the right-hand side of an assignment MUST be defined previously; that is, either it is known or it will have been calculated.

VLE Binary System Question:	Any functional form, like "**vlet**" in **Mathematical Algorithm A**, can be represented one of four ways—graph, table, set of equations, or computer program. Which type of functional "**vlet**" form should be used to solve quickly and accurately for the bubble-point temperatures of the feed and distillate streams?
Option 1:	○ read the temperature from a TXY graph.
Option 2:	○ interpolate the temperature in a table.
Option 3:	○ solve manually a set of equations for the temperature.
Option 4:	○ solve a set of equations for the temperature using a computer program.
Feedback 1:	Select the text of only ONE option and then highlight it. After selecting your option, click this yellow rectangle and then delete it to see the feedback for each option.
Feedback 2:	
Feedback 3:	
Feedback 4:	

Mathematical Algorithm A

$[\bar{X}_D, T_F, T_D, \dot{n}_B] = \text{overall}[\dot{n}_F, P_F, P_D, \bar{X}_F]$

④	1.	$\dot{n}_B \leftarrow 0.02(0.3\dot{n}_F)/0.01$
①	2.	$\dot{n}_D \leftarrow \dot{n}_F - \dot{n}_B$
②	3.	$\dot{n}_{D,BZ} \leftarrow 0.3\dot{n}_F - 0.01\dot{n}_B$
③	4.	$\dot{n}_{D,ST} \leftarrow 0.7\dot{n}_F - 0.99\dot{n}_B$
⑤	5.	$X_{D,BZ} \leftarrow \dot{n}_{D,BZ}/\dot{n}_D$
⑥	6.	$X_{D,ST} \leftarrow \dot{n}_{D,ST}/\dot{n}_D$
⑦	7.	$T_F \leftarrow \text{vlet}[P_F, V_f=0, \bar{X}_F]$
⑧	8.	$T_D \leftarrow \text{vlet}[P_D, V_f=0, \bar{X}_D]$

Mathematical Algorithm B

$[P_B, \bar{Y}_V, \bar{X}_L] = \text{reboiler}[T_B, \dot{n}_B, \bar{X}_B]$

④	1.	$\dot{n}_V \leftarrow 2.5\dot{n}_B$
①	2.	$\dot{n}_L \leftarrow \dot{n}_V + \dot{n}_B$
⑤-⑦	3.	$[P_B, \bar{Y}_V] \leftarrow \text{vlep}[T_B, V_f=0, \bar{X}_B]$
⑧	4.	$\dot{n}_{V,BZ} \leftarrow \dot{n}_V Y_{V,BZ}$
⑨	5.	$\dot{n}_{V,ST} \leftarrow \dot{n}_V Y_{V,ST}$
②	6.	$\dot{n}_{L,BZ} \leftarrow \dot{n}_{V,BZ} + 0.01\dot{n}_B$
③	7.	$\dot{n}_{L,ST} \leftarrow n_{V,ST} + 0.99\dot{n}_B$
⑩	8.	$X_{L,BZ} \leftarrow \dot{n}_{L,BZ}/\dot{n}_L$
⑪	9.	$X_{L,ST} \leftarrow \dot{n}_{L,ST}/\dot{n}_L$

Interaction 8:

Topic: Distillation Column

Background: The fourth step in the problem-solving methodology (PSM) is to generate the numerical solution using the mathematical algorithm as a blueprint or guide.

Please examine **Numerical Solution A** for the overall material balance on Page 5 in your PAPER COPY of the template document. As indicated by the yellow highlights to the right of this script page, you are to determine the bubble-point temperatures of the feed and distillate streams at 1 atm. Do not forget to account for precision when writing the final temperature values.

Click here to examine a general explanation of the Raoult's Law Model for multi-component vapor-liquid equilibrium.

It may be of help to complete your task of determining the two bubble-point temperatures. Two ways exist to complete your task: 1) you could find the bubble-point temperatures using the two TXY graphs on Pages 6 and 7 in your PAPER COPY of the template document, or 2) you could use the "EZ Setup" numerical solutions to the VLE models on Pages 6 and 7. If you would like to run the "EZ Setup" file for these VLE models, click here to save the "bzsmTXY.xls" file to your computer desktop and then open this Excel file that uses the "EZ Setup" and Solver utilities.

Numerical Solution A

Basis: cgs system, $\dot{n}_F = 100$ mol/min

Givens: $T_B = 150°C$

1. $\dot{n}_B = 0.02(0.3)(100 \frac{mol}{min})/(0.1) = \boxed{60 \text{ mol/min}}$
2. $\dot{n}_D = (100 - 60)$ mol/min $= 40$ mol/min

3. $\dot{n}_{D,BZ} = 0.3(100 \frac{mol}{min}) - 0.01(60 \frac{mol}{min}) = 29.4$ mol/min
4. $\dot{n}_{D,ST} = [0.7(100) - 0.99(60)]$ gmol/min $= 10.6$ mol/min
5. $X_{D,BZ} = 29.4 \frac{mol}{min} / 40 \frac{mol}{min} = \boxed{0.74}$
6. $X_{D,ST} = 10.6 \frac{mol}{min} / 40 \frac{mol}{min} = \boxed{0.26}$

7. $T_F = \text{vlet}[1\text{atm}, V_f = 0, \bar{X}_F] = \boxed{\quad °C}$ see Page 6
8. $T_D = \text{vlet}[1\text{atm}, V_f = 0, \bar{X}_D] = \boxed{\quad °C}$ see Page 7

Page 6 referenced in Interaction 8 =====➔

<u>Vapor-Liquid Equilibrium Model</u> for the Feed Stream:

// Total and Two Component Material Balances   EZ Setup File   HYSYS File   Excel File

1.0 = Vf + Lf

zBZ = Vf * yBZ + Lf * xBZ
zST = Vf * yST + Lf * xST

// Vapor-Liquid Equilibrium using Raoult's Law
yBZ = kBZ * xBZ
yST = kST * xST

kBZ = PsatBZ / P
kST = PsatST / P

// Antoine Equations for the Two Components, Table B.4, F&R, 3rd Ed.
ln(PsatBZ) / 2.303 = 6.89272 - 1203.531 / (T + 219.888)   // 14.5 to 80.9 C
ln(PsatST) / 2.303 = 7.06623 - 1507.434 / (T + 214.985)   // 29.9 to 144.8 C

// Two mixture equations for the liquid and vapor phases
xBZ + xST - yBZ - yST = 0

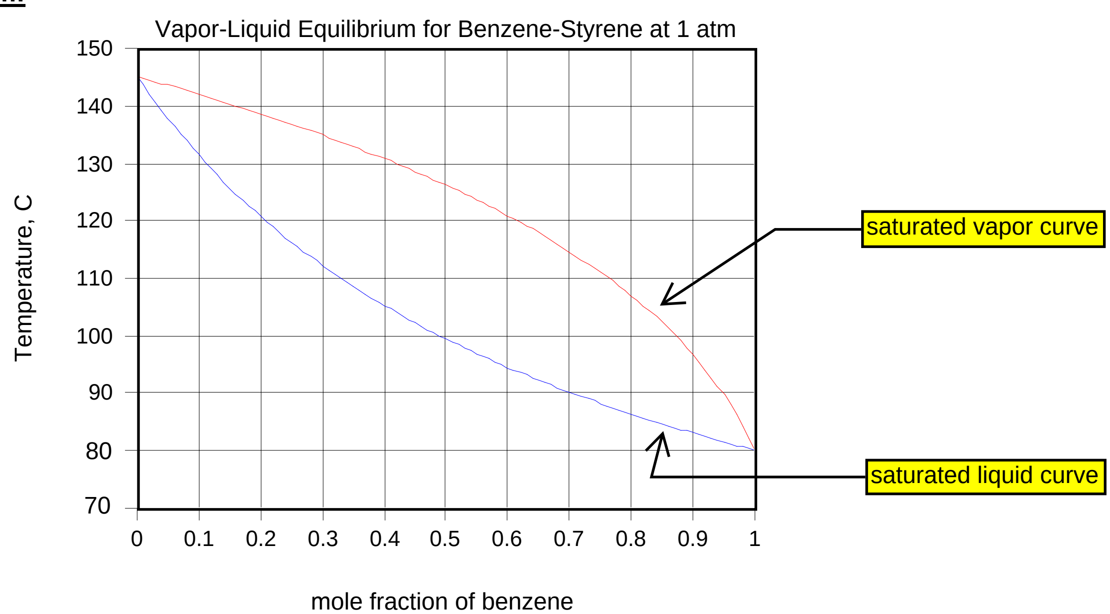
// Given Information
Vf = 0.0
P = 760 // mmHG or 1 atm
zBZ = 0.30
zST = 1.0 - zBZ

<u>Numerical Solution</u> as given by EZ Setup:

T	kBZ	kST	xBZ	xST	yBZ	yST	zST
112.241	2.44796	0.379444	0.3	0.7	0.734389	0.265611	0.7

P	Vf	zBZ
760	0	0.3

<u>TXY Diagram:</u>



Page 7 referenced in Interaction 8 =====➔

Vapor-Liquid Equilibrium Model for the Distillate Stream:

EZ Setup File HYSYS File Excel File

// Total and Two Component Material Balances
1.0 = Vf + Lf

zBZ = Vf * yBZ + Lf * xBZ
zST = Vf * yST + Lf * xST

// Vapor-Liquid Equilibrium using Raoult's Law
yBZ = kBZ * xBZ
yST = kST * xST

kBZ = PsatBZ / P
kST = PsatST / P

// Antoine Equations for the Two Components, Table B.4, F&R, 3rd Ed.
ln(PsatBZ) / 2.303 = 6.89272 - 1203.531 / (T + 219.888) // 14.5 to 80.9 C
ln(PsatST) / 2.303 = 7.06623 - 1507.434 / (T + 214.985) // 29.9 to 144.8 C

// Two mixture equations for the liquid and vapor phases
xBZ + xST - yBZ - yST = 0

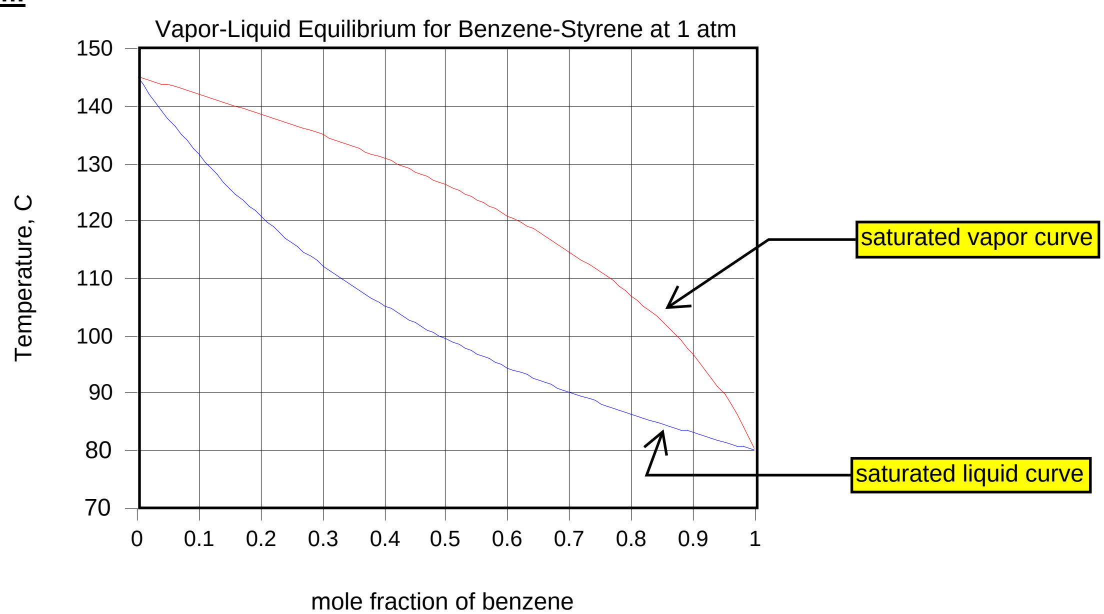
// Given Information
Vf = 0.0
P = 760 // mmHG or 1 atm
zBZ = 0.735
zST = 1.0 - zBZ

Numerical Solution as given by EZ Setup:

T	kBZ	kST	xBZ	xST	yBZ	yST	zST
88.8318	1.30014	0.167549	0.735	0.265	0.9556	0.0444004	0.265

P	Vf	zBZ
760	0	0.735

TXY Diagram:



Interaction 9:

Topic:	Distillation Column
Background:	Please examine **Numerical Solution B** for the reboiler on Page 5 in your PAPER COPY of the template document. As indicated by the yellow highlight to the right of this script page, you are to determine the bubble-point pressure of Stream B and the composition of Stream V. Do not forget to account for precision when writing the final pressure and composition values. Click here to examine a general explanation of the Raoult's Law Model for multi-component vapor-liquid equilibrium. It may be of help to complete your task of determining the bubble-point pressure and composition. Two ways exist to complete your task: 1) you could find the bubble-point pressure using the PXY graph on Page 8 in your PAPER COPY of template document, or 2) you could use the "EZ Setup" numerical solution to the VLE model on Page 8. If you would like to run the "EZ Setup" file for this VLE model, click here to save the "bzsmTXY.xls" file to your computer desktop and then open this Excel file that uses the "EZ Setup" and Solver utilities.
VLE Binary System Question:	What causes the blue curve for the saturated liquid in the PXY diagram on Page 8 in your PAPER COPY of the template document to be shaped as it is shown? Note that the third page in the Raoult's Law document might provide some insight for you.
Option 1:	○ Because the total pressure is only a non-linear function of the benzene mole fraction when using Raoult's Law.
Option 2:	○ Because the total pressure is only a linear function of the benzene mole fraction when using Raoult's Law.
Feedback 1: **Feedback 2:**	Select the text of only ONE option and then highlight it. After selecting your option, click this yellow rectangle and then delete it to see the feedback for each option.

Before continuing, close ALL browser and other windows that you opened thus far in the session.

Numerical Solution A

Basis: cgs system, $\dot{n}_F = 100$ mol/min

Givens: $T_B = 150°C$

1. $\dot{n}_B = 0.02(0.3)(100 \frac{mol}{min})/(0.1) = $ **60 mol/min**
2. $\dot{n}_D = (100 - 60)$ mol/min $= 40$ mol/min
3. $\dot{n}_{D,BZ} = 0.3(100 \frac{mol}{min}) - 0.01(60 \frac{mol}{min}) = 29.4$ mol/min
4. $\dot{n}_{D,ST} = [0.7(100) - 0.99(60)]$ gmol/min $= 10.6$ mol/min
5. $X_{D,BZ} = 29.4 \frac{mol}{min} / 40 \frac{mol}{min} = $ **0.74**
6. $X_{D,ST} = 10.6 \frac{mol}{min} / 40 \frac{mol}{min} = $ **0.26**
7. $T_F = \text{vlet}[1\text{atm}, V_f = 0, \bar{X}_F] = $ **110 °C** see Page 6
8. $T_D = \text{vlet}[1\text{atm}, V_f = 0, \bar{X}_D] = $ **89 °C** see Page 7

Numerical Solution B

1. $\dot{n}_V = 2.5(60$ mol/min$) = 150$ mol/min
2. $\dot{n}_L = (150 + 60)$ mol/min $= 210$ mol/min
3. $[P_B, \bar{Y}_V] = \text{vlep}[150°C, V_f = 0, \bar{X}_B]$ see Page 8

   $P_B = 899.207$ mmHg $=$

   $Y_{V,BZ} =$ $\qquad$ $Y_{V,ST} =$ $\quad$ $=$

4. $\dot{n}_{V,BZ} = 0.0485(150 \frac{mol}{min}) = 7.275$ mol/min
5. $\dot{n}_{V,ST} = 0.9515(150 \frac{mol}{min}) = 142.725$ mol/min
6. $\dot{n}_{L,BZ} = 7.275 \frac{mol}{min} + 0.01(60 \frac{mol}{min}) = 7.875$ mol/min
7. $\dot{n}_{L,ST} = 142.725 \frac{mol}{min} + 0.99(60 \frac{mol}{min}) = 202.125$ mol/min
8. $X_{L,BZ} = 7.875 \frac{mol}{min} / 210 \frac{mol}{min} = 0.0375 = $ **0.04**
9. $X_{L,ST} = 202.125 \frac{mol}{min} / 210 \frac{mol}{min} = 0.9625 = $ **0.96**

Page 8 referenced in Interaction 9 =====➔

Vapor-Liquid Equilibrium Model for the Bottoms Stream:

// Total and Two Component Material Balances   EZ Setup File   HYSYS File   Excel File

1.0 = Vf + Lf

zBZ = Vf * yBZ + Lf * xBZ
zST = Vf * yST + Lf * xST

// Vapor-Liquid Equilibrium using Raoult's Law
yBZ = kBZ * xBZ
yST = kST * xST

kBZ = PsatBZ / P
kST = PsatST / P

// Antoine Equations for the Two Components, Table B.4, F&R, 3rd Ed.
ln(PsatBZ) / 2.303 = 6.89272 - 1203.531 / (T + 219.888)   // 14.5 to 80.9 C
ln(PsatST) / 2.303 = 7.06623 - 1507.434 / (T + 214.985)   // 29.9 to 144.8 C

// Two mixture equations for the liquid and vapor phases
xBZ + xST - yBZ - yST = 0

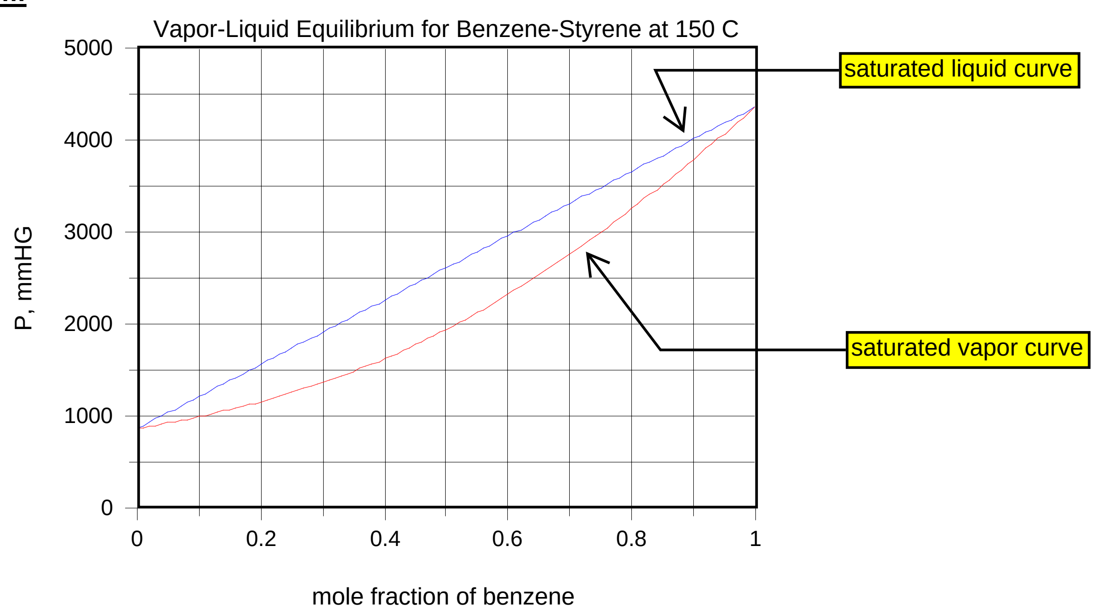
// Given Information
Vf = 0.0
T = 150 // C
zBZ = 0.01
zST = 1.0 - zBZ

Numerical Solution as given by EZ Setup:

P	PsatBZ	PsatST	kBZ	kST	xBZ	xST	yBZ
899.207	4361.18	864.238	4.85003	0.961111	0.01	0.99	0.0485003

yST	zST	T	Vf	zBZ
0.9515	0.99	150	0	0.01

PXY Diagram:



Interaction 10:	
Topic:	Distillation Column
Background:	The fifth and final step in the problem-solving methodology (PSM) is to generate the Heuristic Observations about the numerical solution, the mathematical algorithm, the mathematical model, and the conceptual model. Please examine the **Heuristic Observations** on Pages 9 and 10 in your PAPER COPY of template document. As indicated by the yellow highlight on Page 10, which is beyond Page 9 to the right of this script page, you are to complete writing the bubble-point temperatures of the feed and distillate streams at 1 atm and the bubble-point pressure of the bottoms stream at 150ºC.
Conceptual Model Question:	In the conceptual model, an overall system boundary around the distillation process (see Page 1) was used FIRST to solve the material balances, because a flow rate was known for Stream F. Could a system boundary around just the column (crossing Stream F, E, R, L, and V) be used FIRST to solve the material balances?
Option 1:	○ yes.
Option 2:	○ no.
Feedback 1:	Select the text of only ONE option and then highlight it. After selecting your option, click this yellow rectangle and then delete it to see the feedback for each option.
Feedback 2:	

Heuristic Observation

1. Numerical Solution

Model A: $\sum_{j=1}^{2} X_{D,j} = 0.735 + 0.265 \overset{ok!}{=} 1.00$

Model B: $\sum_{j=1}^{2} X_{V,j} = 0.0485 + 0.9515 \overset{ok!}{=} 1.000$

$\sum_{j=1}^{2} X_{L,j} = 0.0375 + 0.9625 \overset{ok!}{=} 1.000$

Check T_F :
Check T_D

For pure BZ, $T_{NBP} = 80.09\,°C$ } HYSYS 2004
For pure ST, $T_{NBP} = 145.20\,°C$

$T_F = 112\,°C$ and $T_D = 88.8\,°C$ must be between the normal boiling points of the pure components, for a binary VLE system that is assumed to follow Raoult's Law at 1 atm.

Check P_B:

BZ at 150°C, boils at 5.71 atm } HYSYS 2004
ST at 150°C, boils at 1.13 atm

$P_B = 1.18$ atm must be between these two boiling pressure for the pure components. Also, the VLE system must follow Raoult's Law at 150°C.

2. Math Algorithm

What if P_B were given and not T_B?

Then Step 3 in Math. Algorithm B would be replaced with

$$[T_B, \bar{Y}_V] \leftarrow \text{vlet}[P_B, V_f = 0, \bar{X}_B]$$

Page 10 referenced in Interaction 10 =====➔

3. Math Model

What if the Raoult's Law assumption did not apply?

Then, the following two functional forms would be modelled differently:

$$[T] = \text{vlet}\,[P, V_f, \bar{z}]$$

$$[P, \bar{y}] = \text{vlep}\,[T, V_f, \bar{z}]$$

For the PRSV equation of state in HYSYS, you get the following values:

	PRSV	Raoult's Law
T_F =	113.00 °C	°C
T_D =	89.33 °C	°C
P_B =	1.162 atm	atm

Thus, Raoult's is a good assumption, because the benzene-styrene system behaves like an ideal solution.

4. Conceptual Model

What if the boil-up ratio was not given, but reflux ratio was given instead?

In the distillation diagram, the reflux ratio is:

$$R_R = \dot{n}_R / \dot{n}_D$$

and the boil-up ratio is:

$$B_R = \dot{n}_V / \dot{n}_B$$

Assuming $\dot{n}_L = \dot{n}_F + \dot{n}_R$ and $\dot{n}_E = \dot{n}_V$

then you can solve the altered problem.

P03 eLEAPS Problem Session Script

Interaction 11:

Topic: Distillation Column

Background: Thank you for completing this problem session. Please place your filled-in PAPER COPY of the template document in your technical journal. Click here for the correct solution to the template document.

If you so desire, you could print this eLEAPS script (two pages per sheet and on both side of a sheet) and place it also in your technical journal.

If you have any questions or concerns about the problem session, please contact your instructor.

Read the Important Observations below and consult the Reference Readings and Review Materials.

Problem Session Observations

- A distillation column contains a reboiler, equilibrium trays, and a condenser.
- The less volatile components concentrate in the reboiler; that is, the high boilers.
- The more volatile components migrate up through the equilibrium trays.
- The more volatile components concentrate in the condenser; that is, the lower boilers.

- The simplest model for VLE is Raoult's Law coupled with the Antoine equation.
- A binary VLE system is represented by a temperature-composition (TXY) diagram for a fixed pressure of the system.
- A binary VLE system is represented by a pressure-composition (PXY) diagram for a fixed temperature of the system.

Reference Readings

- Felder and Rousseau, 3rd Edition, Section 6.4, Multi-Component Gas-Liquid Systems.
- Felder and Rousseau, 3rd Edition, Section 6.1, Single-Component Phase Equilibrium.

- Distillation Column - "Visual Encyclopedia of Chemical Engineering Equipment" On the CD-ROM in the textbook by Felder and Rousseau

Review Materials

- Hanyak's "Rigorous Model for Multi-Component VLE," CinChE Manual, Chapter 6.
- Hanyak's "Raoult's Law Model for Multi-Component VLE," CinChE Manual, Chapter 6.
- Hanyak's "Pure-Component Phase Equilibrium," CinChE Manual, Chapter 6.