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

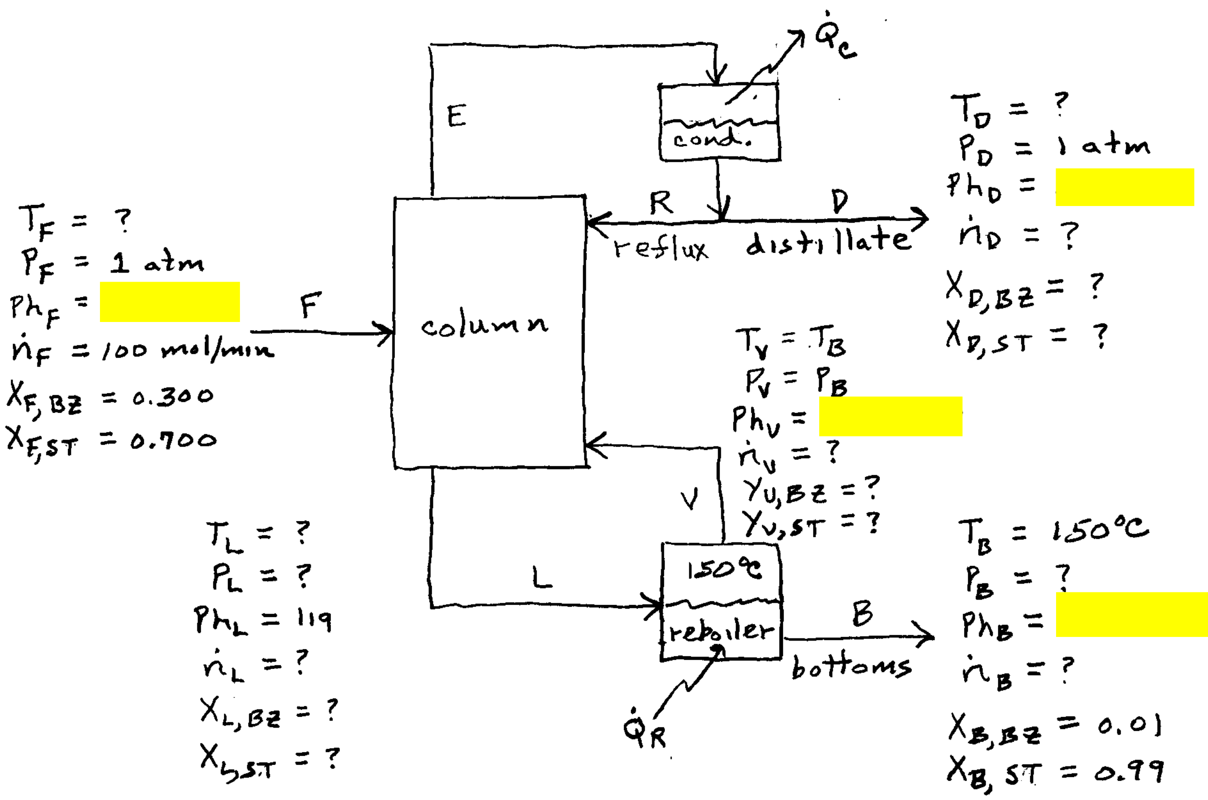
Similar to Problem 6.60 in F&R, 3rd Ed.

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



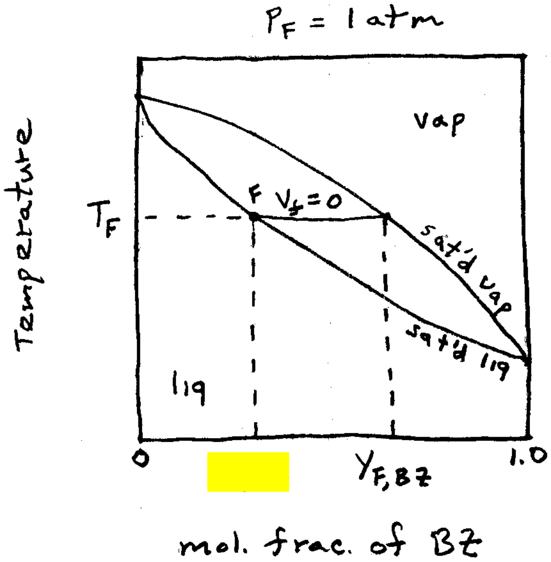
Other Givens: $\dot{n}_V / \dot{n}_B = 2.5$ boilup ratio

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

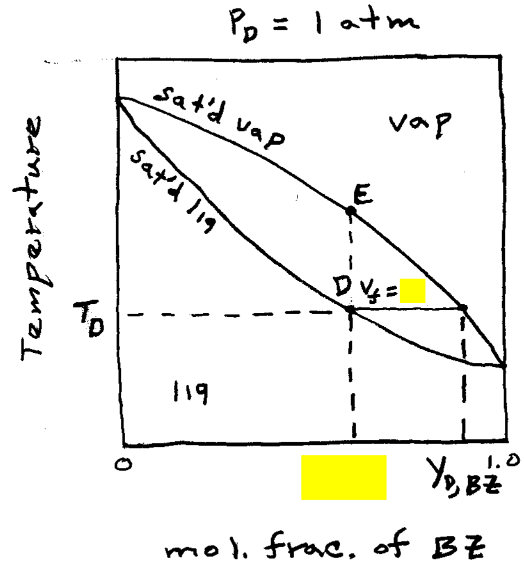
Finds:

$X_{D,BZ}$ 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

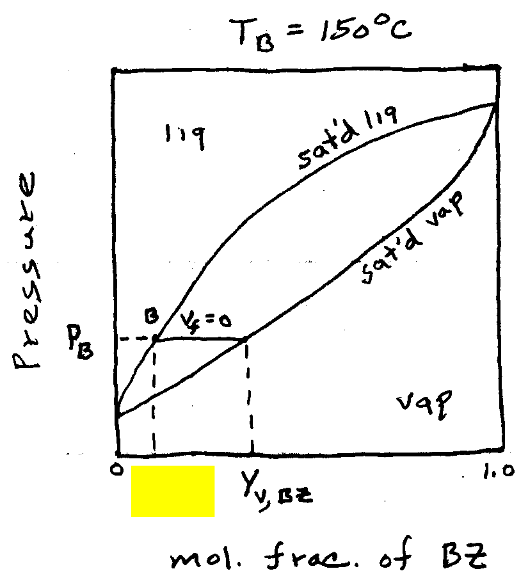
Feed Condition



Distillate Condition



Bottoms Condition



Assumptions

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

Mathematical Model A, Overall Balance

①	Total:	$\dot{n}_F - \dot{n}_D - \dot{n}_B = 0$	
②	benzene:	$0.3\,\dot{n}_F - \dot{n}_{D,BZ} - \boxed{\quad} = 0$	# vars = 5
③	styrene:	$0.7\,\dot{n}_F - \dot{n}_{D,ST} - \boxed{\quad} = 0$	# 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:	$\dot{n}_{D,BZ} = \dot{n}_D\, x_{D,BZ}$	# vars = □
⑥		$\dot{n}_{D,ST} = \dot{n}_D\, x_{D,ST}$	# eqns = □; dof = □
⑦	vle of F:	$[T_F] = \text{vlet}\,[P_F, \boxed{\quad}]$	# vars = 13
⑧	vle of D:	$[T_D] = \text{vlet}\,[P_D, \boxed{\quad}]$	# 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
(dep)	Mix V:	$\dot{n}_V = \dot{n}_{V,BZ} + \dot{n}_{V,ST}$	# eqns = 3; dof = 4
(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:	$[P_B, \bar{y}_V] = \text{vlep}\,[\boxed{\quad}]$	
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:	$\dot{n}_{L,BZ} = \dot{n}_L\, x_{L,BZ}$	# vars = 15
⑪		$\dot{n}_{L,ST} = \dot{n}_L\, x_{L,ST}$	# eqns = 11; dof = 4

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

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. $X_{L,ST} \leftarrow \dot{n}_{L,ST}/\dot{n}_L$

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 atm, \psi_f = 0, \bar{X}_F] = $ [ ] °C see Page 6
8. $T_D = \text{vlet}[1 atm, \psi_f = 0, \bar{X}_D] = $ [ ] °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. $[P_B, \bar{Y}_V] = \text{vlep}[150°C, \psi_f = 0, \bar{X}_B]$ see Page 8

   $P_B = 899.207$ mmHg $=$ [ ]

   $Y_{V,BZ} =$ [ ] $\quad Y_{V,ST} =$ [ ] $=$ [ ]

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**

Vapor-Liquid Equilibrium Model for the Feed Stream:

EZ Setup File HYSYS File Excel File

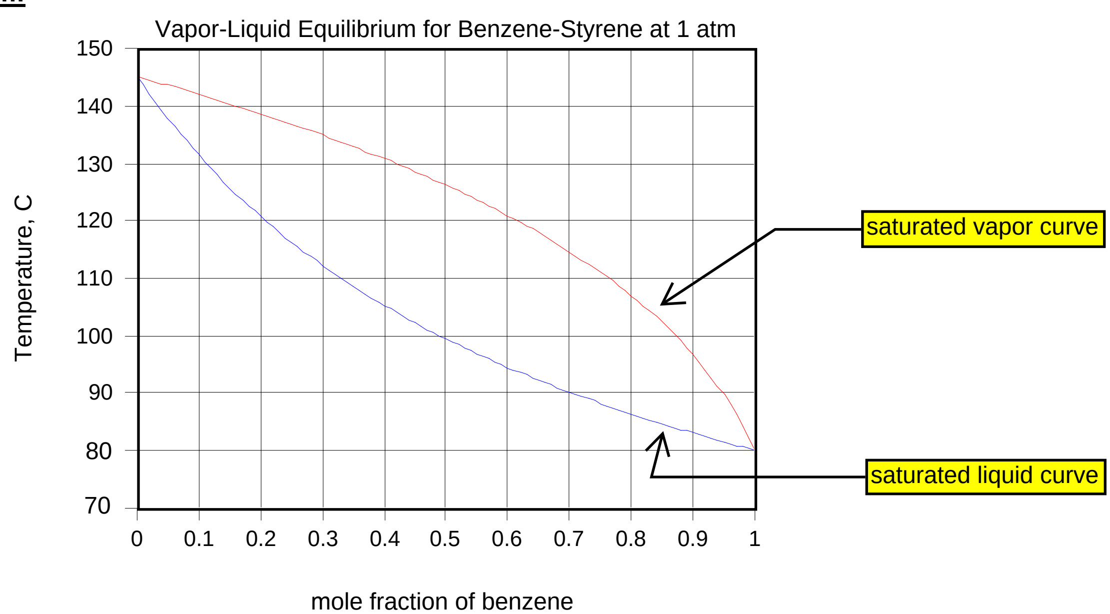
```
   // Total and Two Component Material Balances
   1.0 = Vf + Lf

   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  = 0.30
   zST  = 1.0 - zBZ
```

Numerical Solution 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

TXY Diagram:



Vapor-Liquid Equilibrium Model for the Distillate Stream:

EZ Setup File HYSYS File Excel File

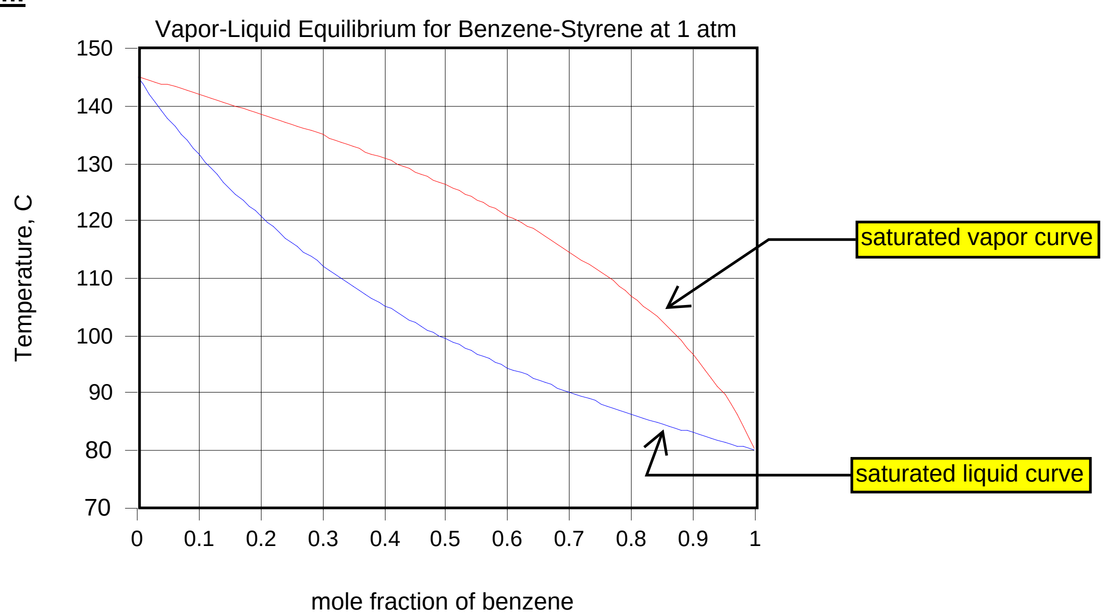
```
    // Total and Two Component Material Balances
    1.0 = Vf + Lf

    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:



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

EZ Setup File   HYSYS File   Excel File

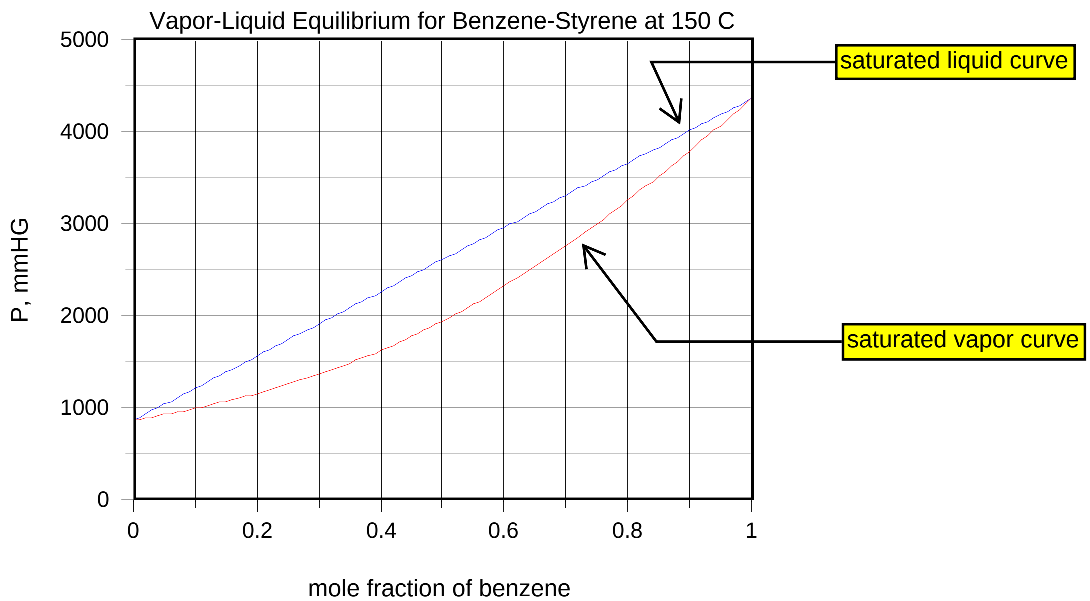
```
    // Total and Two Component Material Balances
    1.0  =  Vf  +  Lf

    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
    T     =  150    // C
    zBZ  =  0.01
    zST  =  1.0  -  zBZ
```

<u>Numerical Solution</u> 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

<u>PXY Diagram:</u>



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: For pure BZ, $T_{NBP} = 80.09\,°C$ } HYSYS 2004
Check T_D: 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

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

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:

		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.