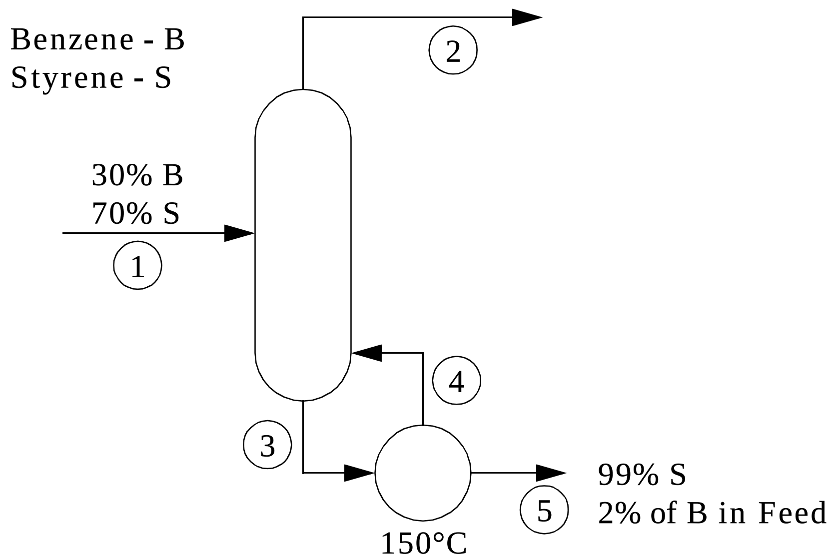
Problem 6.46 Using *Mathematica*

A liquid 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 (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 reboiler are in equilibrium. The boilup ratio, or mole ratio of the vapor and liquid streams leaving the reboiler, is 2.5:1. Using Raoult's law where appropriate, 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.

First we'll draw the PFD and label the streams



Next we'll pick a basis

$$n_1 = 100 \text{ mol/h}$$

so

$$n_{1_B} = x_{1_B} n_1 = 0.3(100) = 30$$

$$n_{1_S} = x_{1_S} n_1 = 0.7(100) = 70$$

In *Mathematica*-ese:

```
(* A Mathematica Solution to Problem 6.46 in Felder &
  Rousseau *)
```

```
n1 = 100 (* Choose a basis & Calculate Feed *)
```

```
100
```

```
n1B = 3 / 10 * n1
```

```
30
```

```
n1S = n1 - n1B
```

```
70
```

Treating the overall system as a separator, we're given the split fraction of B in Stream 5

$$t_{5_B} = 0.02$$

so that

$$t_{2_B} = 1 - t_{5_B} = 1 - 0.02 = 0.98$$

and

$$n_{5_B} = t_{5_B} n_{1_B} = 0.02(30) = 0.6$$

$$n_{2_B} = t_{2_B} n_{1_B} = 0.98(30) = 29.4$$

In *Mathematica*-ese:

```
t5B = 2 / 100 (* Overall Balance on system *)
```

$\frac{1}{50}$

```
t2B = 1 - t5B (* t's are split fractions *)
```

$\frac{49}{50}$

```
n5B = t5B n1B
```

$\frac{3}{5}$

```
n2B = t2B n1B
```

$\frac{147}{5}$

From the definition of mole fraction we have

$$n_5 = \frac{n_{5_B}}{x_{5_B}} = \frac{n_{5_B}}{1 - x_{5_S}} = \frac{0.6}{(1 - 0.99)} = 60$$

and

$$n_{5_S} = x_{5_S} n_5 = 0.99(60) = 59.4$$

In Mathematica-ese:

```
x5S = 99 / 100
99/100
x5B = 1 - x5S
1/100
n5 = n5B / x5B
60
```

Now by an overall mass balance on S

$$n_{2_S} = n_{1_S} - n_{5_S} = 70 - 59.4 = 10.6$$

So the distillate compositions are given by

$$x_{2_B} = \frac{n_{2_B}}{n_2} = \frac{29.4}{(29.4 + 10.6)} = 0.735$$

$$x_{2_S} = 1 - x_{2_B} = 1 - 0.735 = 0.265$$

In *Mathematica*-ese:

```
n2S = n1S - n5S (* Overall balance on S *)
53/5
n2 = n2S + n2B
40
x2B = n2B / n2 (* Composition of Overhead Product *)
147/200
x2S = 1  x2B
53/200
```

From the problem statement Stream 4 is a vapor stream in equilibrium with the liquid Stream 5. We know T and the x_i's, and we need to calculate P and the y_i's, so we need to do a BUBL P calculation. For a BUBL P

$$P = \sum x_k p^*_k$$

and

$$y_k = \frac{x_k p^*_k}{P}.$$

To find p^*_k we'll use the Antoine equation

$$\log_{10}(p^*) = A - \frac{B}{T + C}$$

with T in °C and p^* in mm Hg.

For B

$A = 6.90565$,

$B = 1211.033$,

and

$C = 220.790$

For S

$A = 6.92409$,

$B = 1420.0$,

and

$C = 206$

In *Mathematica*-ese:

```
(* Vapor Pressures from Antoine Equations *)
log10pB = 6.90565 - 1211.033 / (T + 220.790)
```

$$6.90565 - \frac{1211.03}{220.79 + T}$$

```
log10pS = 6.92409 - 1420 / (206 + T)
General::spell1 : Possible spelling error: new symbol
   name "log10pS" is similar to existing symbol "log10pB".
```

$$6.92409 - \frac{1420}{206 + T}$$

```
pB = 10^log10pB
```

$$10^{6.90565 - \frac{1211.03}{220.79 + T}}$$

```
pS = 10^log10pS
```

$$10^{6.92409 - \frac{1420}{206 + T}}$$

```
( [illegible] ,
pressure = x5B pB + x5S pS
```

$$99\ 10^{4.92409-\frac{1420}{206+T}}+10^{4.90565-\frac{1211.03}{220.79+T}}$$

```
(* Composition of BUBL P *)
yB = x5B pB / pressure
```

$$\frac{10^{4.90565-\frac{1211.03}{220.79+T}}}{99\ 10^{4.92409-\frac{1420}{206+T}}+10^{4.90565-\frac{1211.03}{220.79+T}}}$$

```
yS = x5S pS / pressure
```

$$\frac{99\ 10^{4.92409-\frac{1420}{206+T}}}{99\ 10^{4.92409-\frac{1420}{206+T}}+10^{4.90565-\frac{1211.03}{220.79+T}}}$$

We left T as a variable instead of assigning it a value because we may want to play with it later. From the Antoine equation and the BUBL T calculation, we'll know y_{4_S} and y_{4_B}.

In *Mathematica*-ese:

```
(* Could have had T=
  150 but I may want to find T for a given P *)
 y4B = yB /. T -> 150
(* Composition of Vapor leaving Reboiler *)
```

```
0.0486348
```

```
y4S = yS /. T -> 150
```

```
0.951365
```

From the definition of the boilup ratio

$$n_4 = 2.5 n_5$$

and

$$n_{4_S} = y_{4_S} n_4,$$

$$n_{4_B} = y_{4_B} n_4.$$

In *Mathematica*-ese:

```
n4 = 2.5 n5
```

```
150.
```

```
n4S = y4S n4
```

```
142.705
```

```
n4B = y4B n4
```

```
7.29523
```

Once these flows are known a mass balance around the reboiler gives

$$n_{3_S} = n_{4_S} + n_{5_S},$$

$$n_{3_B} = n_{4_B} + n_{5_B}.$$

In *Mathematica*-ese:

```
n3S = n4S + n5S (* S balance around reboiler *)
202.105
n3B = n4B + n5B (* B balance around reboiler *)
7.89523
n3 = n3S + n3B
210.
```

And the composition of the reboiler feed is calculated by the usual definitions.

In *Mathematica*-ese:

```
x3S = n3S / n3 (* Composition of Liquid entering Reboiler *)
0.962404
x3B = n3B / n3
0.0375963
```

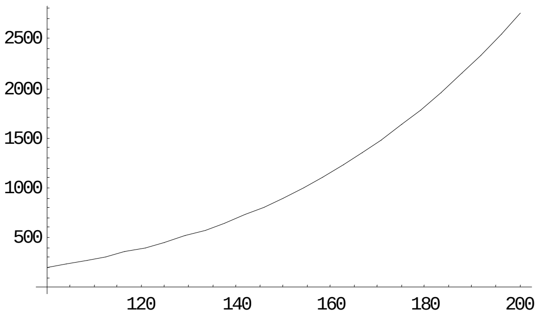
The real value of *Mathematica* for a problem like this is not in the solution of the original problem but in the exploration of what happens for different requirements. For example, it is very common to specify a pressure for the reboiler. Suppose the problem had specified the reboiler pressure as 1000 mm Hg, and asked for the temperature, with all other specifications the same. With the present notebook and *Mathematica's FindRoot* function we can solve that problem. We type simply:

```
FindRoot[pressure == 1000, {T, 150}]
{T → 154.325}
```

We specified the 150 as a starting point for *FindRoot's* algorithm. For those who care, *FindRoot* uses a Newton-Raphson algorithm if the original equation can be differentiated, and the 150 is the starting number for the first iteration. *FindRoot* can easily find any temperature for pressures between 200 torr and 2000 torr.

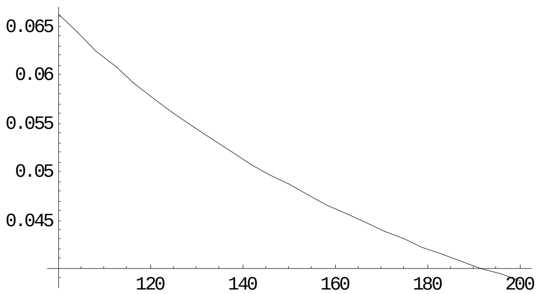
Another *What If* scenario could be to see how the reboiler pressure and the vapor composition change with temperature. We can determine these by plotting P and y_B versus T. In *Mathematica*:

```
Plot[pressure, {T, 100, 200}]
```



- Graphics -

```
Plot[yB, {T, 100, 200}]
```



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