CE 407 Notes
Flash distillation examples

The following problems pertain to binary mixtures of ethylbenzene (component 1, light) and n-propylbenzene (component 2, heavy) at atmospheric pressure. Assume validity of Raoult's law. Use Antoine's equation constants from posted notes as needed.

__1__. Calculate the Txy phase diagram for vapor-liquid equilibria of binary mixtures of ethylbenzene and n-propylbenzene.

__2__. Using the Txy phase diagram you generated for problem __1__, construct the xy equilibrium curve.

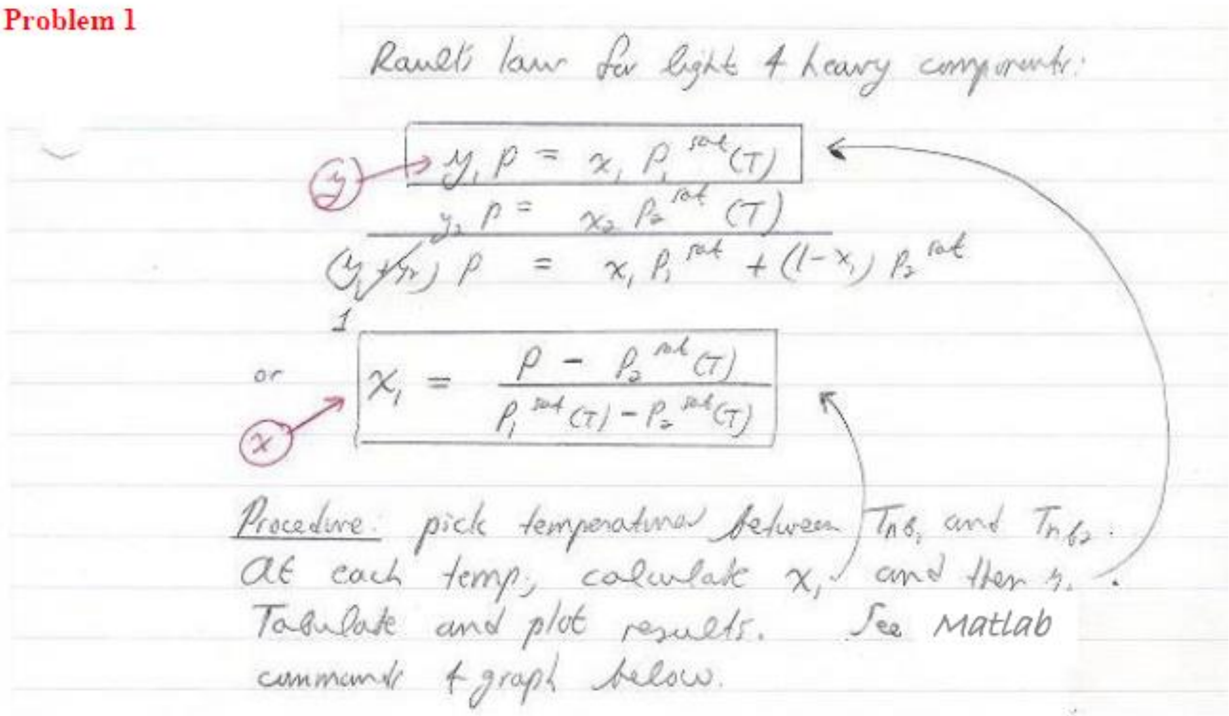
__3__. A feed mixture comprising 35 mole percent ethylbenzene and 65 mole percent n-propylbenzene undergoes flash distillation with 40 percent vaporization (i.e., $f = 0.40$). What is the temperature of the flash, and what are the compositions of the distillate and bottom product? Solve this problem in the following three ways:

[illegible]

(b) by numerical computation according to the analytical (algebraic, non-graphical) flash procedure; and

(c) using the xy equilibrium curve you generated for problem __2__ according to the graphical flash procedure.

Problem 1



Raults law for light + heavy components:

$$\textcircled{y} \rightarrow \boxed{y_1 P = x_1 P_1^{sat}(T)}$$

$$y_2 P = x_2 P_2^{sat}(T)$$

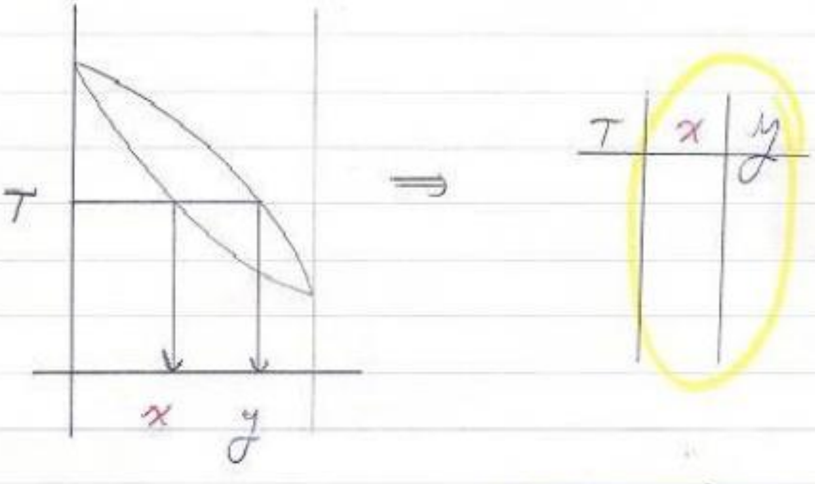
$$\underbrace{(y_1 + y_2)}_{1} P = x_1 P_1^{sat} + (1-x_1) P_2^{sat}$$

or

$$\textcircled{x} \rightarrow \boxed{x_1 = \frac{P - P_2^{sat}(T)}{P_1^{sat}(T) - P_2^{sat}(T)}}$$

Procedure: pick temperatures between T_{nb_1} and T_{nb_2}. At each temp, calculate x_1 and then y_1. Tabulate and plot results. See Matlab commands + graph below.

Problem 2



Then ignore T-column + just plot y as a function of x.

Problem 3

$$\boxed{K_i = \frac{P_i^{sat}(T)}{P}} \qquad \boxed{\begin{array}{l} x_{F_1} = x_F = 0.35 \\ x_{F_2} = 1 - x_F = 0.65 \end{array}}$$

(a) Way too easy. $\boxed{0.4}$

(b) Solve equation $$\sum_{i=1}^{2} \frac{x_{F_i}}{f(K_i - 1) + 1} = 1$$

(where $K_i = P_i^{sat}(T)/P$) for flash temp. T.
When done, calculate

$$x_B = x_{B_1} = \frac{x_{F_1}}{f(K_1 - 1) + 1} = \frac{x_F}{f(K_1 - 1) + 1}$$

$$x_D = x_{D_1} = K_1 x_{B_1} = K_1 x_B .$$

See Matlab commands below. Find

$$\boxed{\begin{array}{ll} T = 424.12 \text{ K} & \text{(temperature of flash)} \\ \left.\begin{array}{l} x_B = 0.295257 \\ x_D = 0.432115 \end{array}\right\} & \text{(composition of bottom and distillate products)} \end{array}}$$

(c) See xy graph below. Material-balance line* passes through the point $(x_F, x_F) = (0.35, 0.35)$ and has slope $-(1-f)/f = -1.5$. See where this line intersects equil. curve to read off x-coord (x_B) and y-coord (x_D). From either x_B or x_D, read temp. off Txy phase diagram. Find

$$\boxed{\begin{array}{l} T = 424 \text{ K} \\ x_B = 0.30 \quad , \quad x_D = 0.43 \end{array}} \leftarrow \text{same}$$

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* $y = -\frac{1-f}{f} x + \frac{x_F}{f}$

General

Psat_Antoine_databank.m

```
(See posted code.)
```

Problem 1

Psat_Antoine.m

```
function Psat = Psat_Antoine( i, T )
%saturated vapor pressures from Antoine's equation for pure substances

%components
%i =  1: ethylbenzene
%i =  2: n-propylbenzene

if i == 1
    ii = 12;
else
    ii = 13;
end

Psat = Psat_Antoine_databank( ii , T );

end
```

boil.m

```
function f = boil( Tb )
%LHS's of nonlinear equations for boiling points of all (both) pure
%components written in the form LHS = 0

for i = 1 : 2
    f(i) = Psat_Antoine(i,Tb(i)) - 760;
end

end
```

calc_Txy.m

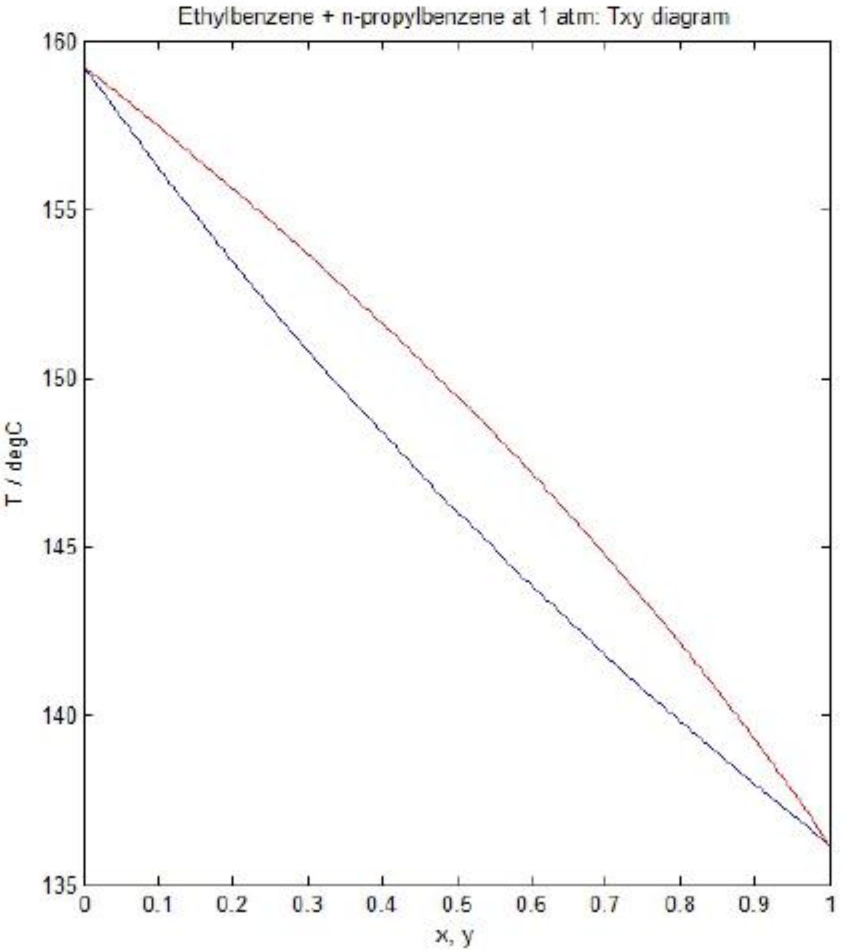
```
%pure-component boiling points
Tb = fsolve(@boil,[100,100])

%Txy data
P = 760;
T = linspace(Tb(1),Tb(2),21);
for k = 1 : 21
    x(k) =    (P                    - Psat_Antoine(2,T(k))) ...
            / (Psat_Antoine(1,T(k)) - Psat_Antoine(2,T(k)));
    y(k) = x(k) * Psat_Antoine(1,T(k)) / P;
end
```

plot_Txy.m

```
%plot Txy diagram
plot(x,T,'-b', ...
     y,T,'-r')
xlim([0 1])
ylim([110 140])
xlabel('x, y')
ylabel('T / degC')
title('Ethylbenzene + n-propylbenzene at 1 atm: Txy diagram')
```

Session

```
>> calc_Txy

Equation solved.

fsolve completed because the vector of function values is near zero
as measured by the default value of the function tolerance, and
the problem appears regular as measured by the gradient.

<stopping criteria details>


Tb =

  136.1934  159.2191

>> plot_Txy
>>
```


Ethylbenzene + n-propylbenzene at 1 atm: Txy diagram
T / degC
160
155
150
145
140
135
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
x, y

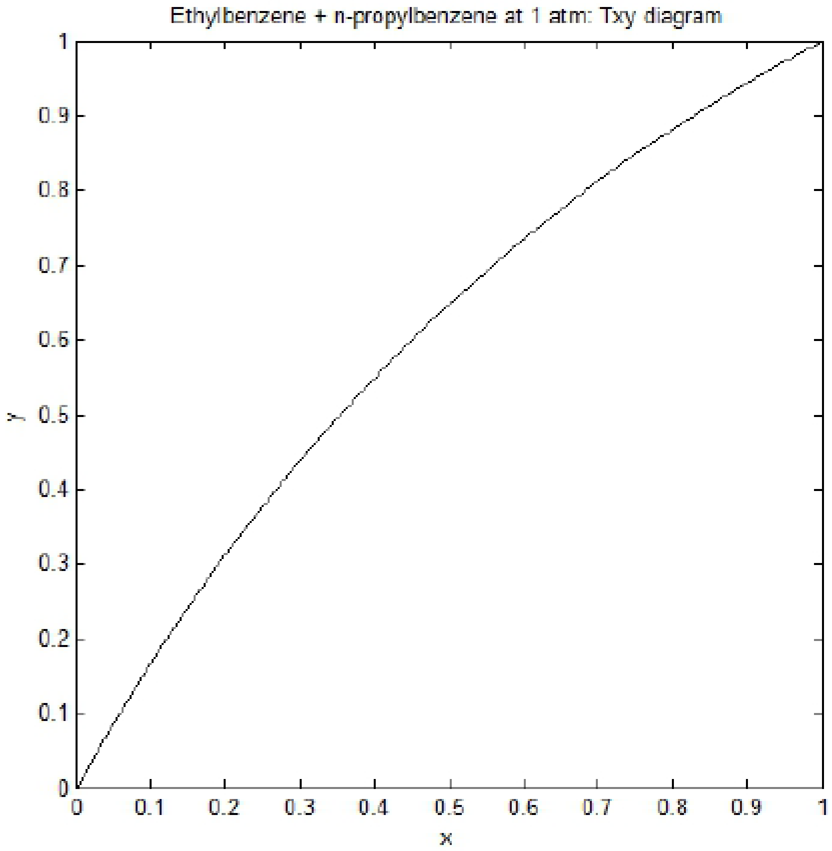
Problem 2

plot_xy.m

```
%plot xy diagram
plot(x,y,'-k')
xlim([0 1])
ylim([0 1])
xlabel('x')
ylabel('y')
title('Ethylbenzene + n-propylbenzene at 1 atm: Txy diagram')
```

Session

```
>> calc_xy
```



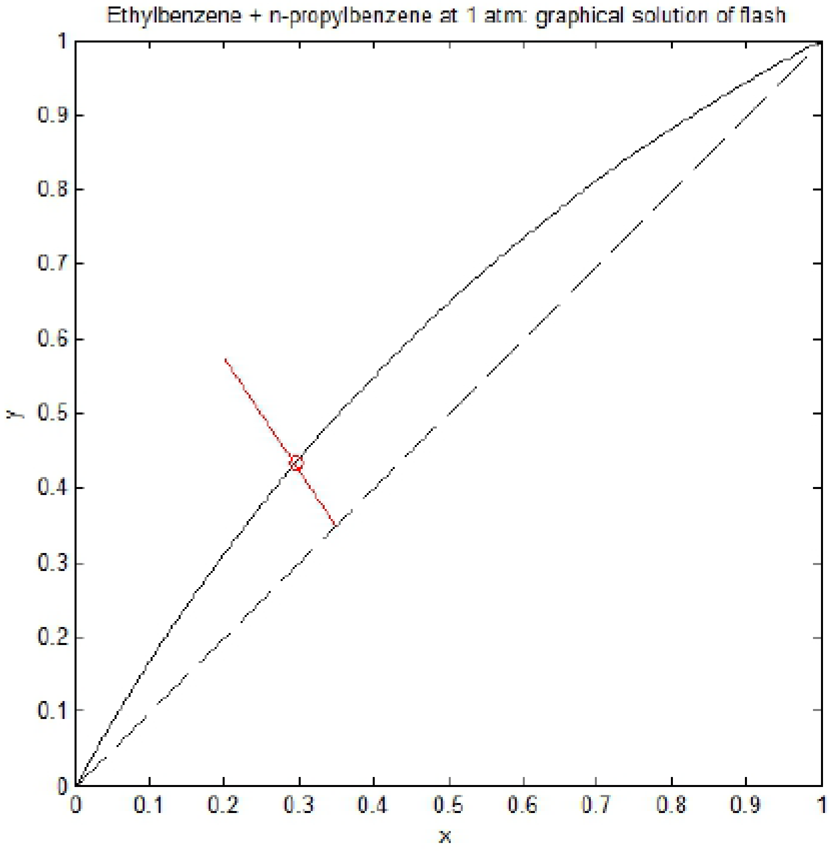
Problem 3(c)

solve_graphical_flash.m

```
%graphical solution of flash problem
fvaporized = 0.4;
xf = 0.35;
xb = 0.20;
yd = (-(1 - fvaporized) * xb + xf) / fvaporized;

plot(x,y,'-k',                   ...
     [0  1 ], [0  1 ], '--k', ...
     [xf xb], [xf yd], '-r',   ...
     [0.295], [0.432], 'ro')
xlim([0 1])
ylim([0 1])
xlabel('x')
ylabel('y')
title('Ethylbenzene + n-propylbenzene at 1 atm: graphical solution of flash')
```

Session

```
>> plot_flash
>>
```



Problem 3(b)

define_flash.m

```
%define flash (feed composition and fraction vaporized)
xf(1) = 0.35;
xf(2) = 0.65;
fvaporized = 0.4;
```

flash.m

```
function f = flash( T )
%LHS of nonlinear equation for flash distillation of multicomponent mixture
%written in the form LHS = 0

%define flash (fraction vaporized and feed composition)
define_flash

%LHS
f = -1;
for i = 1 : 2
    K = Psat_Antoine(i,T) / 760;
    f = f + xf(i) / (fvaporized * (K - 1) + 1);
end

end
```

solve_analytical_flash.m

```
%temperature of flash
T = fsolve(@flash,100.0)

%product compositions from flash
define_flash
for i = 1 : 2
    K = Psat_Antoine(i,T) / 760;
    xb(i) = xf(i) / (fvaporized * (K - 1) + 1);
    yd(i) = xb(i) * K;
end
xb
yd
```

Session

```
>> solve_analytical_flash

Equation solved.

fsolve completed because the vector of function values is near zero
as measured by the default value of the function tolerance, and
the problem appears regular as measured by the gradient.

<stopping criteria details>


T =

  150.9684


xb =

    0.2953    0.7048


yd =

    0.4321    0.5679

>>
```