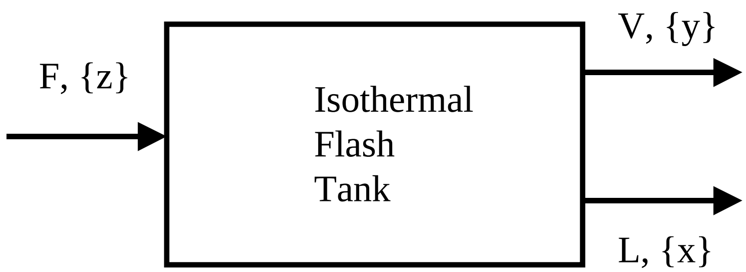
Exam III
Administered: Thursday, November 7, 2014
22 points

For each problem part: 0 points if not attempted or no work shown,
1 point for partial credit, if work is shown,
2 points for correct numerical value of solution

Problem 1. (10 points)

Consider an isothermal flash tank:



This unit takes a pressurized liquid, two-component feed stream and exposes it to a low pressure vessel maintained under isothermal conditions. The net result is that some of the fluid is vaporized, while some fluid remains liquid. The compositions of the liquid and vapor phase are determined by the combined analysis of mass balances and Raoult's Law for vapor-liquid equilibrium. The temperature in the flash tank is $T = 298K$ and the pressure in the tank is $P = 101kPa$.

$$F = 100\, mol/hr \quad V = 40\, mol/hr \quad L = F - \mathrm{V}\, mol/hr$$

$$z_A = 0.4 \qquad y_A = ? \qquad x_A = ?$$

$$z_B = 0.6 \qquad y_B = ? \qquad x_B = ?$$

You have four unknowns, the compositions of the liquid stream, x_A and x_B, and the composition of the vapor stream, y_A and y_B.

You also have four equations.

material balance on moles of A: $0 = Fz_A - Lx_A - Vy_A$

liquid mole fraction constraint: $1 = x_A + x_B$

vapor mole fraction constraint: $1 = y_A + y_B$

one equilibrium constraint: $x_A P_A^{vap} = y_A P$ (Raoults' law for vapor-liquid equilibrium)

where $P_A^{vap} = 60\, kPa\ @\ T = 298K$

(a) Is the system of equations linear or nonlinear in the unknowns?
(b) Solve for the four unknown mole fractions. Show your work. Emphasize the steps in the procedure.

Solution

(a) Equations are linear in the unknowns. Therefore, use linear algebra to solve.
(b) Solve.
Put equations in linear form

$$Lx_A + Vy_A = Fz_A$$
$$x_A + x_B = 1$$
$$y_A + y_B = 1$$
$$x_A P_A^{vap} - y_A P = 0$$

Put equations in matrix form
matrix of coefficients, A, (4x4)

eqn/var	x_A	x_B	y_A	y_B
1	L	0	V	0
2	1	1	0	0
3	0	0	1	1
4	P_A^{vap}	0	$-P$	0

vector of right hand sides, b, (4x1)

eqn	b
1	Fz_A
2	1
3	1
4	0

I then created a matlab script to solve this problem, xm03p01_f14.m.

```
clear all;
F = 100; % mol/hr
V = 40; % mol/hr
L = F - V; % mol/hr

zA = 0.4;
zB = 0.6;

PvapA = 60; % kPa

P = 101; % kPa

A = [L  0   V   0
   1    1   0   0
   0    0   1   1
   PvapA    0   -P  0]

b =[F*zA; 1; 1; 0]

detA = det(A)

x = A\b;

xA = x(1)
xB = x(2)
```

```
yA = x(3)
yB = x(4)
```

Upon execution, the output of this script was as follows,

```
>> xm3p01_f14

A =
    60     0    40     0
     1     1     0     0
     0     0     1     1
    60     0  -101     0

b =
    40
     1
     1
     0

detA =         8460

xA =    0.4775
xB =    0.5225
yA =    0.2837
yB =    0.7163
```

The mole fractions are provided above.

Problem 2. (10 points)

Consider the same system given in Problem 1. In a more realistic version of the problem, not only are the the compositions of the liquid stream, x_A and x_B, and the composition of the vapor stream, y_A and y_B, unknown, but the liquid and vapor stream flowrates, *L* and *V* respectively are also unknown. In this case, you have six unknowns and six equations. The equations are

material balance on total moles:	$0 = F - L - V$	
material balance on moles of A:	$0 = Fz_A - Lx_A - Vy_A$	
liquid mole fraction constraint:	$1 = x_A + x_B$	
vapor mole fraction constraint:	$1 = y_A + y_B$	
equilibrium constraint on A:	$x_A P_A^{vap} = y_A P$	(Raoults' law for A)
equilibrium constraint on B:	$x_B P_B^{vap} = y_B P$	(Raoults' law for B)

where $P_A^{vap} = 60\,kPa\ @\ T = 298K$ and $P_B^{vap} = 140\,kPa\ @\ T = 298K$

(a) Is this set of equations linear or nonlinear in the unknowns?
(b) Come up with a good set of initial guesses for the solution.
(c) Solve for the flowrates and compositions of the liquid and vapor streams. Show your work. Emphasize the steps in the procedure.

Solution

(a) Equations are nonlinear in the unknowns. Therefore, use a multivariate rootfinding technique, such as the multivariate Newton-Raphson method with numerical derivatives to solve.

(b) Come up with a good set of initial guesses for the solution.

A good set of initial conditions comes from the solution to Problem 1.

```
xA =    0.4775
xB =    0.5225
yA =    0.2837
yB =    0.7163
L =     60
V =     40
```

(c) Solve for the flowrates and compositions of the liquid and vapor streams. Show your work. Emphasize the steps in the procedure.

Put equations in appropriate form

$$f_1(x_1, x_2, y_1, y_2, L, V) = F - L - V = 0$$
$$f_2(x_1, x_2, y_1, y_2, L, V) = Fz_A - Lx_A - Vy_A = 0$$
$$f_3(x_1, x_2, y_1, y_2, L, V) = x_A + x_B - 1 = 0$$
$$f_4(x_1, x_2, y_1, y_2, L, V) = y_A + y_B - 1 = 0$$
$$f_5(x_1, x_2, y_1, y_2, L, V) = x_A P_A^{vap} - y_A P = 0$$
$$f_6(x_1, x_2, y_1, y_2, L, V) = x_B P_B^{vap} - y_B P = 0$$

I then created a matlab script to solve this problem, xm03p02_f14.m. Note that this script first solves problem 1 again in order to obtain a consistent guess for the six variables.

```
clear all;
%
%  come up with good initial guess from problem 1
%
xA =    0.4775;
xB =    0.5225;
yA =    0.2837;
yB =    0.7163;
L =     60;
V =     40;
%
%  create initial guess vector
%
x0=[xA,xB,yA,yB,L,V];
tol = 1.0e-6;
iprint = 1;
%
%  call multivariate Newton-Raphson with Numerical derivatives
%
[x,err,f] = nrndn(x0,tol,iprint);
%
%  identify solutions
%
xA = x(1)
xB = x(2)
yA = x(3)
yB = x(4)
L = x(5)
V = x(6)
```

The input file for `nrndn.m` is given by

```
function f = funkeval(x)
n = max(size(x));
f = zeros(n,1);
%
%  identify variables
%
xA = x(1);
xB = x(2);
yA = x(3);
yB = x(4);
L = x(5);
V = x(6);
%
%  assign constants
%
F = 100; % mol/hr
zA = 0.4;
PvapA = 60; % kPa
PvapB = 140; % kPa
P = 101; % kPa
%
%  write equations
%
f(1) = F - L - V;
```

```
f(2) = F*zA - L*xA - V*yA;
f(3) = xA + xB - 1;
f(4) = yA + yB - 1;
f(5) = xA*PvapA - yA*P;
f(6) = xB*PvapB - yB*P;
```

Upon execution, the output of this script was as follows,

```
>> xm3p02_f14

iter =    1, err =  2.48e+00 f =  3.25e-01
iter =    2, err =  5.08e-02 f =  7.10e-03
iter =    3, err =  3.11e-14 f =  4.35e-15

xA =    0.4875
xB =    0.5125
yA =    0.2896
yB =    0.7104
L =   55.7849
V =   44.2151
```

The mole fractions are provided above. The flowrates, *L* and *V*, are also given with units of mol/hr.

Problem 3. (2 points)

An even more realistic version of this problem occurs when the flash tank is operated under adiabatic rather than isothermal conditions. In this case, the temperature of the system is unknown. Discuss briefly how one might solve this problem. What kind of equation would be added to account for the new variable? What kind of additional parameters would be needed? What technique could you use to solve this?

Solution

The new equation would be an energy balance. We would need vapor pressures for pure components as a function of temperature, not just at one point, from something like the Antoine equation. The system of seven equations and seven unknowns (at least for a binary system) would be nonlinear and would require a technique like the multivariate Newton Raphson method with numerical derivatives as used in problem 2.