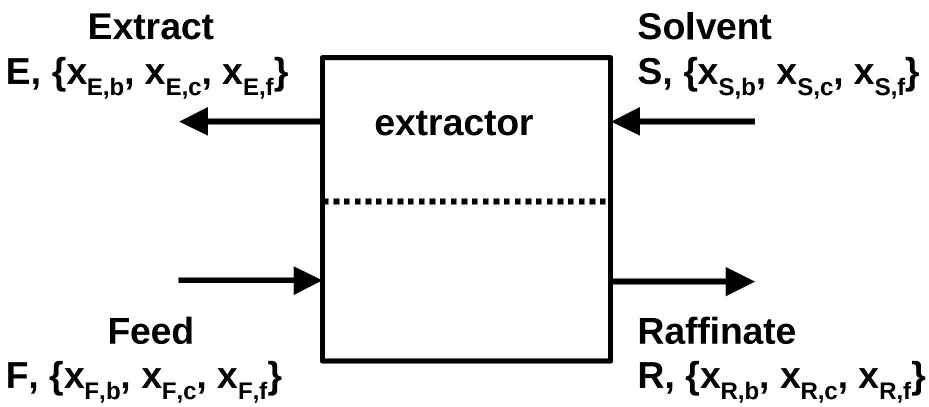
Applied Statistics and Numerical Methods for Engineers
ChE 301, Fall 1998
Midterm Exam Number Three
TAKE HOME EXAM
Assigned: Wednesday, November 11, 1998
Due: Friday, November 13, 1998, BEGINNING OF CLASS

THE EXAM HAS 48+54+20=122 POINTS.

Problem 1. (48 points)

Consider an extractor:



This unit removes uses a recycled furfural stream as the solvent to extract benzene from a cyclohexane product stream. The data you are given is

$$F = F_o \text{ mol/hr} \quad S = 150 \text{ mol/hr} \quad R = 95 \text{ mol/hr} \quad E = E_o \text{ mol/hr}$$

$$x_{F,b} = 0.1 \quad x_{S,b} = 0.0010 \quad x_{R,b} = ? \quad x_{E,b} = ?$$

$$x_{F,c} = 0.9 \quad x_{S,c} = 0.0001 \quad x_{R,c} = ? \quad x_{E,c} = ?$$

$$x_{F,f} = 0.0 \quad x_{S,f} = 0.9989 \quad x_{R,f} = ? \quad x_{E,f} = ?$$

You are to consider F_o and E_o as givens defined by:

a = 100
b = 105

$$F_o = \text{rand} \cdot (b - a) + a$$

$$E_o = F_o + S - R$$

where rand is the random number generator function of MATLAB.

The equilibrium constants are: $K_b = \frac{x_{E,b}}{x_{R,b}} = 20.0$ and $K_c = \frac{x_{E,c}}{x_{R,c}} = 0.05$.

Then you have six unknowns, the compositions of the raffinate stream and the composition of the extract stream.

(a) Write equations which will yield the unknowns. Clearly identify the origin of each equation (mass balance, constraint, etc.) (12 points)
(b) Convert these equations to a linear form with unknown terms on the left hand side and constants on the right hand side, if they are not already in that form. (12 points)
(c) Convert the equations to matrices and vectors. (4 points)
(d) Compute the determinant and rank of the matrix, and list the random values of F and E used in the calculation.
(8 points)
(e) Using MATLAB, solve for the steady-state values of the unknowns. (12 points)

(Hint: since you have 3 components, you will have three mass balances. You also have 2 streams with constraints that the sum of the mole fractions must be unity. You also have 2 separation ratio constraints. Therefore, you have 7 equations. However, you only have 6 unknowns. Not all of the 7 equations are independent. You must choose 6 independent equations. Part (d) should indicate to you whether you have selected 6 independent equations.)

Solution:
(a) Write equations

benzene mole balance: $0 = Fx_{F,b} + Sx_{S,b} - Rx_{R,b} - Ex_{E,b}$

cyclohexane mole balance: $0 = Fx_{F,c} + Sx_{S,c} - Rx_{R,c} - Ex_{E,c}$

furfural mole balance: $0 = Fx_{F,f} + Sx_{S,f} - Rx_{R,f} - Ex_{E,f}$ **(not used, dependent)**

raffinate mole fraction constraint: $1 = x_{R,b} + x_{R,c} + x_{R,f}$

extract mole fraction constraint: $1 = x_{E,b} + x_{E,c} + x_{E,f}$

benzene equilibrium constraint: $K_b = \frac{x_{E,b}}{x_{R,b}} = 20.0$

c-hexane equilibrium constraint: $K_c = \frac{x_{E,c}}{x_{R,c}} = 0.05$

(b) Put equations in linear form

benzene mole balance: $Rx_{R,b} + Ex_{E,b} = Fx_{F,b} + Sx_{S,b}$

cyclohexane mole balance: $Rx_{R,c} + Ex_{E,c} = Fx_{F,c} + Sx_{S,c}$

furfural mole balance: $Rx_{R,f} + Ex_{E,f} = Fx_{F,f} + Sx_{S,f}$ **(not used, dependent)**

raffinate mole fraction constraint: $x_{R,b} + x_{R,c} + x_{R,f} = 1$

extract mole fraction constraint: $x_{E,b} + x_{E,c} + x_{E,f} = 1$

benzene equilibrium constraint: $x_{E,b} - x_{R,b}K_b = 0$

c-hexane equilibrium constraint: $x_{E,c} - x_{R,c}K_c = 0$

(c) Put equations in matrix form

matrix of coefficients, A (6 x 6)

eqn/var $x_{R,b}$ $x_{R,c}$ $x_{R,f}$ $x_{E,b}$ $x_{E,c}$ $x_{E,f}$

1	R	0	0	E	0	0
2	0	R	0	0	E	0
3	1	1	1	0	0	0
4	0	0	0	1	1	1
5	$-K_b$	0	0	1	0	0
6	0	$-K_c$	0	0	1	0

vector of right hand sides, b (6x1)

eqn	b
1	$Fx_{F,b} + Sx_{S,b}$
2	$Fx_{F,c} + Sx_{S,c}$
3	1
4	1
5	0
6	0

(d) Compute the determinant and rank of the matrix.
F = 100.9941
E = 160.9941
detA = 3.2453e+005
rankA = 6

(e) Using MATLAB, solve for the steady-state values of the unknowns.

x(1) = 0.003097 = $x_{R,b}$ x(2) = 0.927179 = $x_{R,c}$ x(3) = 0.069724 = $x_{R,f}$

x(4) = 0.061932 = $x_{E,b}$ x(5) = 0.046359 = $x_{E,c}$ x(6) = 0.891709= $x_{E,f}$

Problem 2. (54 points)

Use the data given in the file “file.xm3_pr2.dat” (available on the website) to determine if the data is best fit by a first, second, or third-order single-variable polynomial fit.

For the first order case, determine
- (a) the value of the model parameters (4 points)
- (b) the standard deviation of the model parameters (4 points)
- (c) the measure of fit of the model (2 points)
- and (d) write out the model equation with the parameters you have obtained. (2 points)

For the second order case, determine
- (e) the value of the model parameters (6 points)
- (f) the standard deviation of the model parameters (6 points)
- (g) the measure of fit of the model (2 points)
- and (h) write out the model equation with the parameters you have obtained. (2 points)

For the third order, determine
- (i) the value of the model parameters (8 points)
- (j) the standard deviation of the model parameters (8 points)
- (k) the measure of fit of the model (2 points)
- and (l) write out the model equation with the parameters you have obtained. (2 points)

(m) Based on this data determine which case is best. Justify. (4 points)

Solution:

(a), (b), (c), and (d)

PARAMETER	VALUE	STANDARD DEVIATION
1	2.4068295e+002	1.7077344e+001

2 -5.2241420e+000 2.9358728e-001
MOF = 7.6364612e-001

$$y = 240.7 - 5.22x$$

(e), (f), (g) and (h)

PARAMETER	VALUE	STANDARD DEVIATION
1	5.7142627e+001	8.1842047e+000
2	5.5723477e+000	3.7404040e-001
3	-1.0689594e-001	3.5880269e-003

MOF = 9.7671478e-001

$$y = 57.1 + 5.57x - 0.11x^2$$

(i), (j), (k), and (l)

PARAMETER	VALUE	STANDARD DEVIATION
1	7.1947978e+001	1.0940489e+001
2	3.8558520e+000	9.3343561e-001
3	-6.4619093e-002	2.1417748e-002
4	-2.7905509e-004	1.3943383e-004

MOF = 9.7764739e-001

$$y = 71.9 - 3.86x - 0.06x^2 - 0.0003x^3$$

(m) The linear fit gives a bad MOF of 0.76.
The quadratic and cubic fits give good MOF of 0.977 and 0.978.
This difference is not great enough to justify the use of the additional fitting parameter in the cubic fit.
The quadratic fit is the best model.

Problem 3. (20 points)

Consider the non-linear function:

$$f(x) = 0.001 \cdot \left[\left(\frac{x}{4} - 5 \right)^3 \sin\left(\frac{x}{4} + 4 \right) - \frac{x^2}{16} + 3 \right] \exp\left(\frac{-x}{40} \right)$$

(a) How many roots are there between x = 0 and x =100?
(b) What are the roots of f(x) between x = 0 and x =100?
(c) Plot the function over the range x = 0 to x =100 with the line y=0 and circle the roots.

(a) seven roots
(b) 8.7977, 38.6600, 44.6455, 60.2832, 71.3668, 84.9503, 96.7675

(c)