**ChE 310 Problem Set 6 (15 pts) Due Wed 3/6/19**

Collect all m-files in a single .zip file and upload the .zip file to the course webpage by midnight on Wednesday, March 6, 2019. Please note any collaborations in the Canvas upload comment box. Each student must upload their own individual copy of the work.

Keep in mind that book problems below correspond to the 3rd edition of Chapra’s text; the 4th edition may have different problem numbers.

**6\_1 (6 pts) Optimization.** These are shorter problems, so submit them all within one m-file PS6\_1.m.

1. Problem 7.14 from the text. Report the optimal insulation thickness to the command window; also report the temperature of the wire at the optimum thickness value.
2. Problem 7.26 from the text. Have the answer reported to the command window in this format: “The max growth rate of \_\_\_\_\_ d^-1 occurs at concentration of \_\_\_\_\_\_ mg/L”.
3. Problem 7.30 from the text. Print the location of the peak concentration as well as the value of the peak concentration to the command window.

***Solution:***

%PS6\_1.m

%(A) Solution to Chapra 7.14

clear; clf;

%Input parameters

q = 75; %W/m

r\_w = 6e-3; %m

k = 0.17; %W/m\*K

h = 12 ; %W/m^2\*K

T\_air = 293 ; %K

%Input function

T = @(r\_i) T\_air + q/(2\*pi)\*(1/k\*log((r\_w+r\_i)/r\_w)+1./(h\*(r\_w+r\_i)));

%Optional, but good idea: plot to determine initial guess

fplot(T,[0 .1])

%We have a few tools available to us... let's use fminbnd since bounds are

%clear from the plot.

disp('Part A')

[r\_i\_min T\_min] = fminbnd(T,0.005,0.015)

%(B) Solution to Chapra 7.26

clear; figure();

%Input function

g = @(c) 2\*c./(4+0.8\*c+c.^2+0.2\*c.^3);

%Optional, but good idea: plot to determine initial guess

fplot(g,[0 5])

%Let's try fminsearch this time.

f = @(c) -g(c);

[c\_max f\_min] = fminsearch(f,1.5);

g\_max = -f\_min;

disp('Part B')

fprintf('The max growth rate of %4.3g d^-1 occurs at concentration of %4.3g mg/L.\n',g\_max,c\_max)

%(C) Solution to Chapra 7.30

clear; figure()

%Input function

c = @(x,y) 7.9 + .13\*x + .21\*y - .05\*x.^2 - .016\*y.^2 - .007\*x.\*y;

%Optional, but again we can plot over the suggested range.

x = linspace(-10,10); y = linspace(0,20);

[X,Y] = meshgrid(x,y);

C = c(X,Y);

surfc(X,Y,C);

xlabel('x')

ylabel('y')

%The surface appears to behave well, so a good guess in that range should

%converge to the desired result with fminsearch.

c\_mod = @(V) -c(V(1),V(2));

[V\_min c\_mod\_min] = fminsearch(c\_mod,[1 6]);

disp('Part C')

x\_max = V\_min(1)

y\_max = V\_min(2)

c\_max = -c\_mod\_min

**Outputs:**

>> PS6\_1

Part A

r\_i\_min =

 0.0082

T\_min =

 423.5398

Part B

The max growth rate of 0.37 d^-1 occurs at concentration of 1.57 mg/L.

Part C

x\_max =

 0.8537

y\_max =

 6.3758

c\_max =

 8.6249

**6\_2** **(3 pts) Mass balance/linear systems**. Solve in script PS6\_2.m.

Solve problem 8.9 from the text. Include your mass balance derivations either as comments in the m-file or as an image upload (include the problem number in the image name). Output your vector of concentrations to the command line.

***Solution***:

%PS6\_2.m

%Solution to Chapra 8.9

clear

%Input given flow rates

Q01 = 6 ; Q03 = 7 ; Q12 = 4 ;

Q15 = 5 ; Q23 = 2 ; Q24 = 1 ;

Q25 = 1 ; Q31 = 3 ; Q34 = 6 ;

Q44 = 9 ; Q54 = 2 ; Q55 = 4 ;

%Input the known inlet concentrations

c01 = 20 ; c03 = 50 ;

%Write mass balance equations on each reactor

%Rearrange to put them in the form:

%\_\_ c1 + \_\_c2 + \_\_c3 + \_\_c4 + \_\_c5 = \_\_

%Reactor 1

%Q01c01 + Q31c3 = Q15c1 + Q12c1

%(Q15+Q12)c1 - Q31c3 = Q01c01

%Reactor 2

%Q12c1 = Q25c2 + Q24c2 + Q23c2

%-Q12c1 + (Q25+Q24+Q23)c2 = 0

%Reactor 3

%Q03c03 + Q23c2 = Q31c3 + Q34c3

%-Q23c2 + (Q31+Q34)c3 = Q03c03

%Reactor 4

%Q24c2 + Q34c3 + Q54c5 = Q44c4

%-Q24c2 -Q34c3 + Q44c4 - Q54c5 = 0

%Reactor 5

%Q15c1 + Q25c2 = Q54c5 + Q55c5

%-Q15c1 - Q25c2 + (Q54+Q55)c5 = 0

%Convert to matrix notation and solve

A = [(Q15+Q12) 0 -Q31 0 0;

 -Q12 (Q25+Q24+Q23) 0 0 0;

 0 -Q23 (Q31+Q34) 0 0;

 0 -Q24 -Q34 Q44 -Q54 ;

 -Q15 -Q25 0 0 (Q54+Q55)] ;

b = [Q01\*c01 ; 0 ; Q03\*c03 ; 0 ; 0] ;

c = A\b

***Output:***

>> PS6\_2

c =

 28.4000

 28.4000

 45.2000

 39.6000

 28.4000

**6\_3 (2 pts) Mass balance/linear systems.** Solve in script PS6\_3.m.

Solve problem 9.9 from the text. Include your mass balance derivations either as comments in the m-file or as an image upload (include the problem number in the image name). Output your vector of concentrations to the command line.

***Solution:***

%PS6\_3.m

%Solution to Chapra 9.9

clear

%Input given flow rates

Q33 = 120; Q13 = 40; Q12 = 90;

Q23 = 60; Q21 = 30;

%Input known inlets

c01 = 200; c03 = 500;

%We need unknown flows Q03 and Q01.

%Mass balance on Tank 3:

%Q23 + Q13 + Q03 = Q33;

Q03 = Q33 - Q23 - Q13;

%Overall mass balance:

Q01 = Q33 - Q03;

%Write component balance equations on each reactor

%Rearrange to put them in the form:

%\_\_ c1 + \_\_c2 + \_\_c3 = \_\_

%Reactor 1:

%Q01c01 + Q21c2 = (Q13+Q12)c1

%(Q13+Q12)c1 - Q21c2 = Q01c01

%Reactor 2:

%Q12c1 = Q23c2+Q21c2

%-Q12c1 + (Q23+Q21)c2 = 0

%Reactor 3:

%Q13c1 + Q23c2 + Q03c03 = Q33c3

%-Q13c1 -Q23c2 + Q33c3 = Q03c03

%Put in matrix form and solve

A = [(Q13+Q12) -Q21 0;

 -Q12 (Q23+Q21) 0;

 -Q13 -Q23 Q33];

b = [Q01\*c01;0;Q03\*c03];

c = A\b

***Output:***

>> PS6\_3

c =

 200

 200

 250

**6\_4 (4 pts) Mass balance/linear systems.** Solve in script PS6\_4.m.

A counter-current staged liquid-liquid extraction process is depicted below. In such systems, a stream containing a weight fraction $y\_{in}$ of a chemical enters from the left at a mass flow rate of $F\_{1}$ (this is known as the *raffinate*). Simultaneously, a solvent carrying a weight fraction $x\_{in}$ of the same chemical enters from the right at a flow rate of $F\_{2}$ (this is known as the *extract*). Thus, at steady state for stage $i$, a mass balance can be written as:

$F\_{1}y\_{i-1}+F\_{2}x\_{i+1}=F\_{1}y\_{i}+F\_{2}x\_{i}$ (ps6.4.1)

At each stage, an equilibrium is assumed to be established between $y\_{i}$ and $x\_{i}$, such that

$K=\frac{x\_{i}}{y\_{i}}$ (ps6.4.2)

where $K$ is the distribution coefficient. Equation ps6.4.2 can be solved for $x\_{i}$, and the result substituted into Equation ps6.4.1 and rearranged to yield:

$y\_{i-1}-\left(1+\frac{F\_{2}}{F\_{1}}K\right)y\_{i}+\left(\frac{F\_{2}}{F\_{1}}K\right)y\_{i+1}=0$ (ps6.4.3)

Known parameters include: $F\_{1}=200\frac{kg}{h}$, $y\_{in}=0.2$, $F\_{2}=300\frac{kg}{h}$, $x\_{in}=0$, and $K=5$.

Set up the matrix system for determining the value of $y\_{i}$ at each stage. Note that equation (ps6.4.1) should be used to set up the mass balance for the first and last stage. Solve this problem using (i) ‘tridiag’, (ii) ‘gausspivot’, and (iii) ‘\’ algorithms. Which is most efficient? Output the time taken for each to the command window. (Computation time can be quantified using the ‘tic’ and ‘toc’ commands.)

Then, calculate the corresponding value of $x\_{i}$ at each stage. Create a single plot of log($x\_{i}$) and log($y\_{i}$) vs. stage number; label your plot (axes, legend, title) accordingly.



***Solution***:

%PS6\_4.m

%Input known constants

F1 = 200 ; %kg/h

F2 = 300 ; %kg/h

y0 = 0.2 ;

x7 = 0 ;

K = 5 ;

%Write the mass balances.

%The first 5 are reasonably straightforward from ps6.4.3:

%y0 - (1+F2/F1 K)y1 + (F2/F1 K)y2 = 0

%...

%y4 - (1+F2/F1 K)y5 + (F2/F1 K)y6 = 0

%The last stage doesn't quite fit into the same formula,

%so use ps6.4.1 and manually rearrange using terms we know:

%F1\*y5 + F2\*x7 = F1\*y6 + F2\*x6

%x7 = 0 (from problem statement)

%F1\*y5 - F1\*y6 + F2\*x6 = 0

%We know K = x6/y6, so x6 = K\*y6

%F1\*y5 - F1\*y6 + F2\*K\*y6 = 0

%Divide by F1, so it has the same form as other equations

%y5 - (1+F2/F1 K)y6 = 0

%We now know our matrix A, which has 6 columns corresponding

%to the coefficients on the yi terms (i = 1:6)

%We use F2/F1 \* K often - I'll call that c (for constant)

c = F2/F1 \* K;

A = [-(1+c) c 0 0 0 0 ;

 1 -(1+c) c 0 0 0 ;

 0 1 -(1+c) c 0 0 ;

 0 0 1 -(1+c) c 0 ;

 0 0 0 1 -(1+c) c ;

 0 0 0 0 1 -(1+c)];

%If you noticed a pattern, this could be set up a bit faster:

% -(1+c) on the diagonals

A = -(1+c)\*eye(6);

% 1 directly below the diagonal

A(2:end,1:end-1) = A(2:end,1:end-1) + diag(ones(5,1)) ;

% c directly above the diagonal

A(1:end-1,2:end) = A(1:end-1,2:end) + c\*diag(ones(5,1));

%The b vector is pretty straightforward from our linear equations

b = [-y0 ; 0; 0; 0; 0; 0];

tic

y = chapra\_tridiag([0 1 1 1 1 1],-(1+c)\*ones(1,6),[c c c c c 0],b);

time\_tridiag = toc

tic

y = chapra\_GaussPivot(A,b);

time\_GaussPivot = toc

tic

y = A\b;

time\_leftdiv = toc

x = K\*y ;

plot(1:6,log10(x),'bo--')

hold on

plot(1:6,log10(y),'ro--')

xlabel('stage')

xticks(1:6)

ylabel('log10 Mass Fraction')

legend('x\_i','y\_i')

*Output*:

>> PS6\_4

time\_tridiag =

 1.2820e-04

time\_GaussPivot =

 5.1170e-04

time\_leftdiv =

 9.0400e-05

