Final Exam Solutions
Administered: Tuesday, December 10, 2024
10:30 AM – 12:45 PM
24 points

Problem 1. System of Ordinary Differential Equations (8 points)
Consider the following dimerization reaction

$$2A \rightarrow B$$

The following two mass balances describe the concentrations of A & B in an isothermal reactor as a function of time:

$$\frac{dC_A}{dt} = \frac{F_{in}}{V} C_{A,in} - \frac{F_{out}}{V} C_A - 2r$$

$$\frac{dC_B}{dt} = \frac{F_{in}}{V} C_{B,in} - \frac{F_{out}}{V} C_B + r$$

where the reaction rate, r, is given by

$$r = kC_A^2$$

The following numerical values for the parameters are given in the table below

variable	symbol	value	units
inlet flowrate	F_{in}	1.0	l/s
outlet flowrate	F_{out}	1.0	l/s
inlet concentration of A	$C_{A,in}$	2.0	mol/l
inlet concentration of B	$C_{B,in}$	0.0	mol/l
reactor volume	V	100.0	l
reaction rate	k	20.0	$l/mol/s$

The following initial conditions are given for these two ordinary differential equations

variable	symbol	value	units
Initial reactor concentration of A	$C_{A,o}$	0.0	$mole/l$
Initial reactor concentration of B	$C_{B,o}$	0.0	$mole/l$

(a) Is this system of ordinary differential equations linear or nonlinear?
(b) What is the appropriate technique to solve this system of equations?
(c) Solve the transient behavior of the concentration of A, C_A, and the concentration of B, C_B, up to 1000 seconds, if the initial concentration of A in the reactor is $C_A = C_{A,o}$ and the initial concentration of B in the reactor is $C_B = C_{B,o}$. Plot the concentrations of A & B as a function of time.
(d) Report values of the concentration of A, C_A, and the concentration of B, C_B, at 1000 seconds.

Solution:

(a) Is this system of equations linear or nonlinear?

This system of equations is non-linear in the concentration of A, C_A.

(b) What is the appropriate technique to solve this system of equations?

I would use the classical fourth order Runge-Kutta method to solve this system of two first order ordinary differential equations.

(c) Solve the transient behavior of the concentration of A, C_A, and the concentration of B, C_B, up to 1000 seconds, if the initial concentration of A in the reactor is $C_A = C_{A,o}$ and the initial concentration of B in the reactor is $C_B = C_{B,o}$. Plot the concentrations of A & B as a function of time.
(d) Report values of the concentration of A, C_A, and the concentration of B, C_B, at 1000 seconds.

I wrote a script in the file xm4p01_f24.m

```
clear all;
format long

n = 1000;
xo = 0;
xf = 1.0e+3;
Cao = 0.0; % mol/l
Cbo = 0.0; % K
yo = [Cao, Cbo];

[x,y]=rk4n(n,xo,xf,yo);
Ca_f = y(n+1,1)
Cb_f = y(n+1,2)
```

I modified the input function for rk4n.m as follows

```
function dydx = funkeval(x,y);
CA = y(1);
CB = y(2);
CAin = 2.0; % mol/liter
CBin = 0.0; % mol/liter
k = 20.0; % liter/mol/sec
V = 100.0; % liter
Fin = 1.0; % liter/sec
Fout = 1.0; % liter/sec
rate = k*CA*CA;
dCAdt = 1/V*(CAin*Fin - CA*Fout) -2*rate;
dCBdt = 1/V*(CBin*Fin - CB*Fout) + rate;
dydx(1) = dCAdt;
dydx(2) = dCBdt;
```

I executed the script and received the following output:

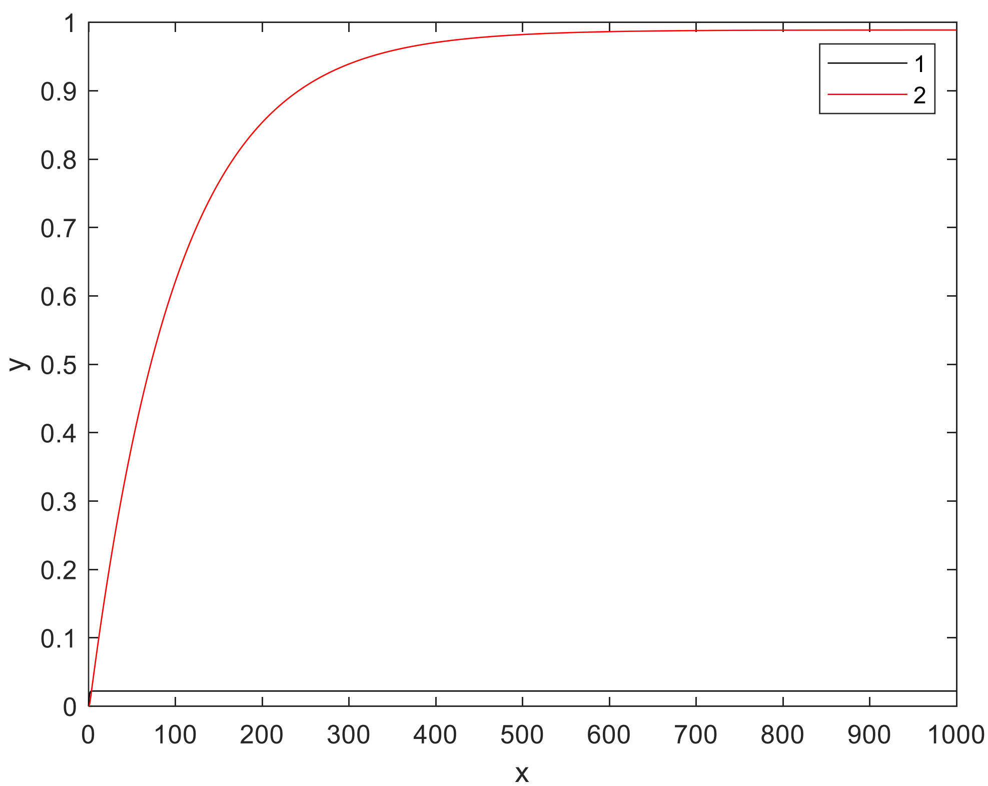
```
>> xm4p01_f24

Ca_f =    0.022236029157890
Cb_f =    0.988836585491254
```

Based on this information, at 1000 seconds, the concentration of A is 0.0222 mol/l and the concentration of B is 0.9888 mol/l.

If I repeat the calculation with n = 10,000 time steps, I get the following result, which is the same to our desired tolerance.

```
Ca_f =    0.022236029157890
Cb_f =    0.988836585491292
```

The plot of the transient behavior looks like this:



Problem 2. System of Algebraic Equations (8 points)

We allow the reactor in problem 1 to reach steady state. In this case, time derivatives in problem 1 become zero. Thus, the ODEs in problem 1 become algebraic equations:

$$0 = \frac{F_{in}}{V} C_{A,in} - \frac{F_{out}}{V} C_A - 2r$$

$$0 = \frac{F_{in}}{V} C_{B,in} - \frac{F_{out}}{V} C_B + r$$

All parameters remain the same as in problem 1.

(a) Is this system of equations linear or nonlinear?
(b) What is the appropriate technique to solve this system of equations?
(c) Determine the steady values of the concentration of A, C_A, and the concentration of B, C_B.
(d) Explain the relationship between the answer for problem 2(c) and problem 1(d).

Solution:

(a) Is this system of equations linear or nonlinear?

This system of equations is non-linear in the concentration of A, C_A.

(b) What is the appropriate technique to solve this system of equations?

I would use the multivariate Newton Raphson method with numerical approximations to the derivatives to solve a set of non-linear algebraic equations,

$$f_1(C_A, C_B) = \frac{F_{in}}{V} C_{A,in} - \frac{F_{out}}{V} C_A - 2r = 0$$

$$f_2(C_A, C_B) = \frac{F_{in}}{V} C_{B,in} - \frac{F_{out}}{V} C_B + r = 0$$

(c) Determine the steady values of the concentration of A, C_A, and the concentration of B, C_B.

I wrote a script in the file xm4p02_f24.m

```
function f = funkeval(x)
n = max(size(x));
f = zeros(n,1);
%
CA = x(1);
CB = x(2);
CAin = 2.0; % mol/liter
CBin = 0.0; % mol/liter
```

```
k = 20.0; % liter/mol/sec
V = 100.0; % liter
Fin = 1.0; % liter/sec
Fout = 1.0; % liter/sec
rate = k*CA*CA;
dCAdt = 1/V*(CAin*Fin - CA*Fout) -2*rate;
dCBdt = 1/V*(CBin*Fin - CB*Fout) + rate;
f(1) = dCAdt;
f(2) = dCBdt;
```

I executed the script and received the following output:

```
>> xm4p02_f24
iter =    1, err =  6.46e-03 f =  2.97e-03
 iter =    2, err =  9.79e-05 f =  1.76e-04
 iter =    3, err =  2.71e-07 f =  4.85e-07

x =    0.0222    0.9889
err =   2.7126e-07
f =   4.8526e-07
```

Based on this information, the steady state concentration of A is 0.0222 mol/l and the steady state concentration of B is 0.9889 mol/l.

(d) The concentrations from problem 2(c) and problem 1(d) are nearly the same because the system in problem 1(d) has almost reached steady state by 1000 second, as evidenced by the very small change in the concentrations with respect to time as shown in the plot reported in problem 1(c).

Problem 3. Numerical Integration (4 points)

Consider the reactor described in problem 1. The total amount of component B, N_B, produced in the first 1000 seconds is given by

$$N_B = \int_{t=0}^{t=1000} F_{out}\left(\frac{dC_B}{dt}\right)dt$$

Substituting in the ODE for C_B and the definition of the reaction rate, r, given in problem 1, yields

$$N_B = \int_{t=0}^{t=1000} F_{out}\left(\frac{F_{in}}{V}C_{B,in} - \frac{F_{out}}{V}C_B + kC_A^2\right)dt$$

Thus knowing the values of C_A and C_B as a function of time (from the solution of problem 1), we can compute the total moles of B produced through numerical integration. For the purposes of this exam, the entire integrand has been calculated from C_A and C_B and is given as a function of time in the file, https://utkstair.org/clausius/docs/mse301/data/xm4p03_f24.txt, on the course website.

(a) What is the appropriate numerical technique to evaluate this integral?
(b) How many moles of B were produced in the first thousand second of reactor operation?

Solution:

(a) What is the appropriate numerical technique to evaluate this integral?

To numerically integrate data, I would use the trapezoidal rule.

(b) How many moles of B were produced in the first thousand second of reactor operation?

I wrote a script in the file xm4p02_f24.m

```
cclear all;
close all;
% perform integration of data by Trapezoidal method
datamat = [0      0
1     0.00787835
2     0.030714499
3     0.066694513
... data omitted for brevity ...
998   0.885329787
999   0.885329783
1000 0.885329778];

n = length(datamat);
```

```
integral = 0.0;
for i = 2:1:n
    base = datamat(i,1) - datamat(i-1,1);
    area = 0.5*base*(datamat(i,2) + datamat(i-1,2));
    integral = integral + area;
end
integral
```

I executed the script and received the following output:

```
>> xm4p03_f24

integral =     8.765470076049994e+02
```

Therefore, during the first 1000 seconds of operation, the reactor generated 876.5 moles of B.

Problem 4. Project Question. (4 points)

Regarding the course project, answer the following questions.

(a) Which project did you work on?
(b) In your opinion, what was the most significant result of your project?