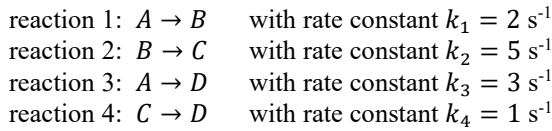


Exam III Solutions  
Administered: Monday, November 2, 2020  
22 points

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. (12 points)**

Consider an isothermal flow reactor with a volume,  $V = 10$  liters, in which the following set of elementary reactions take place



The inlet flow rates are given by

$$F_{A,in} = F_{B,in} = 2 \frac{\text{mole}}{\ell \cdot \text{s}} \quad \text{and} \quad F_{C,in} = F_{D,in} = 0 \frac{\text{mole}}{\ell \cdot \text{s}}$$

The outlet flow rates are given by

$$F_{A,out} = \hat{F}_{out} C_A, F_{B,out} = \hat{F}_{out} C_B, F_{C,out} = \hat{F}_{out} C_C \text{ and } F_{D,out} = \hat{F}_{out} C_D \frac{\text{mole}}{\ell \cdot \text{s}}$$

where  $\hat{F}_{out} = 4 \text{ s}^{-1}$  and concentrations are measured in moles/liter.

The steady state mass balances are

accumulation = in – out + generation – consumption

$$\begin{aligned} 0 &= F_{A,in} - \hat{F}_{out} C_A - k_1 C_A - k_3 C_A \\ 0 &= F_{B,in} - \hat{F}_{out} C_B + k_1 C_A - k_2 C_B \\ 0 &= F_{C,in} - \hat{F}_{out} C_C + k_2 C_B - k_4 C_C \\ 0 &= F_{D,in} - \hat{F}_{out} C_D + k_3 C_A + k_4 C_C \end{aligned}$$

- Write this set of equations in matrix notation,  $\underline{Ax} = \underline{b}$ . Identify all three quantities,  $\underline{A}$ ,  $\underline{x}$  and  $\underline{b}$ .
- Calculate the determinant of  $\underline{A}$ .
- Calculate the rank of  $\underline{A}$ .
- Calculate the rank of  $\underline{A}|\underline{b}$ .
- How many solutions are there to this problem?
- Calculate the steady state concentrations of A, B, C and D in this reactor under these conditions.

**Solution:**

- Write this set of equations in matrix notation,  $\underline{Ax} = \underline{b}$ . Identify all three quantities,  $\underline{A}$ ,  $\underline{x}$  and  $\underline{b}$ .

I rearranged the equations to put constants on the right hand side and grouped the coefficients by variable.

$$\begin{aligned} (\hat{F}_{out} + k_1 + k_3) C_A &= F_{A,in} \\ -k_1 C_A + (\hat{F}_{out} + k_2) C_B &= F_{B,in} \end{aligned}$$

$$\begin{aligned} -k_2 C_B + (\hat{F}_{out} + k_4) C_C &= F_{C,in} \\ -k_3 C_A - k_4 C_C + \hat{F}_{out} C_D &= F_{D,in} \end{aligned}$$

$$\underline{A} = \begin{bmatrix} \hat{F}_{out} + k_1 + k_3 & 0 & 0 & 0 \\ -k_1 & (\hat{F}_{out} + k_2) & 0 & 0 \\ 0 & -k_2 & (\hat{F}_{out} + k_4) & 0 \\ -k_3 & 0 & -k_4 & \hat{F}_{out} \end{bmatrix}, \underline{x} = \begin{bmatrix} C_A \\ C_B \\ C_C \\ C_D \end{bmatrix}, \underline{b} = \begin{bmatrix} F_{A,in} \\ F_{B,in} \\ F_{C,in} \\ F_{D,in} \end{bmatrix}$$

For the remaining parts of this problem, I wrote the following Matlab script, xm3p01\_2015.m

```
clear all;
k1 = 2;
k2 = 5;
k3 = 3;
k4 = 1;
FAin = 2;
FBin = 2;
FCin = 0;
FDin = 0;
Fout = 4;
A = [(Fout+k1+k3) 0 0 0
      -k1 (Fout+k2) 0 0
      0 -k2 (Fout+k4) 0
      -k3 0 -k4 Fout]
b = [FAin; FBin; FCin; FDin]
detA = det(A)
rankA = rank(A)
Ab = [A,b];
rankAb = rank(Ab)
invA = inv(A)
x = invA*b
```

To execute the script, at the Matlab command prompt, I typed

```
>> xm3p01_2020
```

which yielded the following result:

```
A =
     9     0     0     0
    -2     9     0     0
     0    -5     5     0
    -3     0    -1     4
```

```
b =
     2
     2
     0
     0
```

```
detA = 1620
```

```
rankA = 4
```

```
rankAb = 4
```

```
invA =
    0.1111    0    0    0
    0.0247    0.1111    0    0
    0.0247    0.1111    0.2000    0
    0.0895    0.0278    0.0500    0.2500
```

```
x =
    0.2222
    0.2716
    0.2716
    0.2346
```

(b) Calculate the determinant of  $\underline{A}$ .

The determinant of  $\underline{A}$  is 1620.

(c) Calculate the rank of  $\underline{A}$ .

Because the determinant of  $\underline{A}$  is non-zero, you know that the rank of  $\underline{A}$  must be full,  $n=4$ . The Matlab calculation confirms this.

(d) Calculate the rank of  $\underline{A}|\underline{b}$

Because the rank of  $\underline{A}$  is 4, you know that the rank of  $\underline{A}|\underline{b}$  must also be 4. The Matlab calculation confirms this.

(e) How many solutions are there to this problem?

Because the determinant of  $\underline{A}$  is non-zero, there is a one solution.

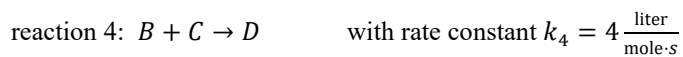
(f) Calculate the steady state concentrations of A, B, C and D in this reactor under these conditions.

We solved for the steady state concentrations in the x vector.

$$\underline{x} = \begin{bmatrix} C_A \\ C_B \\ C_C \\ C_D \end{bmatrix} = \begin{bmatrix} 0.2222 \\ 0.2716 \\ 0.2716 \\ 0.2346 \end{bmatrix} \text{ mole/liter}$$

**Problem 2. (10 points)**

If we rework problem 1 with the single change that we replace reaction 4 with



Then the steady state mass balances become

accumulation = in – out + generation -consumption

$$0 = F_{A,in} - \hat{F}_{out} C_A - k_1 C_A - k_3 C_A$$

$$0 = F_{B,in} - \hat{F}_{out} C_B + k_1 C_A - k_2 C_B - k_4 C_C C_B$$

$$0 = F_{C,in} - \hat{F}_{out} C_C + k_2 C_B - k_4 C_C C_B$$

$$0 = F_{D,in} - \hat{F}_{out} C_D + k_3 C_A + k_4 C_C C_B$$

- (a) Is this system of equation linear or nonlinear?
- (b) What numerical technique is appropriate for solving this problem?
- (c) Solve for the steady state concentrations. (6 points)

**Solution:**

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

This system of equations is nonlinear because of the  $k_4 C_C C_B$  term in the third and fourth equation.

(b) What numerical technique is appropriate for solving this problem?

An appropriate technique for solving a system of nonlinear algebraic equations is the multivariate Newton-Raphson method with numerical approximations to the derivatives.

(c) Solve for the steady state concentrations. (6 points)

For this problem, I wrote the following Matlab script, xm3p02\_2020.m. The initial guess comes from the solution of the linear version in problem 1.

```
clear all;
x0 = [0.2222
      0.2716
      0.2716
      0.2346];
tol = 1.0e-6;
iprint = 1;
[x,err,f] = nrndn(x0,tol,iprint)
```

In the input subroutine for nrndn.m, I put the following code

```
function f = funkeval(x)
%
% these two lines force a column vector of length n
%
n = max(size(x));
f = zeros(n,1);
%
% enter the functions here
%
CA = x(1);
CB = x(2);
CC = x(3);
CD = x(4);
k1 = 2;
k2 = 5;
k3 = 3;
k4 = 1;
FAin = 2;
FBin = 2;
FCin = 0;
FDin = 0;
Fout = 4;
f(1) = FAin - (Fout+k1+k3)*CA;
f(2) = FBin + k1*CA - (Fout+k2)*CB - k4*CC*CB;
f(3) = FCin + k2*CB - Fout*CC - k4*CC*CB;
f(4) = FDin + k3*CA + k4*CC*CB - Fout*CD;
```

To execute the script, at the Matlab command prompt, I typed

```
>> xm3p02_f20
```

which yielded the following result:

```
iter =    1, err = 3.03e-02 f = 1.45e-01
iter =    2, err = 6.85e-05 f = 2.84e-04
iter =    3, err = 7.51e-10 f = 3.11e-09
```

```
x =
  0.2222
  0.2626
  0.3080
  0.1869
```

```
err = 7.5125e-10
```

```
f = 3.1098e-09
```

The error indicates that the value converged. So the steady state concentrations are

$$\underline{x} = \begin{bmatrix} C_A \\ C_B \\ C_C \\ C_D \end{bmatrix} = \begin{bmatrix} 0.2222 \\ 0.2626 \\ 0.3080 \\ 0.1869 \end{bmatrix} \text{ mole/liter}$$