# Birla Institute of Technology and Science, Pilani

Semester I Session: 2016-2017

**CHE G523 Mathematical methods in chemical engineering**

Mid-semester Test (Closed Book)

Date: 08/10/2016 Maximum Marks: 25

Duration: 90 minutes Weightage: 25 %

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**Q 1** **[4]**

Consider a mixture containing a compounds $H_2O$, $C_2H_4$, $C_2H_5OH$, $C_4H_{10}O$, and $CH_4$. The elemental matrix can be formed as

| Elements\Species | $H_2O$ | $C_2H_4$ | $C_2H_5OH$ | $C_4H_{10}O$ | $CH_4$ |
|---|---|---|---|---|---|
| H | 2 | 4 | 6 | 10 | 4 |
| C | 0 | 2 | 2 | 4 | 1 |
| O | 1 | 0 | 1 | 1 | 0 |

Consider an elemental vector as a vector defined by any column of the elemental matrix.

a) Find out the maximum number of independent chemical reactions i.e. linear combination between elemental vectors of elemental matrix.
b) Find out the orthonormal basis of the linearly independent set obtained from the elemental matrix.

**Q 2** **[7]**

Solve for $y(t)$, the altitude of rocket. The differential equation is given by $y'' = -g + 0.1\,y$.

- $g = 9.8$ m/sec$^2$ (acceleration due to gravity)
- $y(0) = 0$ (launch from ground)
- $y(5) = 40$ (fireworks explode after 5 seconds, we want them 40 m off ground)

Using finite difference approximation with $\Delta t = 1.25$ second, find the y ($t$). What should be the launch velocity?

**Q 3** **[7]**

An irreversible first order reaction is taking place in an isothermal tubular reactor with axial mixing. The governing equation with boundary conditions are given below:

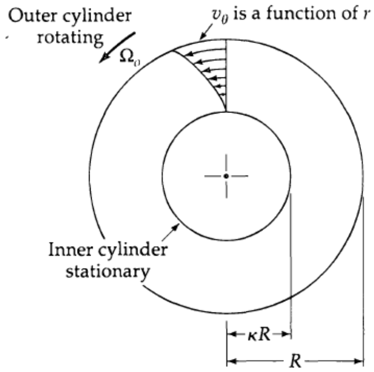
$$\frac{1}{Pe}\frac{\partial^2 w_A}{\partial x^2} - \frac{\partial w_A}{\partial x} - D_A w_A = 0 \qquad \text{where } Pe = 6 \text{ and } Da = 8/3$$

At $x = 0$; $w_A = 1.0$; At $x = 1$; $\frac{\partial w_A}{\partial x} = 0$

Apply the shooting method and solve the set of IVP using eigne value approach. Perform onely one complete iteration. State the assumptions clearly with proper justification.

**Q 4** **[7]**

There is a steady, tangential, laminar flow in the annular region between the two coaxial cylinders a shown in the figure below.




The governing equation is given by $\frac{\partial^2 v_\theta}{\partial r^2} - \frac{1}{r}\frac{\partial v_\theta}{\partial r} - \frac{v_\theta}{r^2} = 0$. The boundary conditions are:

At $r = kR$, $v_\theta = 0$; At $r = R$, $v_\theta = \Omega R$.

Apply orthogonal collocation method with N = 4 and convert the differential equations in a set of algebraic equations.

The OC matrices for N = 4 are given below.

X=

| |
|---|
| 0 |
| 0.0694 |
| 0.33 |
| 0.67 |
| 0.9306 |
| 1 |

A=

| | | | | | |
|---|---|---|---|---|---|
| -21.007 | 23.636 | -3.678 | 1.811 | -1.763 | 1.000 |
| -8.784 | 6.671 | 2.839 | -1.232 | 1.161 | -0.655 |
| 2.497 | -5.186 | 0.769 | 2.941 | -2.250 | 1.230 |
| -1.230 | 2.250 | -2.941 | -0.769 | 5.186 | -2.497 |
| 0.655 | -1.161 | 1.232 | -2.839 | -6.671 | 8.784 |
| -1.000 | 1.763 | -1.811 | 3.678 | -23.636 | 21.007 |

B=

| | | | | | |
|---|---|---|---|---|---|
| 220.088 | -311.867 | 132.221 | -70.695 | 70.266 | -40.013 |
| 135.949 | -183.121 | 59.670 | -20.539 | 18.189 | -10.149 |
| -11.293 | 31.828 | -36.967 | 21.824 | -10.954 | 5.562 |
| 5.562 | -10.954 | 21.824 | -36.967 | 31.828 | -11.293 |
| -10.149 | 18.189 | -20.539 | 59.670 | -183.121 | 135.949 |
| -40.013 | 70.266 | -70.695 | 132.221 | -311.867 | 220.088 |

Ans 1

**Example 3.9:** Maximum number of independent chemical reactions.

Consider a mixture containing the compounds $H_2O$, $C_2H_4$, $C_2H_5OH$, $C_4H_{10}O$ and $CH_4$. Number the compounds in the order given here and the elements such that hydrogen is number 1, carbon number 2 and oxygen number 3. The elemental matrix becomes

| | $H_2O$ | $C_2H_4$ | $C_2H_5OH$ | $C_4H_{10}O$ | $CH_4$ |
|---|---|---|---|---|---|
| $H$ | 2 | 4 | 6 | 10 | 4 |
| $C$ | 0 | 2 | 2 | 4 | 1 |
| $O$ | 1 | 0 | 1 | 1 | 0 |

Specifying a chemical reaction between any of the components in the system is equivalent to specifying a linear combination between columns of this matrix. For instance, the reaction $H_2O + C_2H_4 \leftrightarrow C_2H_5OH$, is equivalent to the linear combination $v_1 + v_2 - v_3 = 0$, where $v_n$ is the vector defined by the $n$'th column of the elemental matrix. One might say that $H_2O$, $C_2H_4$ and $C_2H_5OH$ are linearly

dependent compounds and the problem is to find a set of linearly independent compounds from which all other compounds are formed through chemical reactions. The maximum number of linearly independent compounds or columns is the rank of the elemental matrix. Doing standard row operations, the elemental matrix is reduced to the from

| | $H_2O$ | $C_2H_4$ | $C_2H_5OH$ | $C_4H_{10}O$ | $CH_4$ |
|---|---|---|---|---|---|
| $H$ | 1 | 2 | 3 | 5 | 2 |
| $C$ | 0 | 1 | 1 | 2 | $\frac{1}{2}$ |
| $O$ | 0 | 0 | 0 | 0 | 1 |

The rank is 3. Thus, one can specify 3 compounds that can form all remaining compounds in the system through chemical reactions. Since there are 5 compounds in the system or equivalently 5 columns in the elemental matrix, $5 - 3 = 2$ reactions must be specified. One cannot randomly pick the 3 compounds from which the remaining compounds are formed, the 3 compounds must be linearly independent. Inspection of the reduced matrix shows that columns 1, 2 and 5 in the non-reduced matrix are linearly independent and the linearly independent compounds can therefore be picked as $H_2O$, $C_2H_4$ and $CH_4$. Through chemical reactions, these three compounds can form all other compounds in the mixture.

To specify the reactions needed to form the remaining compounds, write the

To specify the reactions needed to form the remaining compounds, write the columns of the remaining compounds (taken from the elemental matrix in non-reduced form as linear combinations of the columns that correspond to the 3 linearly independent compounds. Thus $v_3 = v_1 + v_2$ which represents the reaction

$$C_2H_5OH \leftrightarrow H_2O + C_2H_4$$

and $v_4 = v_1 + 2v_2$ which represents

$$C_4H_{10}O \leftrightarrow H_2O + 2C_2H_4$$

Thus, given the concentrations of $CH_4$, $H_2O$ and $C_2H_4$, all other equilibrium concentrations can be found. To be a bit more concrete: Assume we mix $M_{0,CH_4}$ moles of $CH_4$, $M_{0,H_2O}$ moles of $H_2O$ and $M_{0,C_2H_4}$ in a vessel with volume $V$. What are the concentrations after equilibrium has been reached?

The concentration of the inert is trivial

$$C_{CH_4} = \frac{M_{0,CH_4}}{V}$$

Four equations are needed to find the remaining four concentrations. The equilibrium constants of the two reaction we determined above provide two equations

$$\frac{C_{H_2O}C_{C_2H_4}}{C_{C_2H_5OH}} = K_1; \qquad \frac{C_{H_2O}C^2_{C_2H_4}}{C_{C_4H_{10}O}} = K_2$$

The stoichiometry of the reactions provide 2 more

$$M_{H_2O} = M_{0,H_2O} - M_{C_2H_5OH} - M_{C_4H_{10}O} \;\Rightarrow$$





$$C_{H_2O} = C_{0,H_2O} - C_{C_2H_5OH} - C_{C_4H_{10}O}$$

$$M_{C_2H_4} = M_{0,C_2H_4} - M_{C_2H_5OH} - 2M_{C_4H_{10}O} \;\Rightarrow$$

$$C_{C_2H_4} = C_{0,C_2H_4} - C_{C_2H_5OH} - 2C_{C_4H_{10}O}$$

All that remains is to solve the last four equations for the four unknown concentrations.