Ref. No.: Ex/ChE/T/412/2019

B.E. CHEMICAL ENGINEERING FOURTH YEAR FIRST SEMESTER EXAMINATION 2019

MATHEMATICAL MODELING IN CHEMICAL ENGINEERING

Full Marks: 100

Answer Question No.1 and any four from the rest

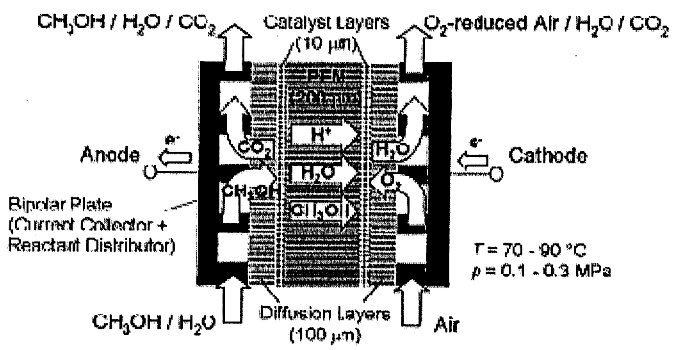
Time 3 hours

Assume any missing data

All symbols have usual significance, if not stated otherwise

1. The reaction scheme for the direct methanol fuel cell is given below (Ref. Chemical Engineering Science 56 (2001) p.333-341)

Anode:	$CH_3OH(l) + H_2O(l)$	$\xrightarrow{Pt/Ru}$	$CO_2(g) + 6H^+ + 6e^-$	$U^{0,25°C}_{CH_3OH \to CO_2} = 0.02$ V
Cathode:	$3/2\, O_2(g) + 6H^+ + 6e^-$	$\xrightarrow{Pt}$	$3H_2O(l)$	$U^{0,25°C}_{O_2 \to H_2O} = 1.23$ V
Overall:	$CH_3OH(l) + 3/2\, O_2(g)$	$\longrightarrow$	$CO_2(g) + 2H_2O(l)$	$U^{0,25°C}_{cell} = 1.21$ V



Reaction mechanisms are provided below:

(R1) $3Pt + CH_3OH \rightleftharpoons Pt_3 - COH + 3H^+ + 3e^-$

(R2) $3Ru + 3H_2O \rightleftharpoons 3Ru - OH + 3H^+ + 3e^-$

(R3) $Pt_3 - COH + 2Ru - OH \rightleftharpoons Pt - COOH + H_2O + 2Pt + 2Ru$

(R4) $Pt - COOH + Ru - OH \rightleftharpoons CO_2 - H_2O + Pt + Ru$

(R5) $3/2O_2 + 6H^+ + 6e \rightleftharpoons 3H_2O$

Develop the model equations stating the phenomena and assumptions under your consideration. 12

2. In a packed bed tubular reactor of length L and unit cross sectional area, a reactant enters with a superficial velocity v. The reactor is packed with catalyst particles. Te reaction is of zero order with respect to the reactant concentration. Develop the mathematical model stating all assumptions and information flow diagram to predict the steady state temperature profile along the reactor length through analytical and numerical methods. Because of the effect of catalysts the thermal

dispersion in the axial direction cannot be neglected. The boundary conditions are as follows: At z=0, T=T0; at z=L, $\frac{dT}{dz} = 0$. 22

3. The mole balance equation of gaseous reactant A reacting with liquid reactant B during diffusion through liquid is $\frac{\partial C_A}{\partial t} = D_{AB}\frac{\partial^2 C_A}{\partial z^2} - kC_A$.

The initial and boundary conditions are:

$$C_A(z,0) = 0 \quad for \quad z > 0$$
$$C_A(0,t) = C_{A0} \quad for \quad t \geq 0$$
$$\frac{\partial C_A}{\partial z}(L,t) = 0 \quad for \quad t \geq 0$$

Describe the algorithm to determine the axial concentration profile at different time using Crank - Nicolson implicit method of solution. 22

4. The governing equation for steady state two-dimensional conductive heat transfer is as follows: $\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = 0$ .The boundary conditions are : T(x,0)=T1; T(x,1)=T2 0≤x≤1 and T(0,y)=T3; T(1,y)=T4 0≤y≤1. Use orthogonal collocation technique to find the temperature profile in the x-y plane describing the algorithm of the solution method. 22

5. Population dynamics of two competing species are as follows:

$$\frac{dx}{dt} = x(\alpha_1 - \beta_1 x - \gamma_1 y)$$
$$\frac{dy}{dt} = y(\alpha_2 - \beta_2 y - \gamma_2 x)$$

Analyze the stability of all possible steady states using linear stability analysis. (x and y stand for the concentrations of species X and Y respectively and $\alpha_1, \alpha_2, \beta_1, \beta_2, \gamma_1, \gamma_2$ are constants). 22

6. For the non-isothermal CSTR(Figure1) determine the condition for Hopf bifurcation with respect to Damkohler number,Da.

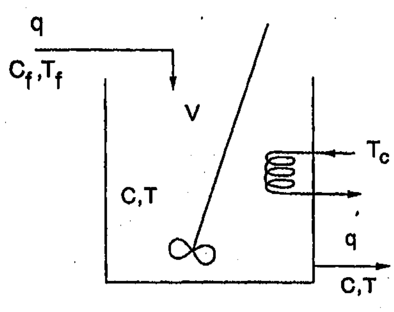


Figure 1

Using dimensionless variables,

$$x_1 = \frac{T - T_f}{T_f}\frac{E}{R_g T_f}, \qquad x_2 = \frac{C_f - C}{C_f}, \qquad \theta = \frac{V}{q}, \qquad \tau = \frac{t}{\theta}$$

$$x_{1c} = \frac{T_c - T_f}{T_f}\frac{E}{R_g T_f}, \qquad \gamma = \frac{E}{R_g T_f}, \qquad \mathrm{Da} = k_0 e^{-\gamma}\theta$$

$$B = \frac{(-\Delta H)C_f}{C_p \rho T_f}\frac{E}{R_g T_f}, \qquad \delta = \frac{Ua}{qC_p\rho}$$

The dynamic equations are as follows:

$$\frac{dx_1}{d\tau} = -x_1 - \delta(x_1 - x_{1c}) + B\,\mathrm{Da}(1 - x_2)\exp\left(\frac{x_1}{1 + x_1/\gamma}\right)$$

$$\frac{dx_2}{d\tau} = -x_2 + \mathrm{Da}(1 - x_2)\exp\left(\frac{x_1}{1 + x_1/\gamma}\right)$$

Consider γ to be much greater than x1.

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