BIRLA INSTITUTE OF TECHNOLOGY AND SCIENCE, PILANI

SECOND SEMESTER 2017-2018

CHE F418 Modeling and Simulation in Chemical Engineering

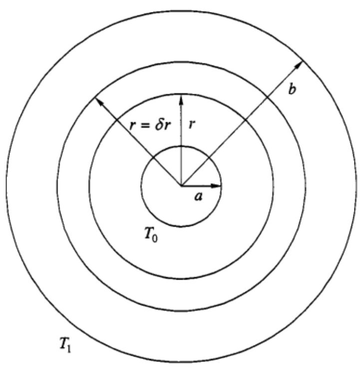
Comprehensive Exam (Close Book) Date: 09.05. 2018

Duration: 8:00 AM – 11:00 AM Maximum Marks: 80

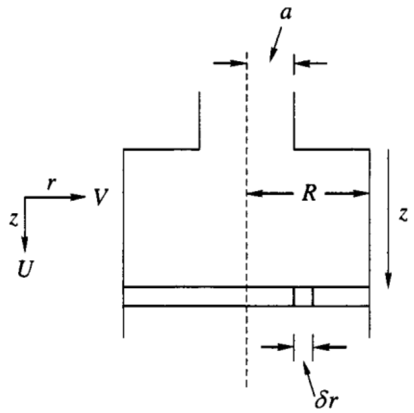
Note: *State your assumptions clearly* and ***check the mathematical consistency*** of a model if necessary

1. An irreversible, exothermic reaction is carried out in a single perfectly mixed variable hold-up CSTR. The reaction is n^{th}-order in reactant A and has a heat of reaction λ (kJ/ mol of A reacted). Negligible heat losses and constant densities are assumed. To remove the heat of reaction, a cooling jacket surrounds the reactor. Cooling water is added to the jacket at a volumetric flow rate F_J and with an inlet temperature of T_{J0}. The volume of water in the jacket V_J is constant. The mass of the reactor metal walls is assumed negligible. The outlet flow is controlled by a ***P* controller**. Develop a mathematical model for the following
   a. Case A. Perfectly mixed cooling jacket
      Case B. Plug flow cooling jacket
   b. Write MATLAB code for solving case (A) modeling equations (5 + 5 = 10 M)

2. Two concentric cylindrical metallic shells are separated by a solid material. If the two metal surfaces are maintained at different temperatures, what is the steady state temperature distribution within the separating material? (10 M)



3. Liquid is distributed within a central core of radius *a* with velocity U_0 and flows through a packed column of radius *R.* At the position *(r,* z), the horizontal and vertical components of velocity are *V* and ***U.*** It is also given that $V = -D\left(\partial U/\partial r\right)$ where *D* is a constant characteristic of the liquid and the packing material. Obtain a mathematical model in the differential form for *U* at steady state. (10 M)



4. A chemical process is represented by the following set of equations,

$$f1(x1, x2, x3, x6) = 0\ , f2(x2, x5, x6) = 0, f3(x1, x2, x3, x4) = 0; f4(x4) = 0,$$

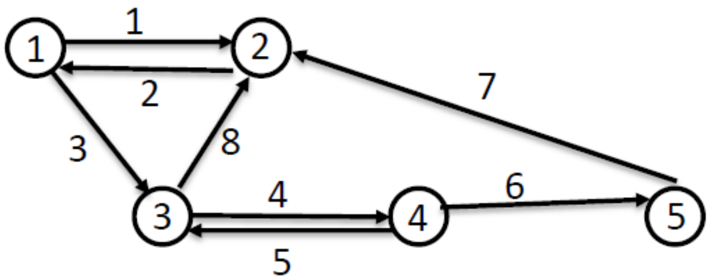
$$f5(x2, x4) = 0, \quad f6(x6, x7, x8) = 0, \quad f7(x3, x6) = 0, f8(x7, x8) = 0$$

Determine the following: (a) Associated incidence matrix with output-set encircled.

(b) Digraph of the process.

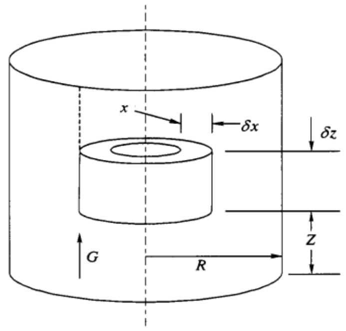
(c) Associated adjacency matrix (3+3+4= 10 M)

5. For the reduced digraph given below (Fig. 12.9), find the following: (a) Signal flow graph. (b) Cut-set using the *Kehat and Shacham* algorithm. (10 M)



6. Using the data given below, obtain a preliminary estimate of the diameter of the tubes to be installed in a fixed bed catalytic reactor which is to be used for the synthesis of vinyl chloride from acetylene and hydrogen chloride. The tubes are to contain mercuric chloride catalyst deposited on 2.54 mm particles of carbon and the heat of the reaction is to be employed to generate steam at 121 ^{o}C for the remainder of the process. To do this, the temperature of the inside surface of the tubes should be constant at 149 ^{o}C. The effective thermal conductivity of the bed, k_e = 6.92 W/m^{2}C, the heat of reaction at bed temperature, ΔH_R = 1.075 x 10^{8} J/ kmol , and the bulk density of the bed, ρ = 288 kg/m^{3}. The rate of reaction is a function of temperature, concentration, and the various adsorption

coefficients, but for the preliminary estimate assume that the rate of reaction can be expressed as $r = r_0(1 + AT)$ where r_o = 0.12, A = 0.024, and T is the temperature in degrees Fahrenheit above a datum of 200°F (93.3 °C). The maximum allowable catalyst temperature to ensure a satisfying life is 252 °C (i.e., T = 252 - 93.3 = 158.7 °C above the datum temperature). (Data: Zeroth Bessel function value = 1.55) (15 M)



T (°C)	0	100	121	141	149	252	93.3
$r \times 10^{-4}$ (kmol/s kg-catalyst)	0.589	2.031	2.33	2.614	2.73	4.214	1.933

7. Using the ***Murthy& Hussain- I*** algorithm for the decomposition of MCN, find the cut-set for the digraph of a process plant (15 M)