Department of Chemical Engineering, IIT Kharagpur

CH49019: CAPE Laboratory Autumn 2021

Assignment 3: Due on September 26, 2021

Email Your Assignment (pdf only) to

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1. Consider an ideal plug flow reactor (PFR) where the following reaction takes place:

   A → Products

   The model of the system and kinetic parameters are given as

$$u\frac{dC_A}{dz} = -\frac{kC_A}{\sqrt{1+K_r C_A^2}}$$

$$k = 2\,\mathrm{s}^{-1}, \quad K_r = 1\,\mathrm{mol}^2/\mathrm{m}^6$$

   The velocity *u* is given by, *u* = *Q/A* where *Q* is inlet volumetric flowrate and *A* is the area of cross-section of the PFR. Consider a PFR with length z = 1m, A = 0.40 m^2, Q = 0.2 m^3/s, C_{A0} = 1 mol/m^3. Determine and PLOT the concentration C_A and conversion (X_A) along the length (*z*) of the PFR.

   (a) Implement 4th order RK method to solve this.

   (b) Compare your results with that obtained using MATLAB function `ode45`

2. Consider the following system of ODE representing autocatalytic reactions. Consider the following initial conditions: *x* = 1, *y* = 0, z = 0.

   (a) Implement 4th order RK method to solve this.

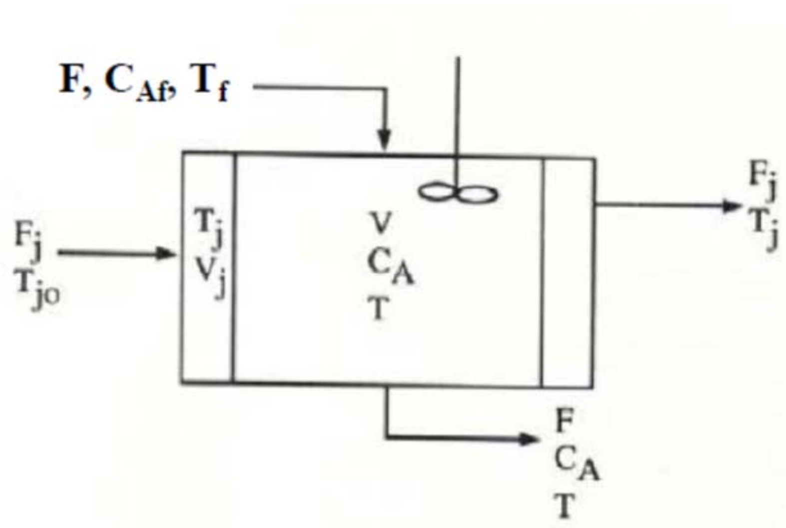
   (b) Compare your results with that obtained using MATLAB function `ode15s`

   (c) Analyse your results.

$$\frac{\mathrm{d}x}{\mathrm{d}t} = -0.04x + 10^4 yz,$$
$$\frac{\mathrm{d}y}{\mathrm{d}t} = 0.04x - 10^4 yz - 3 \times 10^7 y^2,$$
$$\frac{\mathrm{d}z}{\mathrm{d}t} = 3 \times 10^7 y^2.$$

3. Consider again the problem in Assignment – 2. The perfectly mixed CSTR where a first-order exothermic irreversible reaction takes place (r = rate of reaction).

$$A \rightarrow B, \quad r = k_0 e^{\left(\frac{-E}{RT}\right)} C_A$$



Heat generated by reaction is being removed by the jacket fluid. The reactor volume (V) is constant.

<u>Governing Equations</u>:

(Subscript j indicates parameters related to jacket. Symbols carry their usual significance. Refer to the figure.)

$$V\frac{dC_A}{dt} = FC_{Af} - FC_A - rV$$

$$\rho C_p V\frac{dT}{dt} = \rho C_p F\left(T_f - T\right) + \left(-\Delta H\right)Vr - UA\left(T - T_j\right)$$

$$\rho_j C_j V_j\frac{dT_j}{dt} = \rho_j C_j F_j\left(T_{j0} - T_j\right) + UA\left(T - T_j\right)$$

Model Parameter Values:

Parameter	Value	Parameter	Value
F (m^3/h)	1	C_{Af} (kgmol/m^3)	10
V (m^3)	1	UA (kcal/°C h)	150
k_0 (h^{-1})	36×10^6	T_{j0} (K)	298
(-ΔH) (kcal/kgmol)	6500	($\rho_j C_j$) (kcal/m^3 °C)	600
E (kcal/kgmol)	12000	F_j (m^3/h)	1.25
(ρC_p) (kcal/m^3 °C)	500	V_j (m^3)	0.25
T_f (K)	298		

Given the above parameter values, there are three steady states for this system. Perform linear stability analysis for the obtained 3 steady states. If you are not familiar with linear stability analysis, please open any process control/dynamics book.

Here are the key steps for a system with 2 state variables (C_A and reactor temperature, T). You have to extend it for 3 state variables (including jacket temperature as another state variable). Linearize the nonlinear differential equations around the steady states. Introduce deviation variables, and write the linearized ODE as follows (state space model).

$$\begin{bmatrix} \dfrac{dc'_A}{dt} \\ \dfrac{dT'}{dt} \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix}\begin{bmatrix} c'_A \\ T' \end{bmatrix} + \begin{bmatrix} 0 \\ b_2 \end{bmatrix} T'_j$$

The elements of matrix A will be: $$A_{ij} = \left.\frac{\partial f_i}{\partial x_j}\right|_{\text{steady state}}$$

Here f represents differential equation and x represent state variables. If all the eigenvalues of matrix A are negative, the system is stable. If any eigenvalue is positive, the system is unstable.

You can use MATLAB command `eig(A)` to find eigenvalues of matrix A.

Present your results using a table as follows:

Steady State (C_A, T, T_j)	Eigenvalues of Linearized System	Stable/Unstable