Spring Semester CAPE Laboratory 2024 - 2025

Assignment - 3

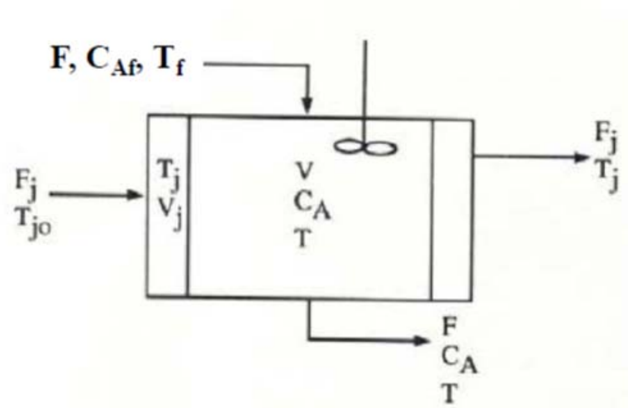
Objective: Solution of Ordinary Differential Equations: Initial Value Problems

This Assignment contains two problems. Solve both the problems.

Problem-1

Consider the perfectly mixed CSTR where a first-order exothermic irreversible reaction takes place (r = rate of reaction). Heat generated by reaction is being removed by the jacket fluid. The reactor volume (V) is constant.

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



Governing Equations:

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

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

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

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

Cont'd

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
($-\Delta H$) (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		

There are three steady states for this system and you should have identified all the three steady states in Assignment 2. Now study the dynamic behaviour of the system by solving the above ODEs as follows.

1. First consider any one steady state that you have obtained. Now obtain 3 different initial conditions by perturbing the selected steady state by 1%, 5%, and 25%. Simulate the system with these three different initial conditions for time t = 0 to t = 50 and plot the three state variables vs time. Does the system go to new steady state? Or does it return to the same steady state? How much time it takes to reach the steady state? **Repeat for other two steady states.**

   Write your own code implementing **4th order Runge Kutta method** and compare your results using MATLAB function `ode45`. Analyse the effect of step size of your RK-4 method on the accuracy of your solution (compare against MATLAB `ode45` function).

2. Comment on the stability of each steady state. Categorise the steady states as stable or unstable steady states.

Cont'd

Problem-2

Consider the following system of first-order ODEs (van der Pol equation rewritten).

$$\frac{dy_1}{dt} = y_2$$

$$\frac{dy_2}{dt} = 1000(1 - y_1^2)y_2 - y_1$$

$$y_1(0) = 2, \;\; y_2(0) = 0, \qquad t = [0 \quad 3000]$$

1. Use your own code (4th order Runge Kutta method) and also the MATLAB function `ode45` to solve this system of ODEs with the given initial conditions. Are you able to solve it? If so, plot y_1 vs time and y_2 vs time.

2. Implement Forward Euler and Backward Euler method for solving the above system of ODEs. Note your observation and plot y_1 vs time and y_2 vs time.

3. Now use the `ode15s` function of MATLAB to solve the same problem and plot y_1 vs time and y_2 vs time.

4. Learn what are "Stiff Differential Equations" and explain the difficulty you faced while solving the given system of ODEs.

----The End ----