CAPE Laboratory

Spring Semester 2025 - 2026

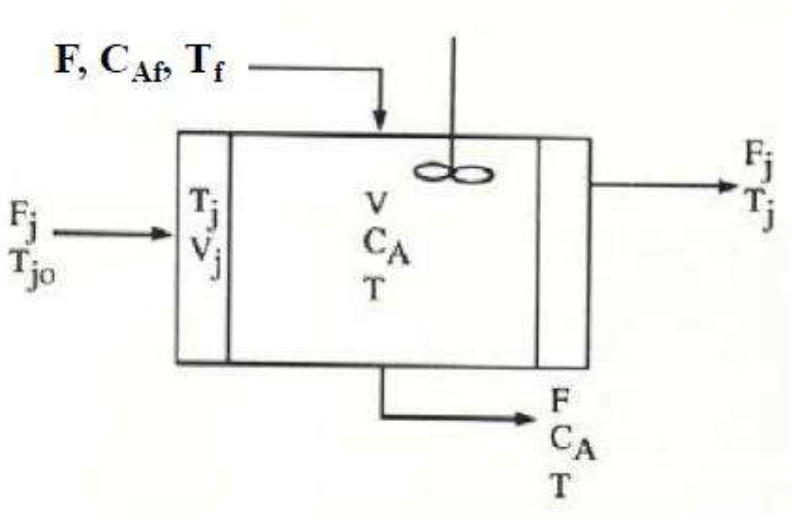
Assignment - 2

Objective: Numerical solution of a system of nonlinear algebraic equations.

Problem - 1:

Consider a perfectly mixed CSTR where a first-order exothermic irreversible reaction takes place (r = rate of reaction).

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



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

Governing Equations:

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

Cont'd

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

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

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

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		

1. There are three steady states for this system. Identify all the steady states by setting LHS of the above ODE to zero and then solving the resulting algebraic equations simultaneously using Newton-Raphson method. Write your own code.

2. Solve the same problem using MATLAB function `fsolve` and compare your results.