Department of Chemical Engineering, IIT Kharagpur

CH49019: CAPE Laboratory Autumn 2021

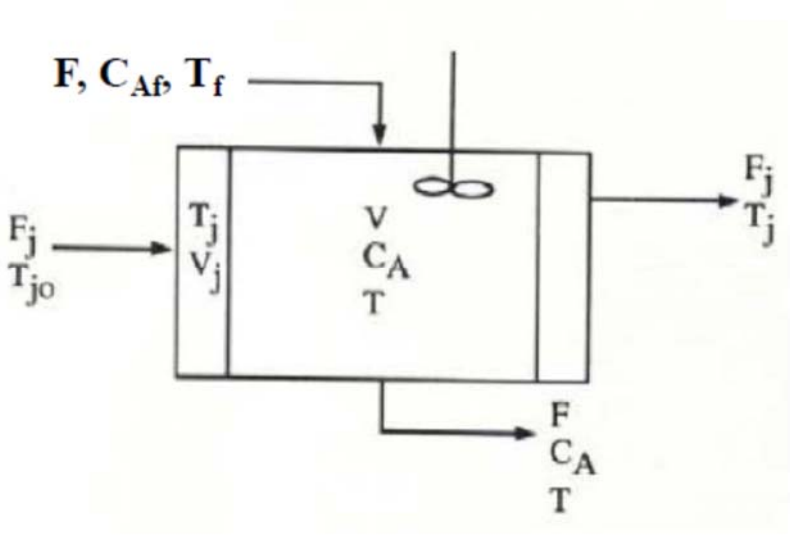
Assignment 2: Due on September 19, 2021

**Email Your Assignment (pdf only) to**

ID-swayamisra@gmail.com **AND** kowsalya123@kgpian.iitkgp.ac.in

1. Consider 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 |
| $k_0$ ($h^{-1}$) | $36\times10^6$ | $T_{j0}$ (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 |
| ($\rho C_p$) (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. Identify all the steady states by setting LHS of the above ODE to zero and then solving the resulting algebraic equations simultaneously for ($C_A$, $T$, $T_j$) by using:

1. Newton's method. Write your own code using any programming language.
2. MATLAB function `fsolve`.
3. Compare your results (all 3 steady states) obtained by two methods in a Table.

**Use of MATLAB function `fsolve`:**

First write the function to describe the 3 algebraic equations and save it as `cstrsteady.m`

```
function F = cstrsteady(x)

F(1) = ....
F(2) = ....
F(3) = ....
```

Next execute the following command:

```
X0 = .... % Initial guess
xout = fsolve(@cstrsteady, X0)
```

`xout` contains the solution (steady state). Note it is a vector with 3 elements.