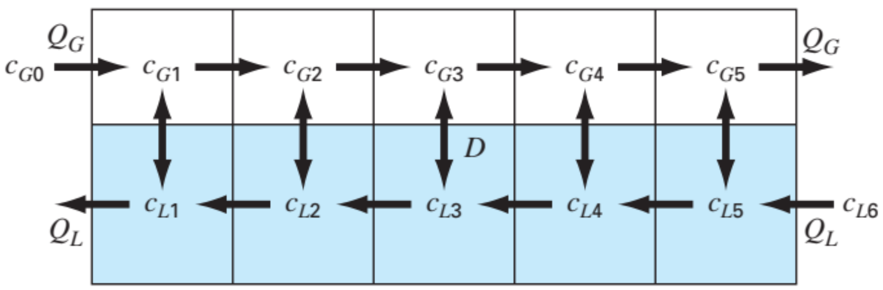
IIT ROPAR
SEMESTER I 2021-22
NUMERICAL SIMULATION LAB (CH230)
Assignment 3   Max Marks: 10

Note: Marks will be awarded for well written codes. Ensure that the files submitted are complete in all respects and only needed to be executed to get the required answers.

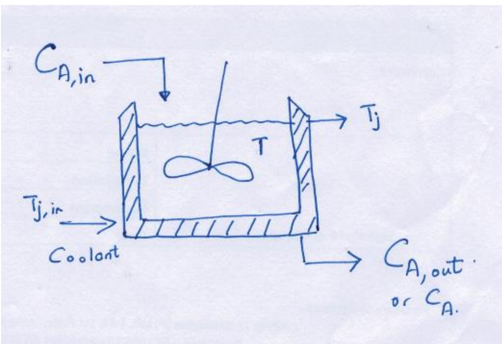
Note: Please write the expressions for the material balances in your MATLAB code as a comment. Codes with no material balances will be awarded zero marks.

1. The figure below depicts a chemical exchange process consisting of a series of reactors in which a gas flowing from left to right is passed over a liquid which is flowing from right to left. The transfer of chemical from the gas into the liquid occurs at a rate that is proportional to the difference between the gas (c_G) and liquid (c_L) concentrations in each reactor. Assuming a proportional constant of D (gas liquid exchange rate), write mass balances for each reactor for the gas and liquid phases. Q_G and Q_L are the gas and liquid flow rates (can be assumed to remain constant across all reactors). Solve for the steady state concentrations in the gas and liquid phase in each reactor given the following: $Q_G=2$; $Q_L=1$; $D=0.8$; $c_{G0}=100$; $c_{L6}=20$ (4M)



Hint: Use the concept of material balances, Input + Generation = Output + Accumulation +Consumption.

2. A first order exothermic reaction A→B takes place in a stirred tank reactor (shown below) provided with a cooling jacket. A coolant flows through this jacket to maintain the temperature inside the reactor to the desired level. The temperature inside the reactor (T) and the exit of the cooling jacket (Tj) and the concentration of A (C_A) inside the reactor at steady state can be obtained by solving the following set of equations. (6M)



$$\frac{F(C_{A,in}-C_A)}{V} - 2kC_A = 0 \qquad (1)$$

$$\frac{F(T_{In}-T)}{V} + 2\frac{(-\Delta H)kC_A}{\rho Cp} - \frac{UA(T-T_j)}{V\rho Cp} = 0 \qquad (2)$$

$$\frac{F_{WS}(T_{j,In}-T)}{V_W} + \frac{UA(T-T_j)}{V_W\rho_W Cp_W} = 0 \qquad (3)$$

Other parameters are given below:

Inlet feed concentration, $C_{A,in}$	1	mol/L
Reactor Volume, V	100	L
Feed Inlet Temperature, T_{in}	275	K
Enthalpy of reaction, ($-\Delta H$)	596619	J/mol
Density of feed, ρ	1	Kg/L
Specific heat capacity of feed, C_p	4200	J/kg.K
Heat Transfer Coefficient, UA	20000*60	J/min .K
Volume of jacket, Vw	10	L
Specific heat capacity of coolant, C_{pw}	4200	J/kg.K
Inlet temperature of coolant, $T_{j,in}$	250	K
Density of coolant, ρ_w	1	kg/L
Inlet feed flow rate, F	120	L/min
Coolant Flow rate, F_{ws}	30	L/min
Reaction rate constant, k	15	min^{-1}

a) Determine the steady state values of C_A,T, Tj. How does the reactor temperature (T) change if the inlet coolant temperature (Tj, in) is varied from 250 K to 315 K. Make a **well labelled** plot of the reactor temperature as a function of the coolant temperature.

b) Assume that the cooling system suddenly fails (UA=0; F_{ws}=0), what would be the new steady state reactor temperature?