Sharif University of Technology

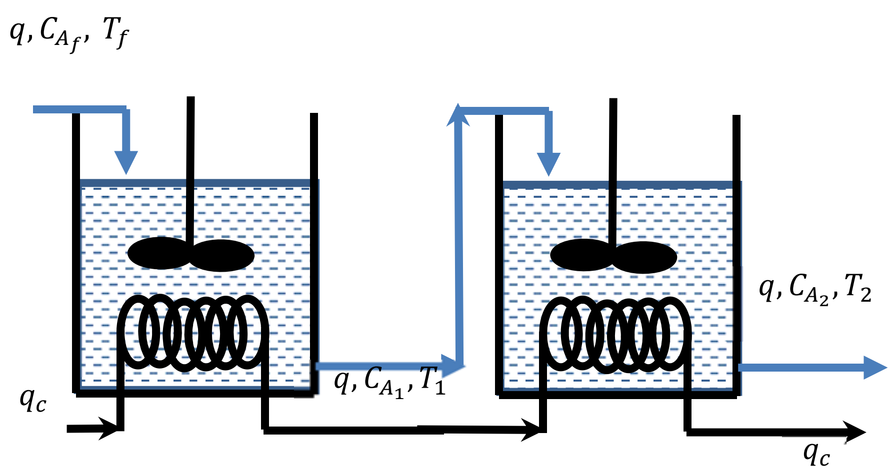
Chemical & Petroleum Eng. Dept.

Advanced Numerical Methods In Chem. Eng.

Fall 2022

Assignment #3

Consider the follwing two CSTR's in series in which a first order exothermic reaction ($A \rightarrow B$) takes place. The simplified mathematical model of this system is also presented by the following four ordinary differential equations. Model parameters of the system along with its operating conditions are given in Table 1. Based on this model you are supposed to:



1. Obtain the open loop response of the system variables (i.e., C_{A1}, T_1, C_{A2},T_2) when each of the inputs (i.e., Feed Flowrate (q), Concentration (C_{A_f}), Temperature (T_f)and Coolant Flowrate (q_c)is perturbed by ±10% step change).
2. Design an optimal PI controller for this system such that outlet concentration of the second reactor is kept at its desired value, by manipulation of coolant flow rate.
3. Evaluate the closed loop behavior of the designed PI controller for both servo and regulatory modes of the system. For servo mode make a ±10% step change in desired value of C_{A_2} while for regulatory mode use the scenario mentioned in part 1.

You should keep in mind that providing the maximum value of the coolant flow rate does not mean that it is constant at this value, it means the value of this variable can be any number from zero to 500 lit./min.

$q = 100\,\frac{lit.}{min.}$	$V_1 = V_2 = 100 lit.$	$\rho = \rho_c = 1000\,\frac{g}{lit.}$	$C_{A_{2ss}} = 0.005\,\frac{mol.}{lit.}$
$C_{A_f} = 1\,\frac{mol.}{lit.}$	$hA_1 = hA_2 = 1.67 \times 10^5\,\frac{j}{min.\,°K}$	$\frac{E}{R} = 10^4\ °K$	
$T_f = 350°K$	$C_p = C_{p_c} = 0.239\,\frac{j}{g°K}$	$k_0 = 7.2 \times 10^{10}\,\frac{1}{min.}$	
$T_{c_f} = 350°K$	$(-\Delta H) = 4.78 \times 10^4\,\frac{j}{mol.}$	$q_{c_{max}} = 500\,\frac{lit.}{min.}$	

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$$
\begin{cases}
\dfrac{dC_{A_1}}{dt} = \dfrac{q}{V_1}\left(C_{A_f} - C_{A_1}\right) - k_0 exp\left(\dfrac{-E}{RT_1}\right) C_{A_1} \\
\dfrac{dT_1}{dt} = \dfrac{q}{V_1}\left(T_f - T_1\right) - \dfrac{k_0(-\Delta H)C_{A_1}}{\rho C_p} exp\left(\dfrac{-E}{RT_1}\right) + \dfrac{\rho_c C_{p_c}}{\rho C_p V_1} q_c \left[1 - exp\left(\dfrac{-hA_1}{\rho_c C_{p_c} q_c}\right)\right]\left(T_{c_f} - T_1\right) \\
\dfrac{dC_{A_2}}{dt} = \dfrac{q}{V_1}\left(C_{A_1} - C_{A_2}\right) - k_0 exp\left(\dfrac{-E}{RT_2}\right) C_{A_2} \\
\dfrac{dT_2}{dt} = \dfrac{q}{V_2}\left(T_1 - T_2\right) - \dfrac{k_0(-\Delta H)C_{A_2}}{\rho C_p} exp\left(\dfrac{-E}{RT_2}\right) + \dfrac{\rho_c C_{p_c}}{\rho C_p V_2} q_c \left[1 - exp\left(\dfrac{-hA_2}{\rho_c C_{p_c} q_c}\right)\right]\left[T_1 - T_2 + exp\left(\dfrac{-hA_1}{\rho_c C_{p_c} q_c}\right)\left(T_{c_f} - T_1\right)\right]
\end{cases}
$$

Good Luck