Design-II lab

Lab 1 - MATLAB functions for Initial Value Ordinary Differential Equations

MATLAB can be used very effectively to solve a single or a system of initial value ordinary differential equations using built-in functions. This week's problem will introduce you to the use of such functions to solve initial value problems of interest to chemical engineering community.

A first order chemical reaction of $A \rightarrow B$ type takes place in two continuous stirred tank reactors (CSTRs) which are connected in series. The contents in the two CSTRs are well mixed but the reactors are not at steady state. The unsteady state mass balance equations for each stirred tank reactor is given as

$$\frac{dCA_1}{dt} = \frac{1}{\tau}(CA_O - CA_1) - kCA_1$$
$$\frac{dCB_1}{dt} = -\frac{1}{\tau}CB_1 + kCA_1$$
$$\frac{dCA_2}{dt} = \frac{1}{\tau}(CA_1 - CA_2) - kCA_2$$
$$\frac{dCB_2}{dt} = \frac{1}{\tau}(CB_1 - CB_2) + kCA_2$$

where CA_O = concentration of A at the inlet of first reactor

CA_1 = concentration of A at the outlet of the first reactor or inlet of the second reactor

CA_2 = concentration of A at the outlet of the second reactor

CB_1 = concentration of B at the outlet of the first reactor

CB_2 = concentration of B in the second reactor

k = the reaction rate constant

τ = residence time for each reactor

(a) Determine the evolutions of concentrations of A and B in both reactors during their first 10 minutes of the operation with the initial concentration of reactant A is given as $CA_O = 20$ mol/lit. Use $k = 0.12$/min and $\tau = 5$ min and assume that the initial conditions of all the other dependent variables are zero.

(b) Determine the steady state concentrations and the corresponding time requirements as functions of k and τ. Choose suitable values of k and τ from the literature.