

University of Alberta  
Department of Chemical Engineering

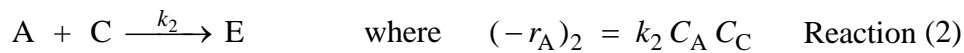
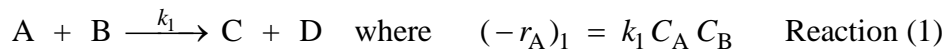
Ch E 345 - Chemical Reactor Analysis

February 10, 2017

Seminar # 4

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1. Consider the following system of series parallel liquid phase reactions occurring in a constant volume transient CSTR.



The rate constants have values of:

$$k_1 = 20 \frac{\text{m}^3}{\text{mol} \cdot \text{s}}, \quad k_2 = 10 \frac{\text{m}^3}{\text{mol} \cdot \text{s}}$$

In this system, the reactant A reacts with one of the products, C, to form a further product, E. Consider a feed stream containing equal concentrations of A and B, such that :

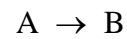
$$C_{A0} = C_{B0} = 1 \times 10^{-3} \frac{\text{mol}}{\text{m}^3}$$

The space time for the reactor is to be 100 seconds. At time zero, the CSTR contains the reactants A and B in an inert solvent with concentrations:

$$C_{A0} = 1 \times 10^{-3} \frac{\text{mol}}{\text{m}^3}, \quad C_{B0} = 5 \times 10^{-4} \frac{\text{mol}}{\text{m}^3}$$

Plot the outlet concentrations of all of the species as a function of time, and calculate the steady state values outlet concentrations.

2. A semi-batch reactor has an inlet feed stream and no effluent stream. A liquid reaction occurs in the reactor:



$$(-r_A) = k C_A \quad k = 1 \times 10^{-3} \text{ s}^{-1}$$

The reactor initially contains  $0.1 \text{ m}^3$  of a solution containing  $1000 \text{ mol/m}^3$  of A . The feed stream flows at  $0.001 \text{ m}^3/\text{s}$  with a concentration of A of  $1000 \text{ mol/m}^3$ . Calculate the number of moles of A and B in the reactor after 900 seconds has passed.

### Solution to Problem 1

The reactor is transient, and it is necessary to write the transient mole balance for each species.

The general mole balance equation for a constant volume CSTR is:

$$F_{j0} - F_{jE} - (-r_j)_E V = V \frac{dC_j}{dt}$$

For a constant density system, the equation written in terms of the space time is:

$$\frac{C_{j0}}{\tau} - \frac{C_{jE}}{\tau} - (-r_j)_E = \frac{dC_j}{dt}$$

where  $(-r_j)_E$  is the rate of disappearance of component  $j$  evaluated at the outlet concentration of the reactor. The rate of disappearance must account for all of the reactions in which the species participates. The mole balance for species A is:

$$\frac{1}{\tau} C_{A0} - \frac{1}{\tau} C_{AE} - k_1 C_{A,E} C_{B,E} - k_2 C_{A,E} C_{C,E} = \frac{dC_{A,E}}{dt}$$

Molecules of A are consumed in both reactions, so the rates of each are included. Component B reacts only in reaction (1) and therefore:

$$\frac{1}{\tau} C_{B0} - \frac{1}{\tau} C_{BE} - k_1 C_{A,E} C_{B,E} = \frac{dC_{B,E}}{dt}$$

C is formed in reaction (1) and consumed in reaction (2). The rate of formation of C in reaction 1 equals minus the rate of disappearance of A in reaction (1). The rate of disappearance of C in reaction (2) equals the rate of disappearance of A in reaction (2). The mole balance for C is:

$$\frac{1}{\tau} C_{C0} - \frac{1}{\tau} C_{CE} + k_1 C_{A,E} C_{B,E} - k_2 C_{A,E} C_{C,E} = \frac{dC_{C,E}}{dt}$$

Component D is formed in reaction 1 at a rate equal to minus the rate of disappearance of A.

$$\frac{1}{\tau} C_{D0} - \frac{1}{\tau} C_{DE} + k_1 C_{A,E} C_{B,E} = \frac{d C_{D,E}}{dt}$$

Component E is formed in reaction (2) at a rate equal to minus the rate of disappearance of A in reaction (2). The mole balance for component E is therefore:

$$\frac{1}{\tau} C_{E0} - \frac{1}{\tau} C_{EE} + k_2 C_{A,E} C_{C,E} = \frac{d C_{E,E}}{dt}$$

We now have a system of five ordinary differential equations to solve simultaneously. Substituting for the known parameters of space time, inlet concentrations and rate constants gives a system of equations to solve:

$$1 \times 10^{-5} - \frac{1}{100} C_{AE} - 20 C_{A,E} C_{B,E} - 10 C_{A,E} C_{C,E} = \frac{d C_{A,E}}{dt}$$

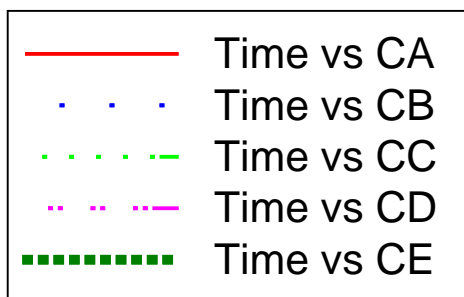
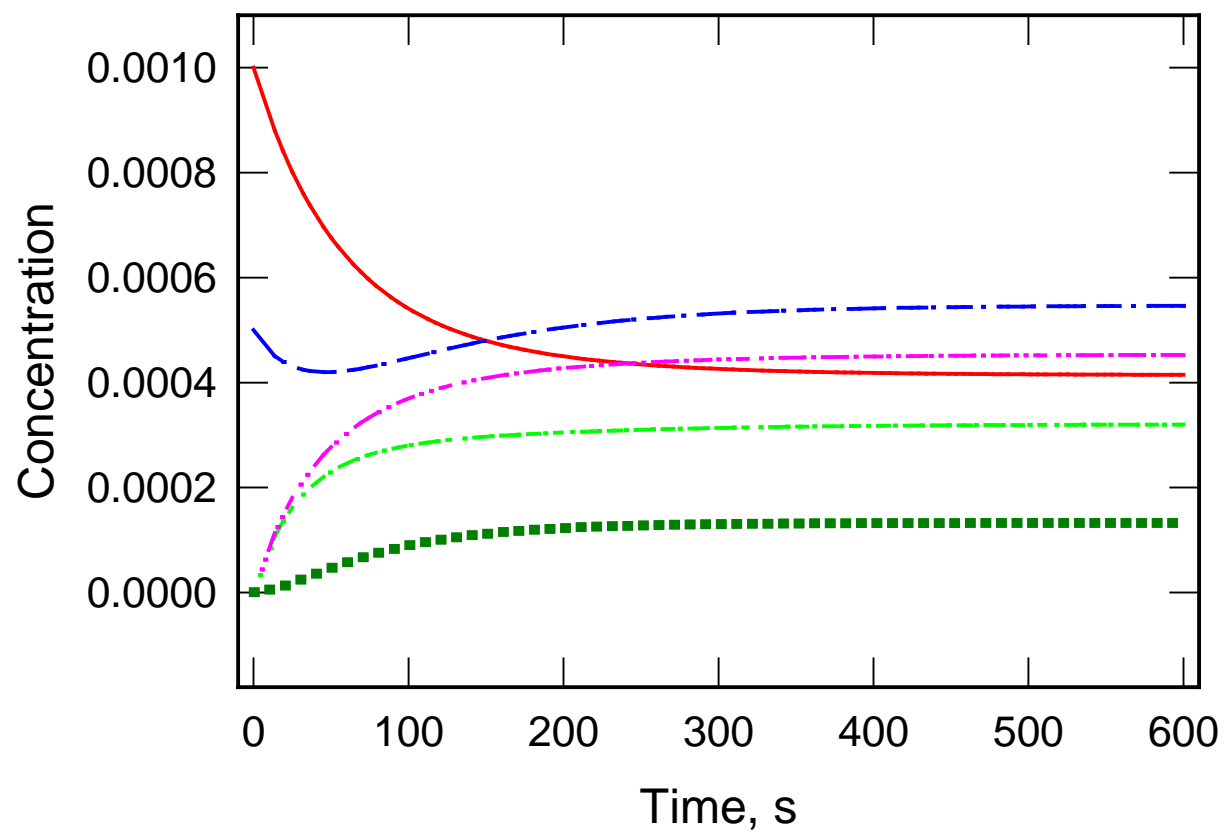
$$1 \times 10^{-5} - \frac{1}{100} C_{BE} - 20 C_{A,E} C_{B,E} = \frac{d C_{B,E}}{dt}$$

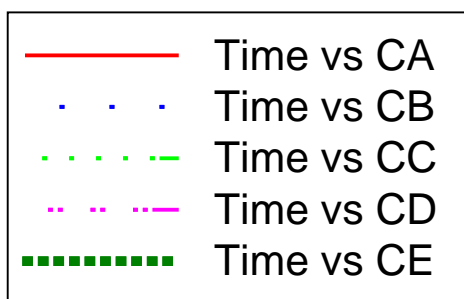
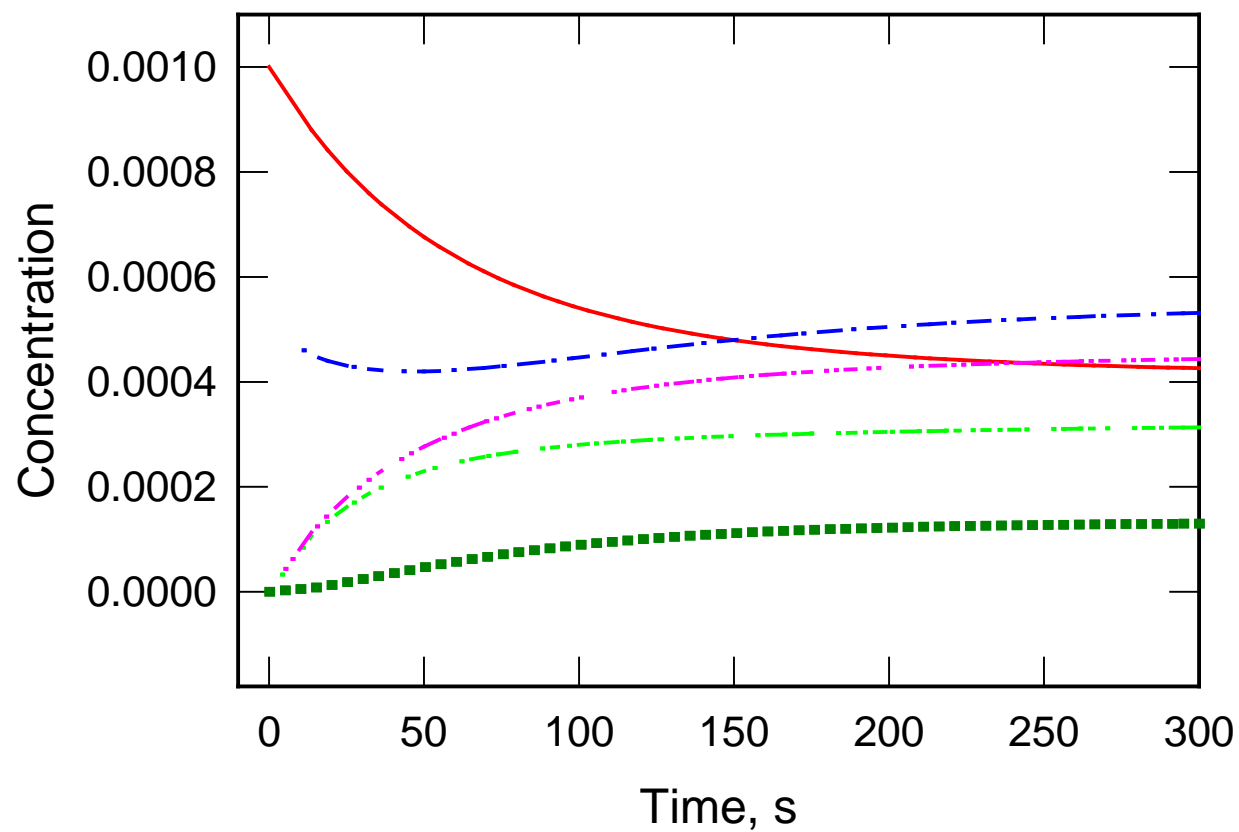
$$-\frac{1}{100} C_{CE} + 20 C_{A,E} C_{B,E} - 10 C_{A,E} C_{C,E} = \frac{d C_{C,E}}{dt}$$

$$-\frac{1}{100} C_{DE} + 20 C_{A,E} C_{B,E} = \frac{d C_{D,E}}{dt}$$

$$-\frac{1}{100} C_{EE} + 10 C_{A,E} C_{C,E} = \frac{d C_{E,E}}{dt}$$

The transient solution generated by Polymath is plotted below, in two time scales:





The steady state solutions can be obtained by running the simulation for a long elapsed time. Alternatively, the steady state solutions can be obtained by setting the time derivatives to zero, to give:

$$1 \times 10^{-5} - \frac{1}{100} C_{AE} - 20 C_{A,E} C_{B,E} - 10 C_{A,E} C_{C,E} = 0$$

$$1 \times 10^{-5} - \frac{1}{100} C_{BE} - 20 C_{A,E} C_{B,E} = 0$$

$$-\frac{1}{100} C_{CE} + 20 C_{A,E} C_{B,E} - 10 C_{A,E} C_{C,E} = 0$$

$$-\frac{1}{100} C_{DE} + 20 C_{A,E} C_{B,E} = 0$$

$$-\frac{1}{100} C_{EE} + 10 C_{A,E} C_{C,E} = 0$$

The steady state solutions generated by Polymath are:

$$C_{AE} = 4.14 \times 10^{-4} \frac{\text{mol}}{\text{m}^3} \quad C_{BE} = 5.47 \times 10^{-4} \frac{\text{mol}}{\text{m}^3} \quad C_{CE} = 3.20 \times 10^{-4} \frac{\text{mol}}{\text{m}^3}$$

$$C_{DE} = 4.53 \times 10^{-4} \frac{\text{mol}}{\text{m}^3} \quad C_{EE} = 1.33 \times 10^{-4} \frac{\text{mol}}{\text{m}^3}$$

## Solution to Problem 2

The mole balance equation for a semi-batch reactor is

$$\frac{dN_A}{dt} = F_{A0} - (-r_A)V$$

For the first order reaction system, we can write

$$\frac{dN_A}{dt} = Q_0 C_{A0} - k C_A V$$

$C_A$  varies with time, as does  $N_A$ . Noting that  $C_A = \frac{N_A}{V}$ , we can write

$$\frac{dN_A}{dt} = Q_0 C_{A0} - k \frac{N_A}{V} V$$

The volume term cancels and we can write

$$\frac{dN_A}{dt} = (0.001)(1000) - 10^{-4} N_A$$

$$\frac{dN_A}{dt} = (1 - 1 \times 10^{-3} N_A)$$

Integrate, noting that the reactor initially contains 100 mol of A.

$$\int_{100}^{N_{Af}} \frac{dN_A}{(1 - 1 \times 10^{-3} N_A)} = \int_0^{900} dt$$

$$-\frac{1}{0.1} \ln(1 - 1 \times 10^{-3} N_A) \Big|_{100}^{N_{Af}} = 900$$

$$-\frac{1}{10^{-3}} \ln\left(\frac{1 - 1 \times 10^{-3} N_{Af}}{1 - 0.1}\right) = 900$$

$$N_{Af} = 634 \text{ mol}$$