Consecutive Reactions for Batch Reactors

Step I – Understanding the Problem

Consider a reaction involving three substances, A, R, and S, which have first-order reaction rates and are carried out isothermically in either the gas or liquid phase in a perfectly mixed batch reactor. The reaction begins with a pure sample of component A.

Schematically, the process can be represented as:

$$\begin{aligned} A &\longrightarrow R, & r_A &= k_1 C_A \\ R &\longrightarrow S, & r_S &= k_2 C_S \end{aligned}$$

where r_A is the reaction rate for the conversion of A into R, r_S is the rate at which R is converted into S; C_A and C_S are the *concentrations* of A and S, respectively.

The primary objective is to determine the amount of each substance in the reactor up to time after the reaction starts. Additional information that is desired includes the time at which the amount of substance R is a maximum, the time at which the amount of S exceeds the amount of A, and the total amount of substance S produced at any time $t > 0$.

Step II – Mathematical Formulation/Modeling

This is really just a three-compartment container problem. Looking at the inflow and outflow for each substance leads to a system of three first-order differential equations with initial conditions.

Let N_A, N_R, and N_S denote the number of moles of A, R, and S at any time in the reactor. The volume of solution in the tank is assumed to be constant. Then, conservation of the total amount of each of the three components can be expressed as

$$\begin{aligned} \tfrac{dN_A}{dt} &= -k_1 N_A \\ \tfrac{dN_R}{dt} &= k_1 N_A - k_2 N_R \\ \tfrac{dN_S}{dt} &= k_2 N_R \end{aligned}$$

with initial conditions $N_A(0) = 1$, $N_R(0) = 0$, $N_S(0) = 0$.

Identify all mathematical information that is needed to answer the questions posed at the end of Step I. (Assume only that you know explicit formulae for N_A, N_R, and N_S.)

Step III – Solution and Analysis

Use the ideas from first-order linear equations to find the solution, N_A, N_R, and N_S, to this system. Be sure to find solutions for all possible combinations of k_1 and k_2 (both positive).

Use your solution, with $k_1 = 1$ and $k_2 = 3$, to answer the questions posed a the end of Step I. Answer the same questions with $k_1 = 3$ and $k_2 = 1$. Are there any differences between the cases when $k_1 < k_2$ and $k_1 > k_2$? Does anything special happen when $k_1 = k_2$?

Step IV – Summary and Conclusion

Use your findings from Step III to provide complete answers to the questions in Step I for any positive constants k_1 and k_2.

Bibliography

[1] Holland, C.D. and R.G. Anthony, Fundamentals of Chemical Reaction Engineering, Prentice–Hall, 1979.