Steady-State Analysis of a Continuous Stirred Tank Reactor under Sequential First-Order Reactions

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Abstract

The continuous stirred tank reactor (CSTR) is one of the fundamental reactor types in chemical reaction engineering. This study presents a steady-state analysis of a CSTR in which a sequential first-order reaction, $A \to B \to C$, occurs. Starting from general mass balance equations, analytical expressions for the steady-state concentrations of all species are derived in terms of the inlet concentration C_{A0}, reaction rate constants k_1 and k_2, and the residence time τ. The resulting relations reveal that the intermediate species B exhibits a concentration maximum for a specific residence time, while the final product C monotonically increases with τ. This work provides a rigorous derivation of the governing equations for sequential first-order kinetics in a continuous reactor and offers insight into the parametric dependence of product yields under steady-state operation.

1 INTRODUCTION

The continuous stirred tank reactor (CSTR) plays a central role in chemical reaction engineering as a model system for analyzing steady-state and dynamic reactor behavior. Due to its assumption of perfect mixing, the CSTR provides a clear theoretical framework for relating input and output concentrations to reaction kinetics and residence time. Such models are essential not only for reactor design but also for studying nonlinear behaviors such as multiple steady states, thermal runaway, and oscillatory dynamics in non-isothermal systems.

Sequential or consecutive reactions, represented by the general scheme $A \to B \to C$, are widely encountered in industrial chemical processes, including oxidation, polymerization, and biochemical conversions. In these reactions, an intermediate species B is produced from A and subsequently consumed to form the final product C. The quantitative behavior of this system is governed by the relative magnitudes of the rate constants k_1 and k_2, as well as by the reactor residence time τ.

Previous studies on reactor modeling have often focused on single-step or parallel reactions. However, the sequential first-order system provides a more realistic representation for multi-step transformations, where the optimization of intermediate yield is of particular industrial interest. Analytical treatment of this system under steady-state conditions enables a direct understanding of how operating parameters influence the concentration profiles of A, B, and C.

The purpose of this work is to present a complete derivation of the steady-state concentration relationships for the sequential first-order reaction $A \to B \to C$ occurring in a single, ideally mixed CSTR. By systematically applying material balance equations and steady-state assumptions, explicit expressions for C_A, C_B, and C_C are obtained as functions of C_{A0}, k_1, k_2, and τ. The derived relations are subsequently analyzed to elucidate the effect of kinetic and residence-time parameters on the reactor performance.

2 Reaction Model Formulation

Consider a continuous stirred tank reactor (CSTR) operating under steady-state conditions, in which two consecutive irreversible first-order reactions take place:

$$A \xrightarrow{k_1} B \xrightarrow{k_2} C \tag{1}$$

where k_1 and k_2 denote the respective rate constants for the first and second reactions. The system is assumed to be isothermal, perfectly mixed, and operated at constant density and volumetric flow rate. Under these assumptions, the reactor volume V and the volumetric flow rate F define the mean residence time:

$$\tau = \frac{V}{F} \tag{2}$$

2.1 Reaction Kinetics

Each reaction step follows first-order kinetics with respect to the reactant species. The rate expressions are therefore given by:

$$r_1 = k_1 C_A \tag{3}$$
$$r_2 = k_2 C_B \tag{4}$$

where C_A, C_B, and C_C denote the molar concentrations of species A, B, and C, respectively.

2.2 Material Balance Equations

At steady state, the general material balance for a species i in the CSTR can be written as:

$$F(C_{i0} - C_i) + V(\text{rate of generation of } i) = 0 \tag{5}$$

Applying this to each component yields the following set of algebraic equations:

For component A:

$$F(C_{A0} - C_A) = V k_1 C_A \tag{6}$$

For component B:

$$F(C_{B0} - C_B) + V k_1 C_A = V k_2 C_B \tag{7}$$

For component C:

$$F(C_{C0} - C_C) + V k_2 C_B = 0 \tag{8}$$

Since there are no inflow streams of B or C, we set $C_{B0} = 0$ and $C_{C0} = 0$. By substituting $\tau = V/F$, the above equations can be expressed entirely in terms of residence time, enabling analytical solutions for the steady-state concentrations of all species.

3 Steady-State Solution

By substituting the residence time $\tau = \frac{V}{F}$ into the material balance equations derived in Section II, the following algebraic expressions for the steady-state concentrations can be obtained.

3.1 Derivation of Component Concentrations

Component A. From Eq. (6), the steady-state balance for A yields:

$$C_{A0} - C_A = k_1 \tau C_A \tag{9}$$

which can be rearranged to give:

$$\boxed{C_A = \frac{C_{A0}}{1 + k_1 \tau}} \tag{10}$$

Component B. Substituting Eq. (8) into the balance for B:

$$0 - C_B + k_1 \tau C_A = k_2 \tau C_B \tag{11}$$

which simplifies to:

$$C_B = \frac{k_1 \tau C_A}{1 + k_2 \tau} \tag{12}$$

and substituting Eq. (9) for C_A:

$$\boxed{C_B = C_{A0} \cdot \frac{k_1 \tau}{(1 + k_1 \tau)(1 + k_2 \tau)}} \tag{13}$$

Component C. The steady-state balance for C can be expressed as:

$$0 - C_C + k_2 \tau C_B = 0 \tag{14}$$

leading to:

$$C_C = k_2 \tau C_B \tag{15}$$

3.2 Validation of Material Conservation

The total molar concentration within the reactor must satisfy the overall mass conservation constraint:

$$C_A + C_B + C_C = C_{A0} \tag{16}$$

which is indeed fulfilled by Eqs. (9)–(13), confirming the consistency of the steady-state formulation.

3.3 Summary of Results

The resulting expressions for the steady-state concentrations are summarized as:

$$C_A = \frac{C_{A0}}{1 + k_1 \tau} \tag{17}$$
$$C_B = C_{A0} \cdot \frac{k_1 \tau}{(1 + k_1 \tau)(1 + k_2 \tau)} \tag{18}$$

These analytical solutions explicitly demonstrate the dependence of each species concentration on the kinetic constants and the residence time, forming the basis for subsequent parametric analysis.