International Journal of Advanced Scientific Research and Engineering Trends

ISSN: 2456-0774

Volume 10 Issue 1s (2026) | Pages: 35-39

Optimization of Process Variables in a Batch Reactor Using Simulation

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Peer Review Information

***Type**: Article*
***Received**: 30 March 2026*
***Revised**: 25 April 2026*
***Accepted**: 03 June 2026*
***Published**: 22 June 2026*

Abstract

In chemical and pharmaceutical industries, consecutively reacting systems are very common where the end-product of interest is usually one or more of the intermediate products. The purpose of this work is to develop a mathematical model of a batch-cooker constant volume-reactor system that is undergoing a first-order reaction series (A → B → C). Analytical formulas for concentration versus time will be derived for both A, B, and C and numerically evaluated. Conversion profiles, intermediate accumulation and batch-time optimization are analyzed with the data from the analytical and numerical analyses to assess the effect of reaction kinetics and total reaction time on maximizing the overall (intermediate) yield. This work provides valuable information that can be applied to improve reactor design and operation.

Keywords: Batch Reactor; Consecutive First-Order Reaction; Kinetic Modelling; Concentration Profiles; Reaction Optimization; Chemical Reactor Simulation.

How to Cite This Article

Lakhadive, S., Khilari, M., Bandpatte, S., & Chaudhari, P. (2026). Optimization of Process Variables in a Batch Reactor Using Simulation. *International Journal of Advanced Scientific Research and Engineering Trends*, 10(1s), 35–39.

Introduction

Various industrial processes have reactions that happen in series, where an intermediate converts from a reactant and reacts again to make the final product. Common examples are the oxidation of materials, degradation of polymers, and the synthesis of pharmaceutical products. If a reaction takes too much time, then it can lead to a lower yield of the desired intermediate from the reaction. A specific example is shown by AIBN (A) decomposing to produce free radicals (B) that then produce stable products (C): AIBN (A)→^(k_1) Free radicals (B)→^(k_2) Stable products (C) Batch reactors are well suited to study these types of reactions as they provide good control over the amount of time taken by the reaction to take place. Information from this work is obtained through simulation of the Azo indicator → B → C system and analysing the resulting concentration profiles to determine conditions to obtain maximum intermediate concentration.

- Azo initiator (AIBN): a compound containing an -N=N- bond that decomposes by heat to create free radicals that begin a chain reaction.
- Free Radicals: free radical are highly active chemicals formed when the initiator decomposes into unpaired electrons, which function as intermediates during the chain reaction process.
- Termination/stable products: termination occurs when free radicals join together to together to produce a stable (non-free radical) material, cutting off the reaction chain.

Reaction Scheme and Kinetics

The reaction system considered is a consecutive first-order reaction:

$$AIBN\ (A) \rightarrow^{k_1} Free\ radicals\ (B) \rightarrow^{k_2} Stable\ termination\ product\ (C)$$

where:
A = reactant (AIBN)
B = intermediate (free radicals)
C = final product (stable termination product)
The rate expressions are:

$$-r_A = k_1 C_A,$$

$$r_B = k_1 C_A - k_2 C_B,$$

$$r_C = k_2 C_B$$

Batch Reactor Design Equations

Reactant A

$$-\frac{dC_A}{dt} = k_1 C_A$$

Integrating with $C_A = C_{A0}$at $t = 0$:

$$C_A = C_{A0} e^{-k_1 t}, X_A = 1 - e^{-k_1 t}$$

Intermediate B

$$\frac{dC_B}{dt} = k_1 C_A - k_2 C_B$$

Substituting $C_A$and integrating with $C_B = 0$at $t = 0$:

$$C_B = \frac{k_1 C_{A0}}{k_2 - k_1}(e^{-k_2 t})$$

Product C

$$\frac{dC_C}{dt} = k_2 C_B$$

Integrating with $C_C = 0$at $t = 0$:

$$C_C = C_{A0}\left[\frac{k_2 e^{-k_1 t} - k_1 e^{-k_2 t}}{k_2 - k_1}\right]$$

Table 1. *Concentration–Time Data for Consecutive First-Order Reaction Simulation*

Time (min)	CA (mol/L)	CB (mol/L)	CC (mol/L)	Conversion (XA)
0	1.000	0.000	0.000	0.00
5	0.368	0.564	0.068	0.63
10	0.135	0.629	0.236	0.87
20	0.018	0.489	0.493	0.98
60	≈ 0	0.066	0.934	≈ 1.00

Simulation Parameters

Table 2. *Simulation Parameters for Batch Reactor Optimization Study*

Parameter	Value
Initial Concentration (CA_0)	1.0 mol·L^{-1}
Rate Constant (k_1)	0.20 min^{-1}
Rate Constant (k_2)	0.05 min^{-1}
Reactor Type	Constant Volume Batch Reactor
Temperature	Constant Temperature

Results and Discussion

Concentration–Time Data (Sample)

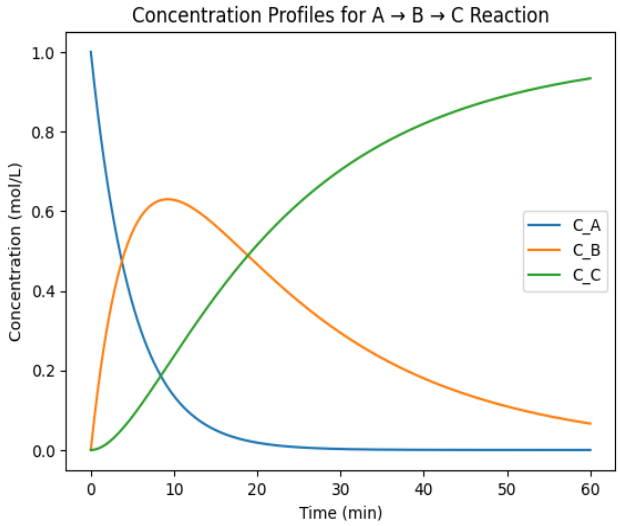

Fig. 1. *Concentration Profiles of Species A, B, and C*

Concentration Profiles

C_A decreases exponentially with time.

C_B rises to a maximum before declining as it converts to C.

C_C increases continuously and dominates at long reaction times.

A (↓) ──k1──> B (↑ then ↓) ──k2──> C (↑)

Conversion vs Time

Conversion rises rapidly in the early stages, approaching unity around 20 minutes.

Beyond this, further operation mainly converts B to C.

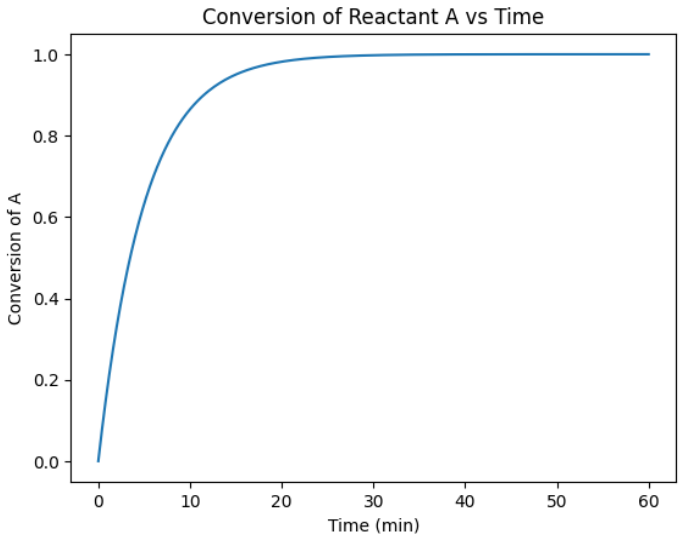

Fig. 2. *Conversion of Reactant A vs Time*

Observations

- The peak concentration of Intermediate B occurs at a definite time after reaction.
- Longer batch times yield more Intermediate B but result in a higher formation of final product.
- The ratio of rate constants (k1/k2) has a significant influence on the accumulation of Intermediate B.
- Determining the optimum batch time is very important if the Intermediate B is the desired product.

Optimization Insight

- For maximum B, run the reactor at the point in time that corresponds to peak values for C_B.
- For maximum C, increase the batch duration to achieve close to complete conversion.
- Utilizing simulation as a method of developing the optimal operating conditions provides a method of implementation that is both safe and cost-effective.

Conclusions

In this study, AIBN (A) was analyzed as it converted, through a free radical intermediate (B), into a final product (C) in a batch reactor. The results clearly demonstrate that intermediate (B) accumulates to a maximum concentration before being converted to the stable end product, (C), at a given reaction time. Longer batch reaction times will favour the production of the complete yield of the final product (C), but will reduce the yield of the intermediate (B) produced; thus, as the ratio of rate constants (k_1/k_2) increases, the accumulation of the intermediate (B) significantly decreases. Therefore, optimization of batch time is critical to obtaining the desired selectivity of the final product and maximizing product yield.

Acknowledgments

I would like to take this opportunity to show my appreciation to Prof. Sagar Bandpatte and Prof. Prashant Chaudari for their invaluable assistance, support and guidance throughout this time of my research. The input and knowledge that they provided for this research study have made it possible for me to carry out the research and also helped me to determine the research direction and the quality of the study.

I would especially like to thank Dr P V Chavan, Dept Head, for his persistent motivation, assistance, and ability to provide the academic environment and the necessary resources to carry out this research.

Next, I would like to extend my heartfelt thanks to Bharati Vidyapeeth (Deemed University) College of Engineering, Pune, India, for providing the institution and the necessary support and resources to enable the completion of the research.

Finally, I would like to express my appreciation to everyone who contributed directly or indirectly to the completion of this research.

Conflict of Interest Statement

This paper was prepared without any conflict of interest or any outside funding or relationships influencing these findings.

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