CLL 122 Chemical Reaction Engineering

CSTR and PFR Modelling Using a Custom CRE Calculator

Project Report

Authors:
Akash - 2023CH10001
Shashi Kumar - 2023CH70980
Harshit Bhatt - 2023CH10471
Surabhi - 2023CH10206

Contents

1 Introduction

Chemical reactors are the heart of any chemical process. Among the different types of reactors, the Continuous Stirred Tank Reactor (CSTR) and the Packed Bed Reactor (PBR) are widely used in industry due to their unique characteristics and application suitability.

2 CSTR Reactor

A Continuous-Stirred Tank Reactor (CSTR), also known as a vat or back-mix reactor, is widely employed in industrial chemical processes, particularly for liquid-phase reactions. Operated under steady-state conditions, it is assumed to be perfectly mixed, ensuring uniform temperature, concentration, and reaction rate throughout the reactor volume. Consequently, the exit stream's properties represent the entire reactor's behavior.

3 General Concepts and Equations

3.1 General Mole Balance Equation

The general mole balance over a system volume V for a species j is given as:

$$F_{j0} - F_j + \int_V r_j \, dV = \frac{dN_j}{dt} \tag{1}$$

where:

- F_{j0}: Inflow molar rate of species j
- F_j: Outflow molar rate of species j
- r_j: Rate of formation of species j per unit volume
- N_j: Number of moles of species j in the system

3.2 CSTR Design Equation

Under steady-state operation with no accumulation ($\frac{dN_j}{dt} = 0$) and assuming uniform reaction rate throughout the reactor:

$$V = \frac{F_{A0} X}{(-r_A)_{\text{exit}}} \tag{2}$$

where:

- F_{A0}: Molar feed rate of species A
- X: Conversion of species A
- $(-r_A)_{\text{exit}}$: Reaction rate of A at the exit

4 PFR Reactor

A Plug Flow Reactor (PFR), also known as a fixed-bed reactor, consists of a bed of solid catalyst particles through which reactant fluids pass. This reactor is widely used for heterogeneous catalytic reactions, where the catalytic surface plays a crucial role in determining the reaction rate.

For a first-order, isothermal reaction $A \rightarrow B$, the design equation is derived from the mole balance:

$$\frac{dF_A}{dV} = r_A \tag{3}$$

Expressing in terms of conversion X:

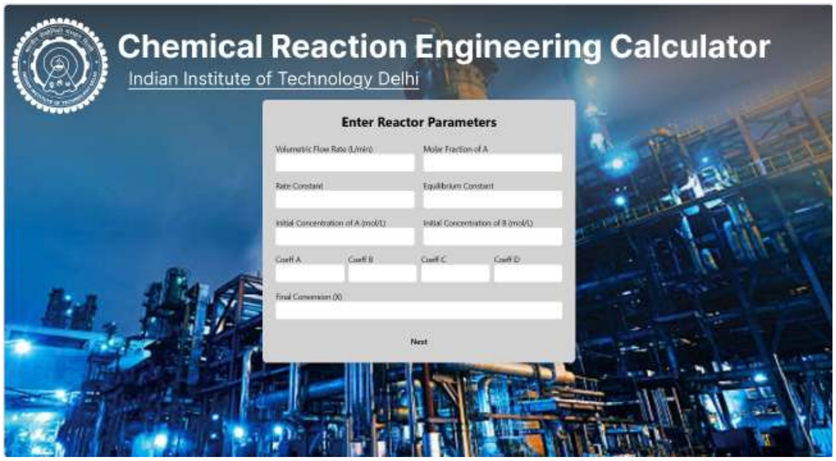
$$V = F_{A0} \int_0^X \frac{1}{-r_A} \, dX \tag{4}$$

Where:

- V: Reactor volume (L or m^3)
- F_{A0}: Inlet molar flow rate of species A (mol/min)
- X: Conversion of A (dimensionless)
- r_A: Rate of disappearance of A (mol/L.min), generally given as $r_A = kC_A$

This equation allows calculation of the volume needed to achieve a desired conversion for a given rate law and operating conditions.

Entering reaction parameters:



5 Types of Reactions

5.1 Irreversible Reactions

In an irreversible reaction, the reactants convert completely to products under given conditions, and the reaction proceeds in one direction. The general rate expression for an irreversible reaction:

$$\text{Rate} = kC_A^n C_B^m \tag{5}$$

where k is the rate constant and C_A, C_B are the reactant concentrations.

5.2 Reversible Reactions

In a reversible reaction, the products can revert back to reactants, making the reaction proceed in both forward and backward directions. The net rate is:

$$\text{Net Rate} = k_f C_A^n - k_r C_P^m \tag{6}$$

where k_f and k_r are the forward and reverse rate constants respectively.

6 Energy Balance

The energy balance for an open system accounts for the heat and work interactions along with the energy carried by mass entering and leaving the system.

$$\frac{d\hat{E}_{\text{sys}}}{dt} = \dot{Q} - \dot{W} + F_{\text{in}}E_{\text{in}} - F_{\text{out}}E_{\text{out}} \tag{7}$$

Where:

- $\frac{d\hat{E}_{\text{sys}}}{dt}$: Rate of energy accumulation within the system (J/s)
- $\dot{Q}$: Rate of heat added to the system from the surroundings (J/s)
- $\dot{W}$: Rate of work done by the system on the surroundings (J/s)
- $F_{\text{in}}E_{\text{in}}$: Energy added via mass flow into the system (J/s)
- $F_{\text{out}}E_{\text{out}}$: Energy leaving via mass flow out of the system (J/s)

This general energy balance is fundamental for analyzing non-isothermal reactors, especially under transient or adiabatic conditions.

7 Isothermal Reactors

An isothermal reactor maintains a constant temperature throughout the reaction. This simplifies energy balance equations and is useful when reaction kinetics are temperature-sensitive but uniform heating or cooling can be maintained.

The reactor design equations (for CSTR or PFR) remain the same as in non-isothermal cases, but with k being constant:

$$k = k_0 e^{-\frac{E_a}{RT}} \tag{8}$$

8 Non-Isothermal Reactors

In non-isothermal reactors, temperature varies with time or position. These require coupled mass and energy balances, as reaction rates are strongly temperature-dependent.

The Arrhenius dependence of rate constant:

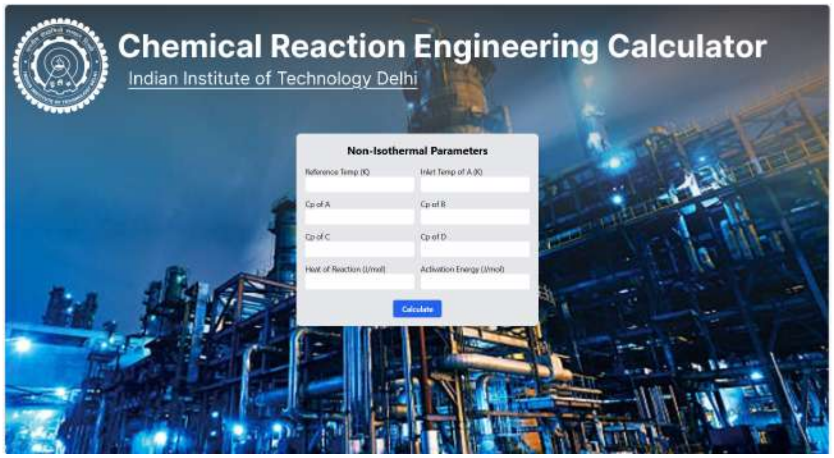
$$k = k_0 e^{-\frac{E_a}{RT}} \tag{9}$$

The energy balance for adiabatic systems (no heat loss or work done):

$$T = T_0 + \frac{-\Delta H_R C_{A0} X}{\sum_i y_i C_{p,i}} \tag{10}$$

Where:

- T_0: Inlet temperature
- ΔH_R: Heat of reaction
- $C_{p,i}$: Heat capacity of species i



9 Conclusion

This report presented fundamental chemical reactor types and equations essential in chemical reaction engineering. Using general mole balance principles, the behavior of CSTR and PFR reactors can be analyzed under various operating conditions—both isothermal and non-isothermal. These analyses form the backbone of reactor design and optimization in real-world chemical processes.

A solid understanding of mole balances, rate laws, energy balances, and design equations enables engineers to predict reactor performance, select appropriate reactor types, and ensure operational safety and efficiency. Furthermore, knowledge of thermodynamic interactions and reaction kinetics allows engineers to enhance conversion, yield, and selectivity in industrial-scale applications.

By integrating theoretical concepts with practical simulation tools and experimental validation, chemical engineers can design sustainable, cost-effective, and scalable reactor systems that meet growing industrial demands and environmental regulations.

10 References

1. Elements Of Chemical Reaction Engineering - H. Scott Fogler
2. Chemical Reaction Engineering - Octave Levenspiel

11 Acknowledgements

We express our sincere gratitude to Prof. Manjesh Kumar, Department of Chemical Engineering, IIT Delhi, for his invaluable guidance, insightful suggestions, and constant support throughout this project. His expertise and encouragement were instrumental in shaping our understanding of Chemical Reaction Engineering (CRE) concepts. We also extend our thanks to the Department of Chemical Engineering, IIT Delhi, for providing the necessary resources and an enriching academic environment. This project would not have been possible without their mentorship and institutional support. We deeply appreciate the knowledge gained and the opportunity to work under such esteemed guidance.