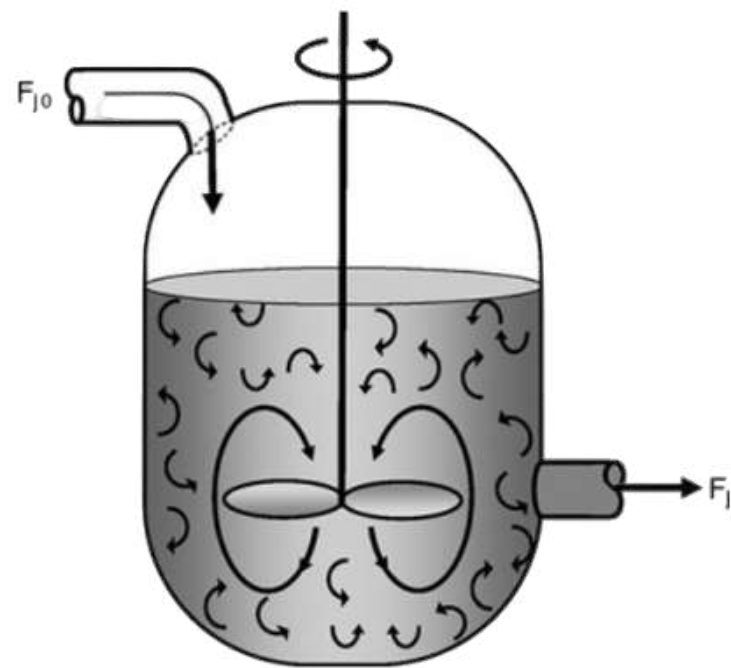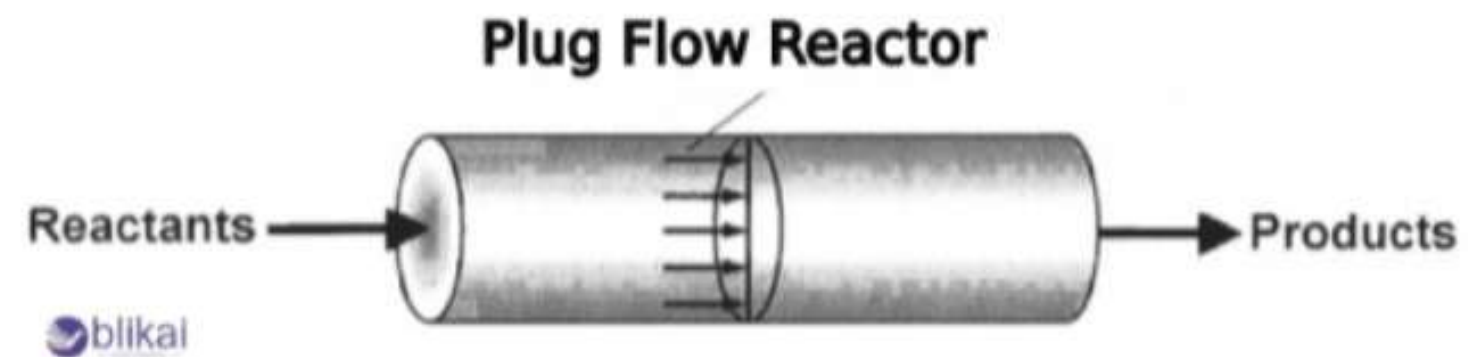# Chemical Reaction Engineering Calculator for CSTR and PFR reactor type

CSTR Reactor

PFR Reactor

Introduction:

- This calculator serves as a valuable tool in the field of chemical engineering, enabling users to estimate **reaction rates** and evaluate the most appropriate reactor type for a given chemical process under specific operating conditions. By simulating various scenarios, it aids in the selection of optimal reactor designs—such as batch, **CSTR**, or **PFR**—based on performance metrics and process requirements. Additionally, the integrated graphical outputs offer clear visual insights, allowing engineers to make informed decisions by analyzing how different variables influence reactor behavior and efficiency.
- In this calculator we have incorporated both **Reversible** and **Irreversible** in case of reversibility of the reaction
- We have also incorporated **Isothermal** and **Non Isothermal** case for given reaction condition

Technology we have used

for web interface development :
we have used HTML and CSS

for back-end development:
we have used **Python** and **flask**

flask is used to intergrate both front end and backend together

Step 1: Choose the Reactor Type

CSTR:

A **Continuous-Stirred Tank Reactor (CSTR)**, also known as a **vat reactor** or **back-mix reactor**, is a commonly used type of reactor in industrial chemical processing, particularly for **liquid-phase reactions**. The CSTR is typically operated at **steady state** and is assumed to be **perfectly mixed**, meaning there is **no variation in temperature, concentration, or reaction rate** with respect to either time or position within the reactor. As a result, the temperature and concentration are **uniform throughout the reactor** and are equal to the values at the reactor's **exit stream**.

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

CSTR
Design

F_{A0}

X
F_A

Equation
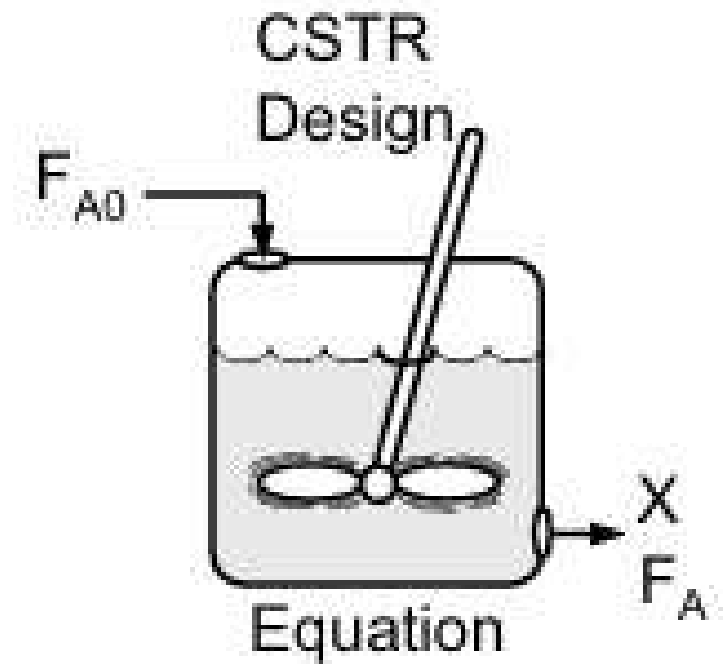
Perfect mixing

PFR:

A **Packed Bed Reactor (PBR)**, also known as a **fixed-bed reactor**, is a type of chemical reactor that consists of a **bed of solid catalyst particles** through which reactant fluids (gases or liquids) flow. It is one of the most common reactor types used in **heterogeneous catalytic reactions**, where the **reaction occurs on the surface of a solid catalyst**.
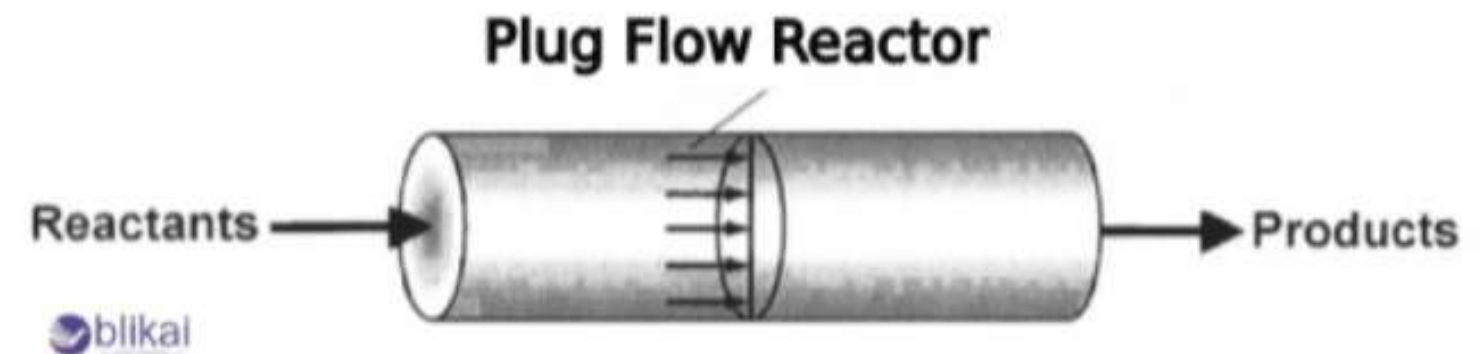
$$\frac{-dF_A}{dV} = -r_A$$

$$F_A = F_{A0} - F_{A0}X$$

$$dF_A = -F_{A0}dX$$

$$V = F_{A0}\int_0^X \frac{dX}{-r_A}$$

$$F_{A0}\frac{dX}{dV} = -r_A$$

Plug Flow Reactor

Reactants → → Products

blikai

Step 2: Choose the reversibility

Reversible Reaction: A reversible reaction is a chemical reaction where the products can react to form the original reactants again. This means the reaction can proceed in both the forward and backward directions.

$$aA + bB \;\rightleftharpoons\; cC + dD$$
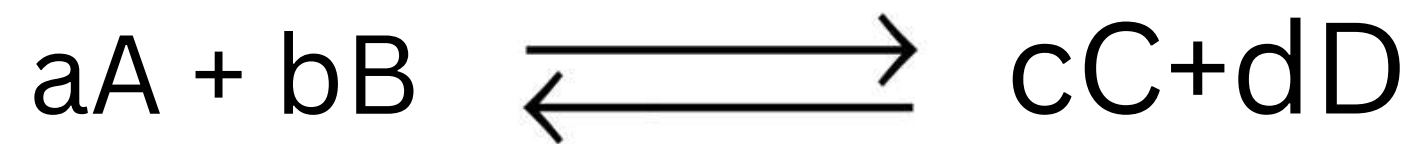
Irreversible Reaction: An irreversible reaction is a chemical reaction where the products cannot easily revert back to the original reactants. The reaction goes in only one direction until the reactants are used up.

$$aA + bB \;\longrightarrow\; cC + dD$$

Without Volume Change

$$C_A = \frac{F_A}{v_0} = \frac{F_{A0}(1-X)}{v_0} = C_{A0}(1-X)$$

$$C_B = C_{A0}(\Theta_B - X)$$

$$C_C = C_{A0}\Theta_C X$$

$$C_D = C_{A0}\Theta_D X$$

With Volume Change

$$v = v_0(1 + \varepsilon X)$$

$$\varepsilon = y_{A0}\,\delta$$

$$C_A = \frac{F_{A0}(1-X)}{v_0(1+\varepsilon X)} = C_{A0}\left(\frac{1-X}{1+\varepsilon X}\right)$$

$$C_B = C_{A0}\left(\frac{\Theta_B - X}{1+\varepsilon X}\right)$$

$$C_C = C_{A0}\left(\frac{\Theta_C + X}{1+\varepsilon X}\right)$$

$$C_D = C_{A0}\left(\frac{\Theta_D + X}{1+\varepsilon X}\right)$$

Step 3: Put all the values according to the requirenment

Chemical Reaction Engineering Calculator
Indian Institute of Technology Delhi

Enter Reactor Parameters

Total molar Flow Rate (Moles/hr)
163000

Molar Fraction of A
0.9

Rate Constant
31.1

Equilibrium Constant
2.51

Initial Concentration of A (moles/cubic metre)
9300

Initial Concentration of B (moles/cubic metre)
0

Coeff of A
1

Coeff of B
0

Coeff of C
1

Coeff of D
0

Final Conversion (X)
0.4

Next

Definition and understanding of all the parameters

Total molar flow rate (moles/hr): This is the volume of fluid that enters the reactor per unit of time, typically measured in liters per minute. It helps determine how quickly reactants are fed into the reactor and is crucial for sizing continuous flow systems and calculating residence time.

Molar Fraction of A: This represents the proportion of component A in a mixture, calculated as the moles of A divided by the total moles of all components. It is a dimensionless quantity and indicates the concentration of A relative to other substances in the system.

Rate Constant: The rate constant is a proportionality factor in the reaction rate equation that indicates how quickly a reaction occurs. It depends on temperature and the presence of catalysts and varies with the order of the reaction.

Equilibrium Constant: The equilibrium constant expresses the ratio of the concentrations of products to reactants at chemical equilibrium. It reflects the extent to which a reaction proceeds and is specific to a given reaction at a particular temperature.

Definition and understanding of all the parameters

Initial Concentration of A (mol/m3):
 This is the starting concentration of reactant A in the reactor, measured in moles per liter. It sets the initial condition for the reaction and influences the reaction rate and conversion.

Initial Concentration of B (mol/m3):
 Similar to A, this is the concentration of reactant B at the start of the reaction. It helps define the stoichiometry and kinetics of the reaction when multiple reactants are involved.
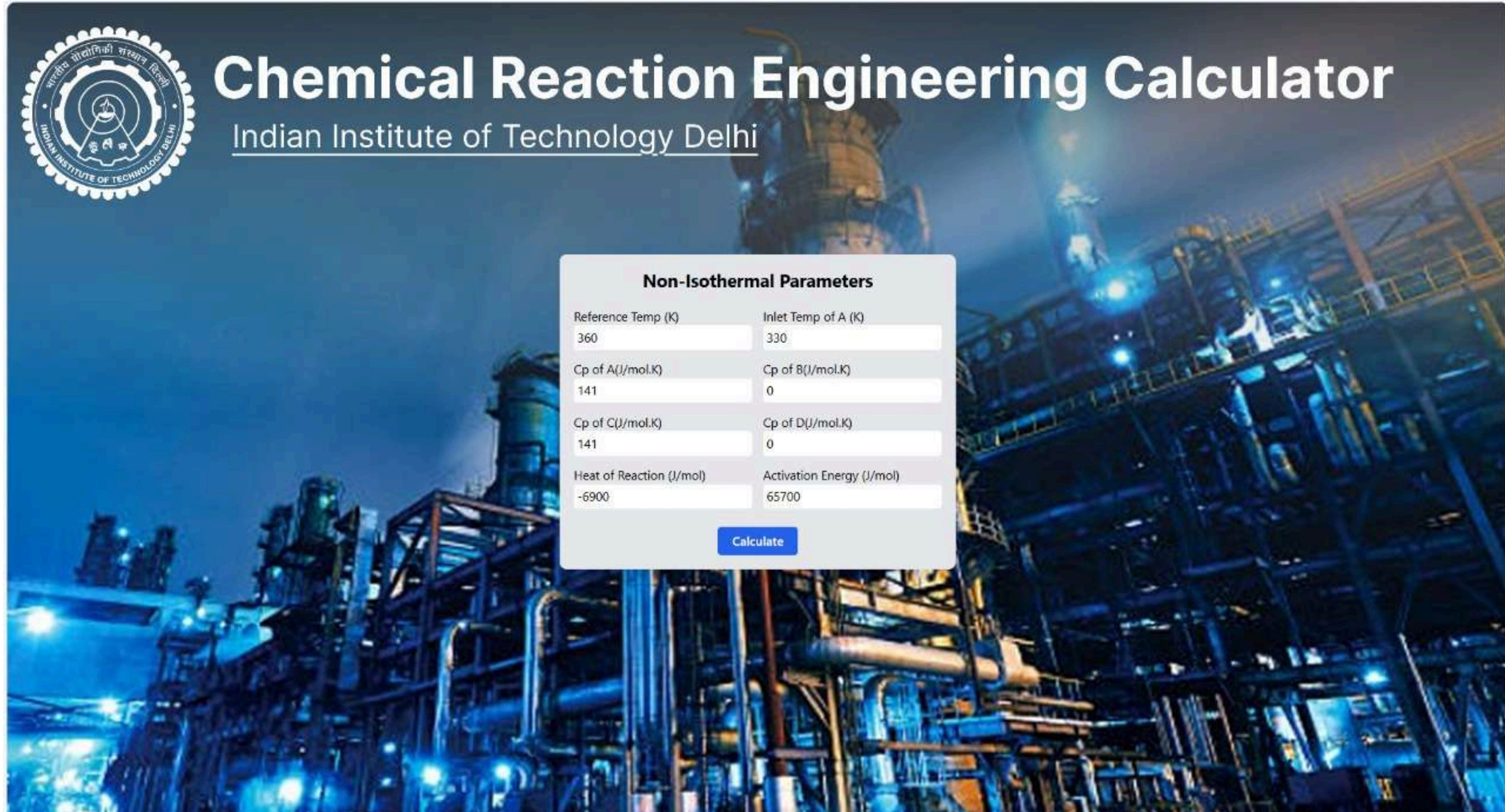
Coeff A, B, C, D:
 These are the stoichiometric coefficients for each species in the balanced chemical equation. They define the molar ratios in which reactants are consumed and products are formed and are essential for reaction rate and equilibrium calculations.

Final Conversion (X):
 Final conversion represents the fraction or percentage of the limiting reactant (usually A) that has been converted into products at the end of the reaction. It's a key indicator of reactor performance.

Step 4(If Non Insothermal): Put all the parameters of Non Isothermal Reaction

Chemical Reaction Engineering Calculator

Indian Institute of Technology Delhi

Non-Isothermal Parameters

Reference Temp (K)
360

Inlet Temp of A (K)
330

Cp of A(J/mol.K)
141

Cp of B(J/mol.K)
0

Cp of C(J/mol.K)
141

Cp of D(J/mol.K)
0

Heat of Reaction (J/mol)
-6900

Activation Energy (J/mol)
65700

Calculate

Definition and understanding of all the parameters

Reference Temperature (K):
 This is a standard or baseline temperature used in calculating temperature-dependent properties such as rate constants through the Arrhenius equation. It provides a fixed point for comparison and simplifies thermal calculations in the system.

Inlet Temperature of A (K):
 The temperature at which reactant A enters the reactor. It directly influences the initial reaction rate and the energy balance, especially important in non-isothermal operations where heat effects are significant.

Cp of A (J/mol·K):
 The specific heat capacity of reactant A, representing the amount of heat needed to raise the temperature of one mole of A by one Kelvin. It is essential in determining how much heat is absorbed or released during the process.

Cp of B (J/mol·K):
 The heat capacity of reactant B, indicating its thermal energy requirements. It's important for calculating the energy needed for heating or cooling B as the reaction proceeds.

Definition and understanding of all the parameters

Cp of C (J/mol·K):
 The specific heat of product C, which is used to estimate how much heat is associated with temperature changes of this component during the reaction and energy balance calculations.

Cp of D (J/mol·K):
 The specific heat capacity of product D, used similarly to the others to compute the energy changes related to heating or cooling this substance in the reactor.

Heat of Reaction (J/mol):
 The enthalpy change that occurs when reactants are converted to products. A negative value indicates an exothermic reaction (releases heat), while a positive value suggests an endothermic reaction (absorbs heat).

Activation Energy (J/mol):
 The minimum energy that molecules must possess to undergo a chemical reaction. It determines how sensitive the reaction rate is to changes in temperature, governed by the Arrhenius equation.

Mechanism and all the formulas used for calculations:

The net rate for reversible reaction is given by :

$$r = r_{\text{f}} - r_{\text{r}} = k_{\text{f}}[A]^a[B]^b - k_{\text{r}}[C]^c[D]^d$$

$$r = k_{\text{f}}\left([A]^a[B]^b - \frac{[C]^c[D]^d}{K_{\text{eq}}}\right)$$

The net rate for irreversible reaction

$$r = r_f = k_f[A]^a[B]^b$$

For Non Isothermal Reactor:

The expression for rate of reaction and its dependence on tempreature $k = k_1(T_1)\,\exp\left[\dfrac{E}{R}\left(\dfrac{1}{T_1} - \dfrac{1}{T}\right)\right]$

The expression for Equilibrium constant and its dependence on tempreature

$$K_{\text{C}} = K_{\text{C2}}(T_2)\,\exp\left[\frac{\Delta H_{\text{Rx}}^\circ}{R}\left(\frac{1}{T_2} - \frac{1}{T}\right)\right]$$

k_0 Inistial Reaction rate

E_a Activation Energy

R gas constant

T absolute temperature

Kc= Equilibrium constant

$\Delta H_{\text{R}}^\circ$=Heat of Reaction at Tr

Energy Balance Equation

$$\begin{bmatrix} \text{Rate of} \\ \text{accumulation} \\ \text{of energy} \\ within \text{ the} \\ \text{system} \end{bmatrix} = \begin{bmatrix} \text{Rate of flow} \\ \text{of heat } to \\ \text{the system} \\ from \text{ the} \\ \text{surroundings} \end{bmatrix} - \begin{bmatrix} \text{Rate of work} \\ done \text{ by} \\ \text{the system} \\ on \text{ the} \\ \text{surroundings} \end{bmatrix} + \begin{bmatrix} \text{Rate of energy} \\ \text{added to the} \\ \text{system by mass} \\ \text{flow } into \text{ the} \\ \text{system} \end{bmatrix} - \begin{bmatrix} \text{Rate of} \\ \text{energy leaving} \\ \text{the system by mass} \\ \text{flow } out \text{ of} \\ \text{the system} \end{bmatrix}$$

$$\dot{Q} - \dot{W}_s + \sum_{i=1}^{n} F_{i0}H_{i0} - \sum_{i=1}^{n} F_i H_i = \frac{d\hat{E}_{sys}}{dt}$$

$$\begin{array}{lccccccc} \text{Energy balance} & \dfrac{d\hat{E}_{sys}}{dt} & = & \dot{Q} & - & \dot{W} & + & F_{in}E_{in} & - & F_{out}E_{out} & (11\text{-}2) \\ \text{on an open} & & & & & & & & & \\ \text{system} & & & & & & & & & \\ & (J/s) & = & (J/s) & - & (J/s) & + & (J/s) & - & (J/s) \end{array}$$

If the process is taken adiabatic and Ws is considered to zero and Cp change is also zero,then the equation becomes:

$$X_{EB} = \frac{\Sigma \Theta_i C_{P_i}(T - T_0)}{-\Delta H^\circ_{Rx}}$$

$$T = T_0 + \frac{(-\Delta H^\circ_{Rx})X_{EB}}{\Sigma \Theta_i C_{P_i}}$$

$$\Delta H_{Rx}(T) = \Delta H^\circ_{Rx}(T_R) + \Delta C_P(T - T_R)$$

$$\Delta C_P = \frac{d}{a}C_{P_D} + \frac{c}{a}C_{P_C} - \frac{b}{a}C_{P_B} - C_{P_A}$$

$$\Delta H^\circ_{Rx}(T_R) = \frac{d}{a}H^\circ_D(T_R) + \frac{c}{a}H^\circ_C(T_R) - \frac{b}{a}H^\circ_B(T_R) - H^\circ_A(T_R)$$

Results

For this case:

F_{T0}	Total molar flow rate (inlet)	16,300	mol/hr
y_{A0}	Mole fraction of species A in feed	0.9	–
C_{A0}	Initial concentration of A	9,300	mol/m³
C_{B0}	Initial concentration of B	0	mol/m³
k	Rate constant at reference temperature T_r	31.1	hr⁻¹
K_c	Equilibrium constant at T_r	2.51	–
X	Conversion of A	0.4	–

T_r	Reference temperature	360	K
C_{pA}	Heat capacity of A	141	J/mol·K
C_{pB}	Heat capacity of B	0	J/mol·K
C_{pC}	Heat capacity of C	141	J/mol·K
C_{pD}	Heat capacity of D	0	J/mol·K
E_a	Activation energy	65,700	J/mol

Reactor Calculation Results

Final Volume: 0.9614405659620661

Final Concentrations & Rate

- **Final Concentration of A**: 5580.0
- **Final Concentration of B**: 0.0
- **Final Concentration of C**: 3720.0
- **Final Concentration of D**: 0.0
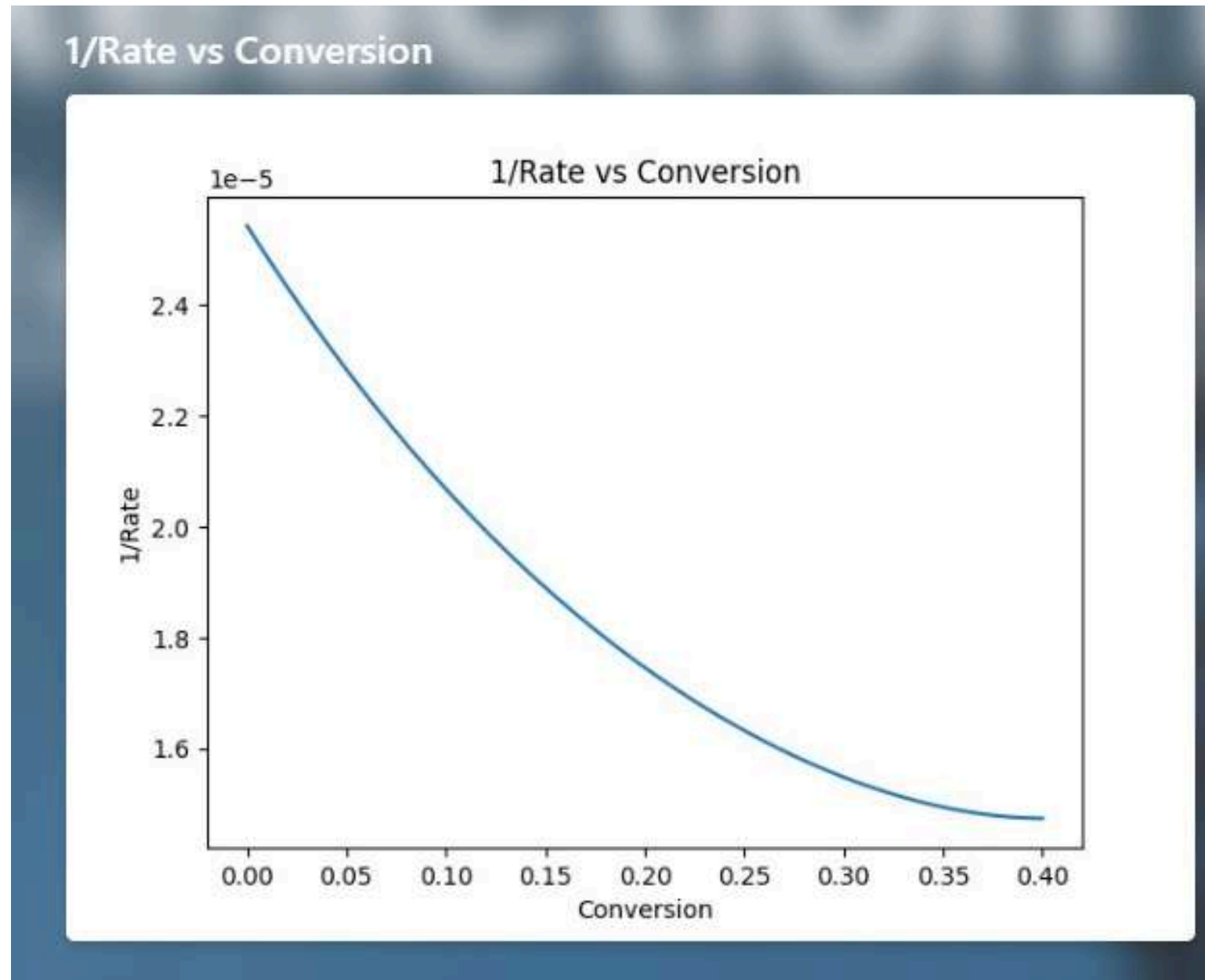- **Final Rate**: 67814.90433031353
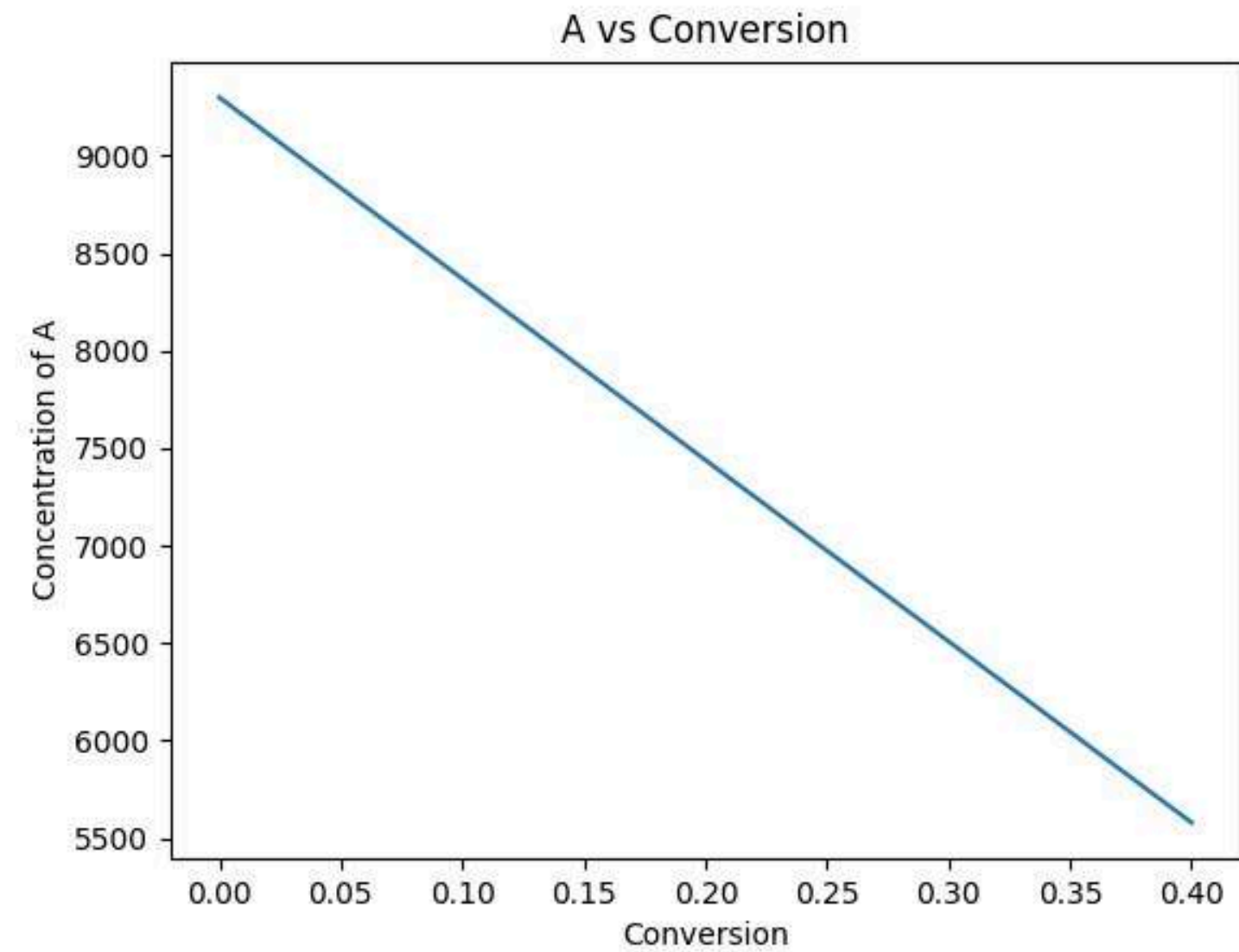
Fig1 graph of 1/rate VS Conversion

Fig2 Concentration of A VS Conversion

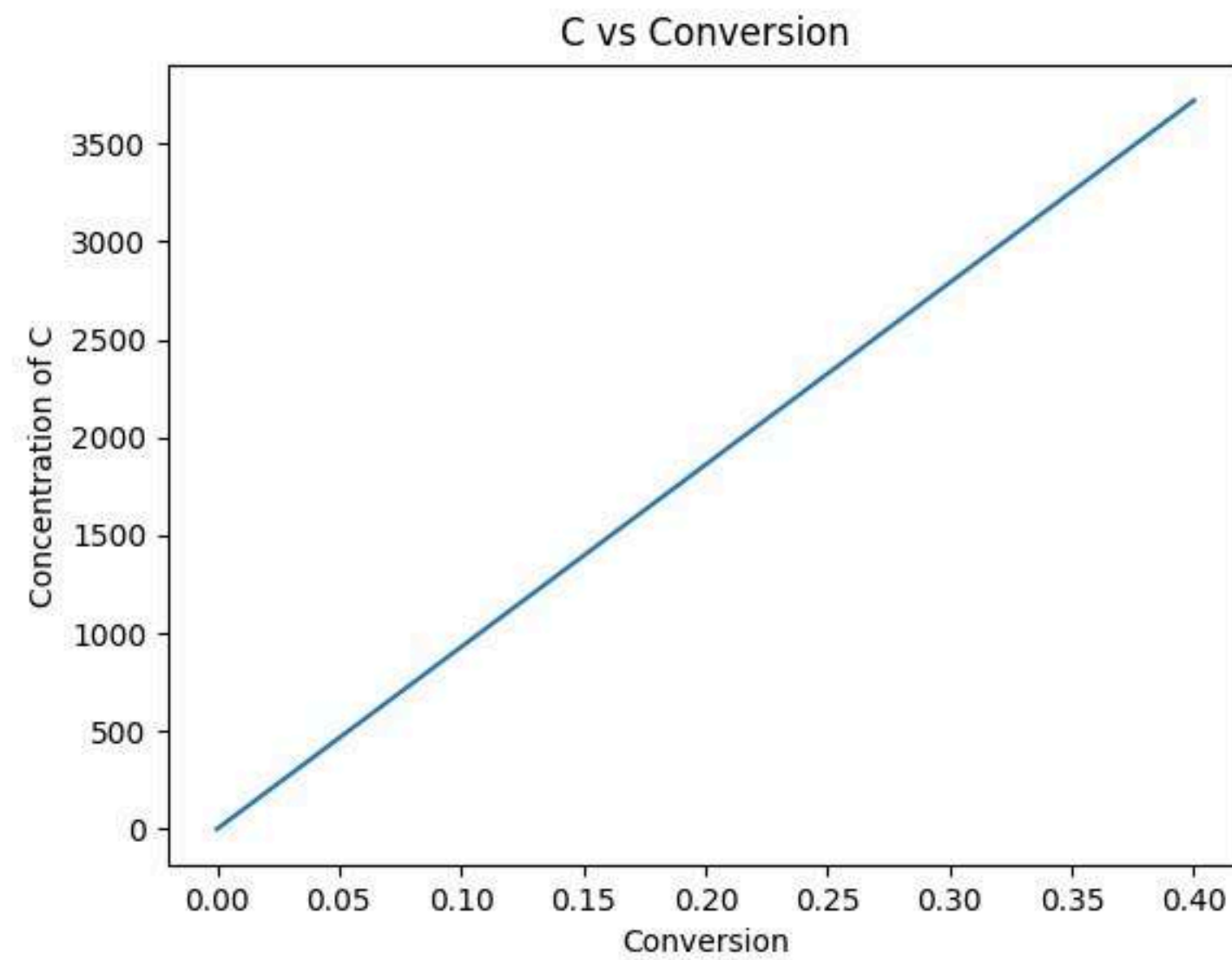$$C_A = \frac{F_A}{v_0} = \frac{F_{A0}(1-X)}{v_0} = C_{A0}(1-X)$$
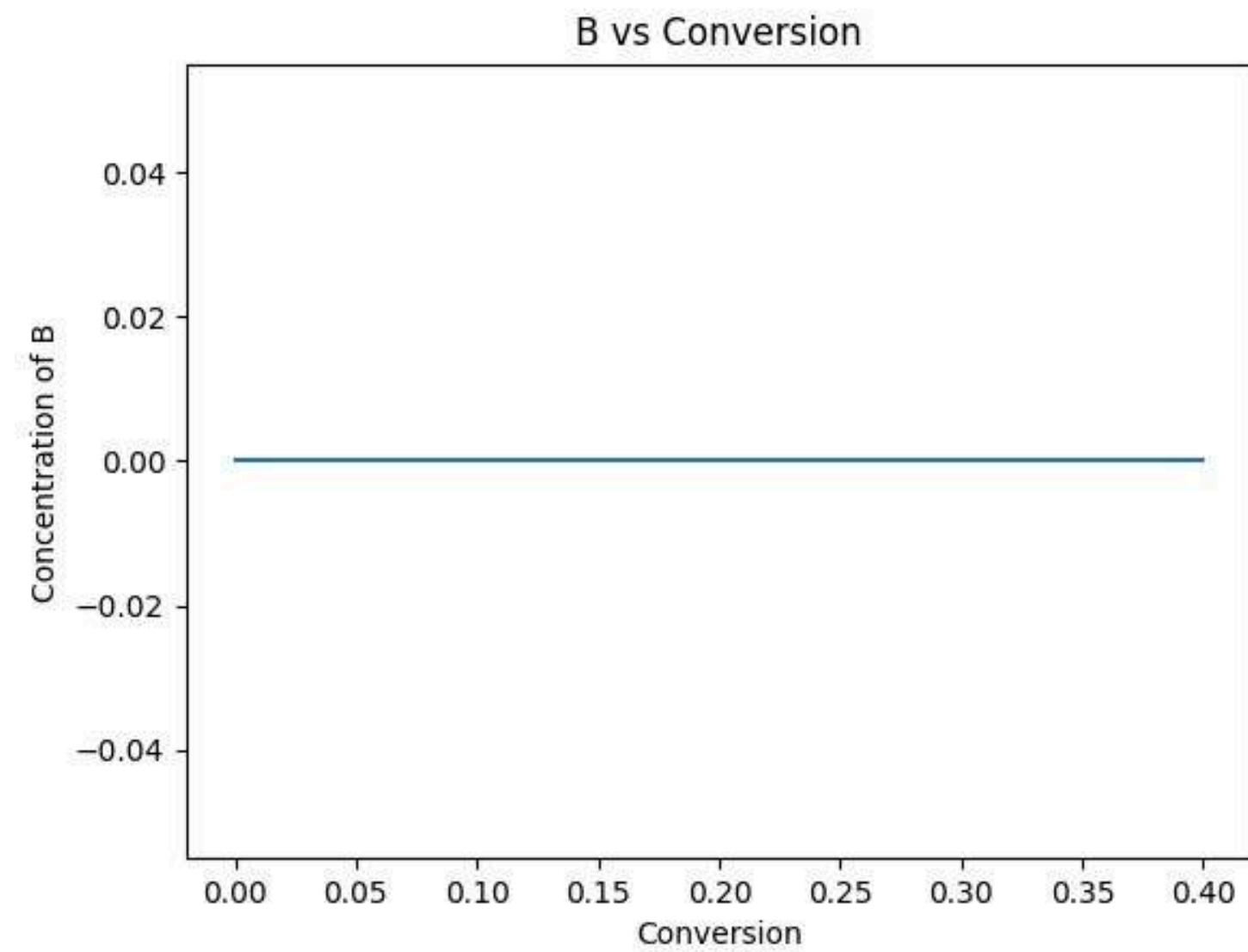
Fig 3 Concentration of C VS Conversion

Fig 4 Concentration of B VS Conversion
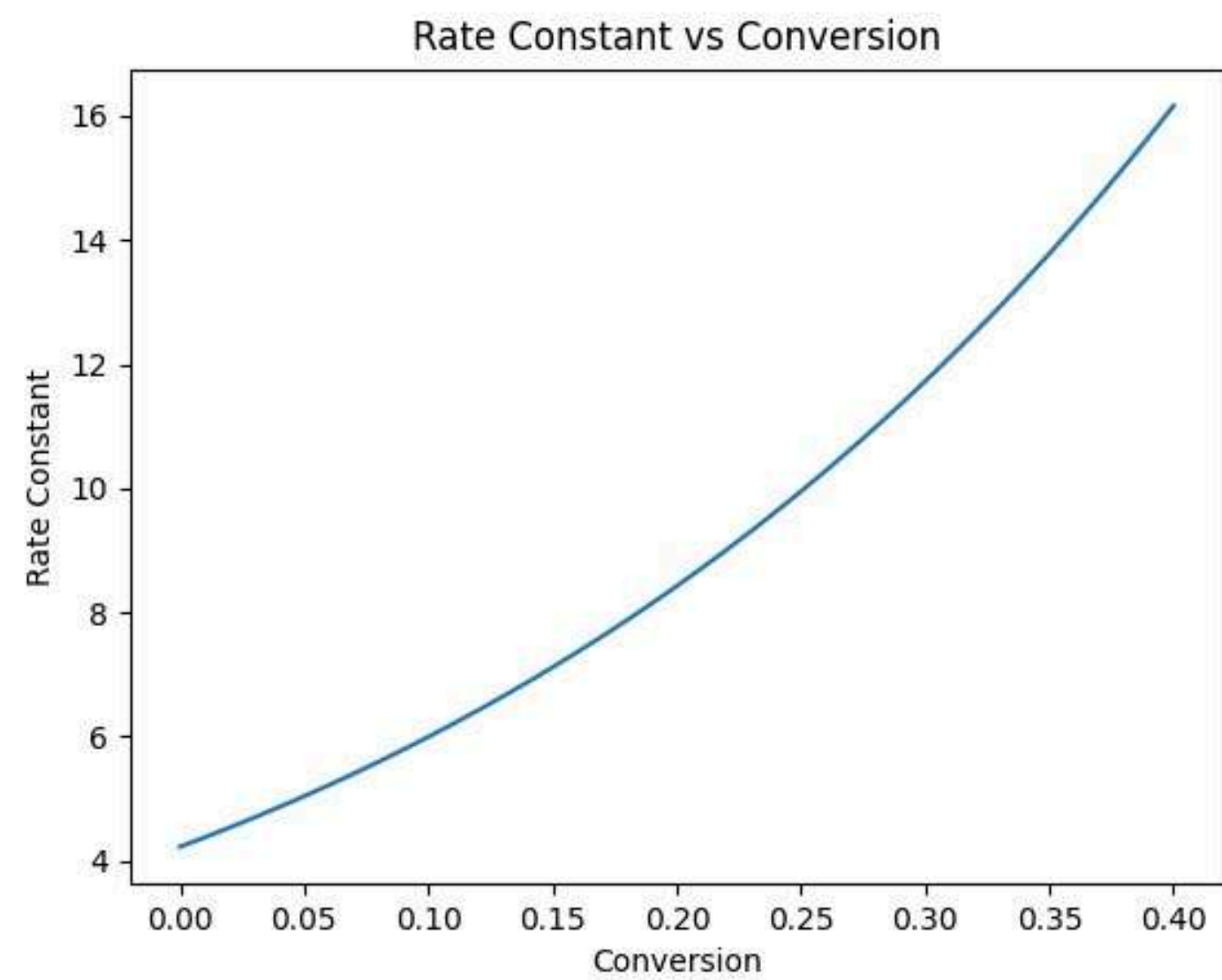
$$C_C = C_{A0}\Theta_C X$$

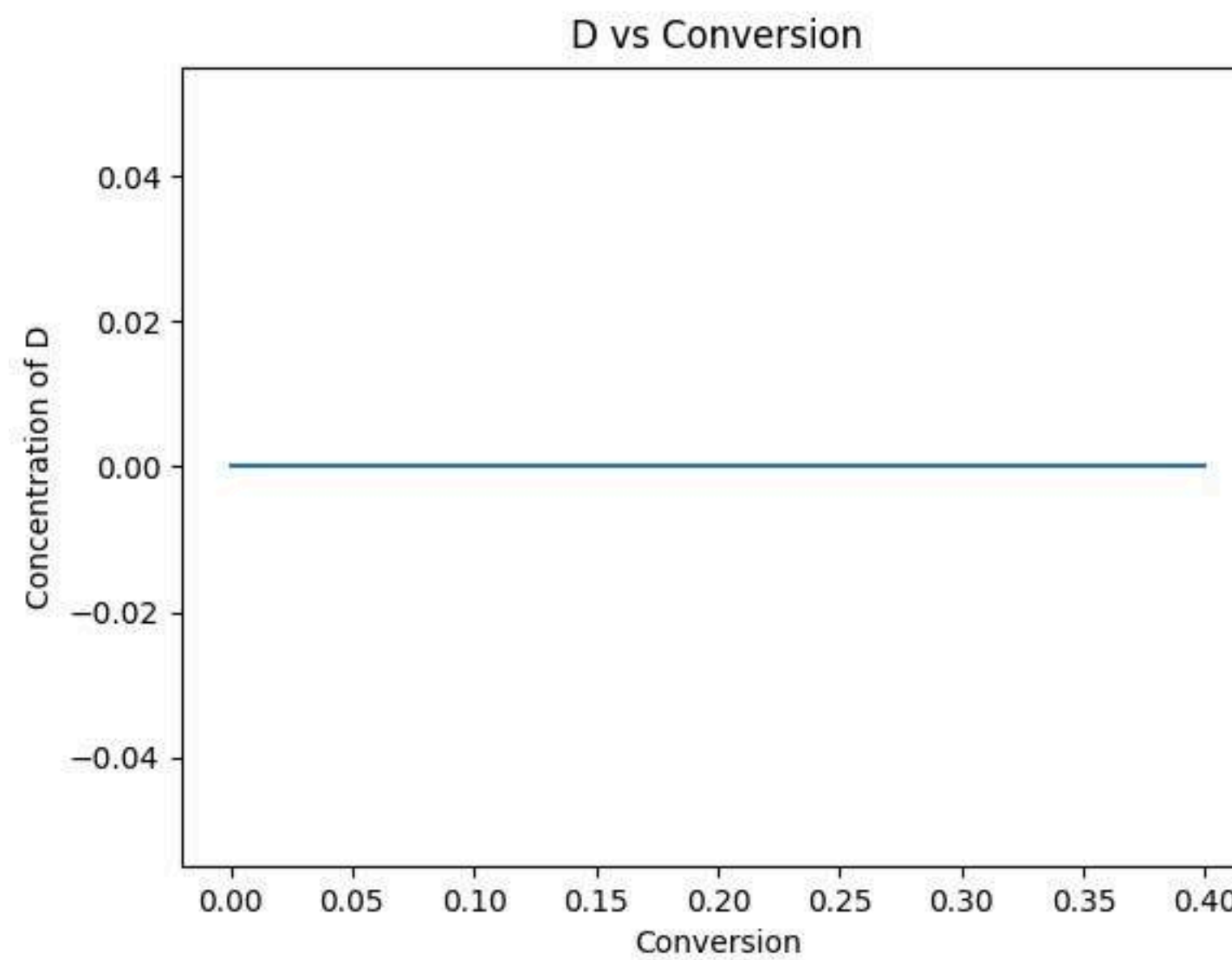Fig 5 Rate Constant VS Conversion
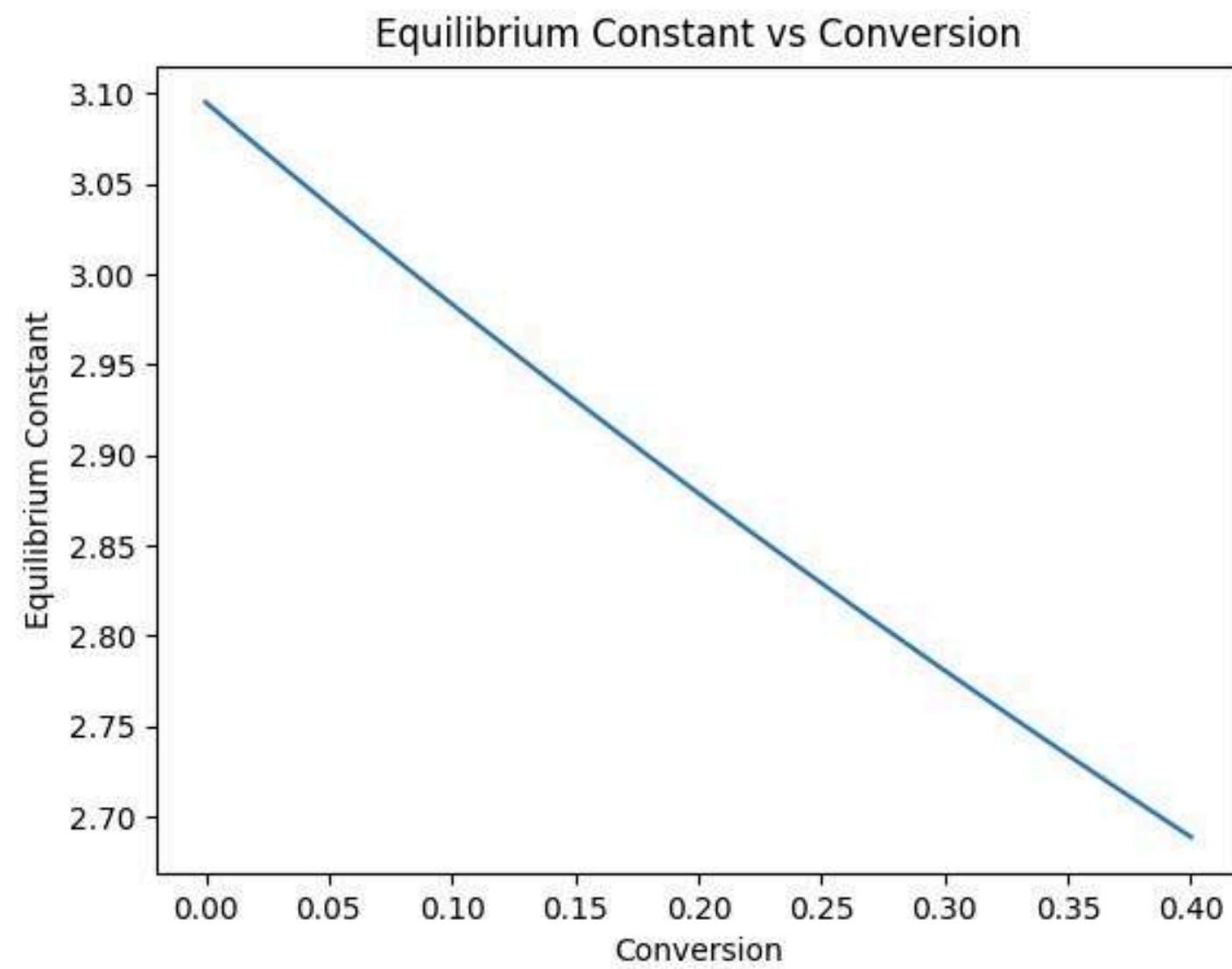

Fig 6 Concentration of D VS Conversion
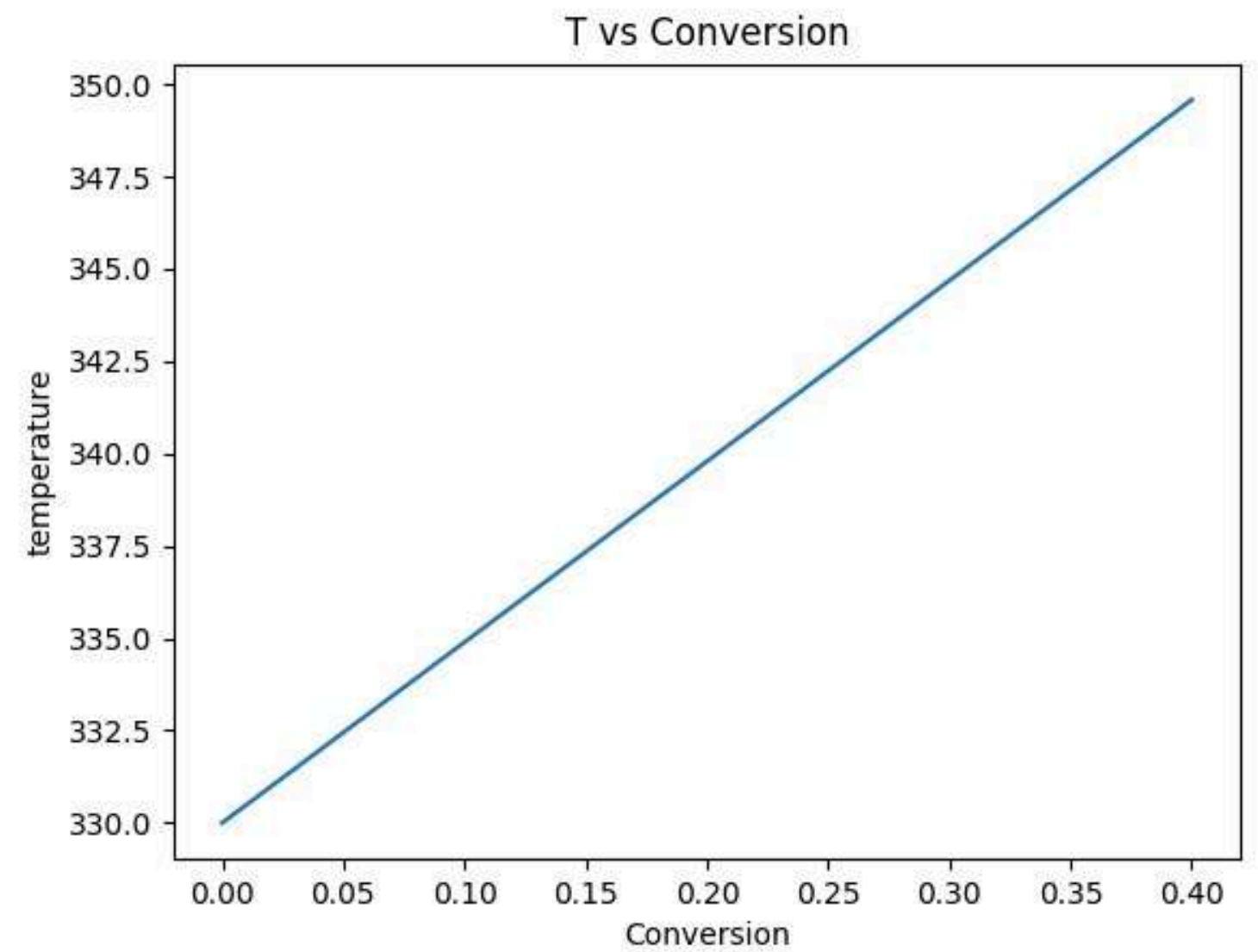
Flig 7 Equilibrium Constant VS Conversion

Fig 8 Tempreature VS Conversion

References:

1.Lecture Notes of Prof. Manjesh Kumar, CHE ,IIT Delhi
2. Elements Of Chemical Reaction Engineering- H. Scott Fogler
3. Chemical Reaction Engineering- Octave Levenspiel

ACKNOWLEDGEMENT

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.