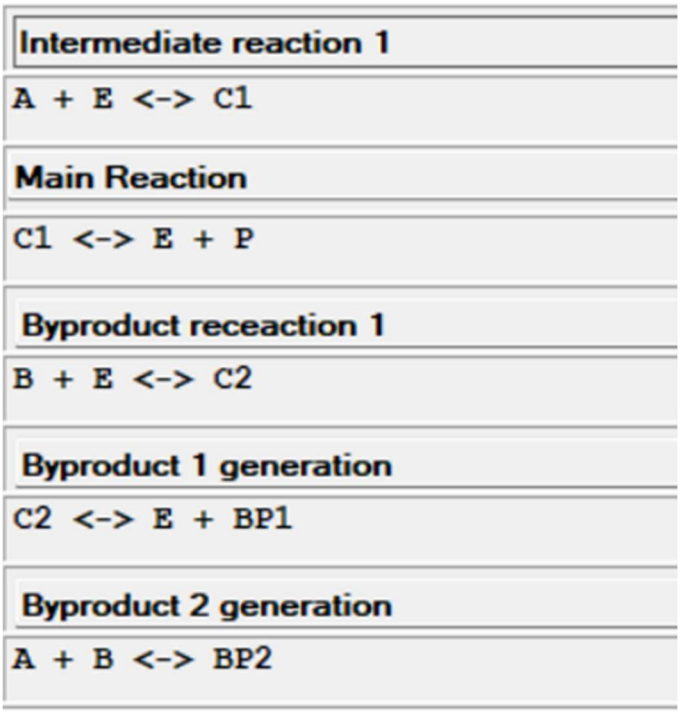
# VISIMIX CHEM
# Continuous flow Process: Enzymatic reaction

**Consider the following enzymatic reaction, which includes a complex intermediate reaction, a main reaction and side reactions that result in by-product formation.**




"Where A and B are the reactants, P is the main product, E is the enzyme, C1 and C2 are the intermediate complexes, and BP1 and BP2 are the by-products".

**Objective:**

To determine the concentration of each reactant, product and by-product as a function of time, analyze the corresponding conversion rates, and generate concentration versus time and conversion versus time graphs to illustrate the kinetics of the enzymatic reaction in the continuous process.

**Initial data:**

Process temperature: 26.85 °C
Solvent: Organic polar (alcohol)
Solvent molar mass: 88 g/mol

Reactant A:
Molecular weight= 101 g/mol
Molar concentration in the Feed 1 = 2 mol/L
Inlet 1 flow rate = 100 L/min

Reactant B:
Molecular weight= 86 g/mol
Molar concentration in the Feed 2= 1 mol/L
Inlet 2 flow rate = 100 L/min

Main Product (P):
Molecular weight= 101 g/mol

Enzyme(E):
Molecular weight= 1800 g/mol
Initial concentration in the tank = 0.01 mol/L
Molar concentration in the Feed 2 = 0.05 mol/L

By-products:
BP1 molecular weight= 86 g/mol
BP2 molecular weight= 187 g/mol

Intermediates:
Intermediate 1 molecular weight= 1900 g/mol
Intermediate 2 molecular weight= 1890 g/mol

Tank: Flat Bottom
Inside diameter = 1000 mm;
Total tank height = 2001 mm;
Fluid level = 1600 mm;

Baffles: Flat baffles
Number of baffles= 4
Baffle length= 1800 mm
Baffle width= 100 mm
Distance from the tank bottom= 0 mm
Angle between baffle and radius= 0°

Impeller: Paddle
Tip diameter = 400 mm
Number of blades = 2
Blade width = 50 mm
Distance from bottom = 305 mm.
Number of impellers= 3

Distance between the stages= 400 mm
Rotational speed = 60 rpm
Motor power = 1111 W

Fluid properties:
Average density= 814 kg/$m^3$
Dynamic viscosity= 3.5 cP (Newtonian fluid)

It is a continuous process. The process duration is 2000 seconds.

**The Solution:**

Application of VisiMix Chem program starts with Opening of a Project. StartVisiMix program. The main menu appears on the screen (Figure 1).


**Figure 1. The main menu bar**

Select **Project** in the Menu bar. Figure 2 appears.

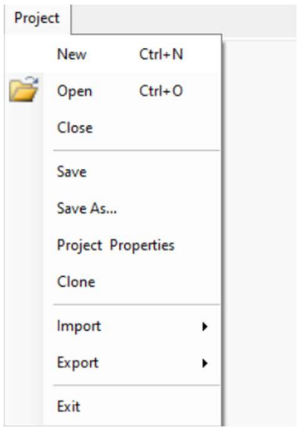



**Figure 2. The Project sub-Menu.**

Select **New** from the sub-Menu. A dialogue box will appear where we need to enter the project name and description as shown in Figure 3

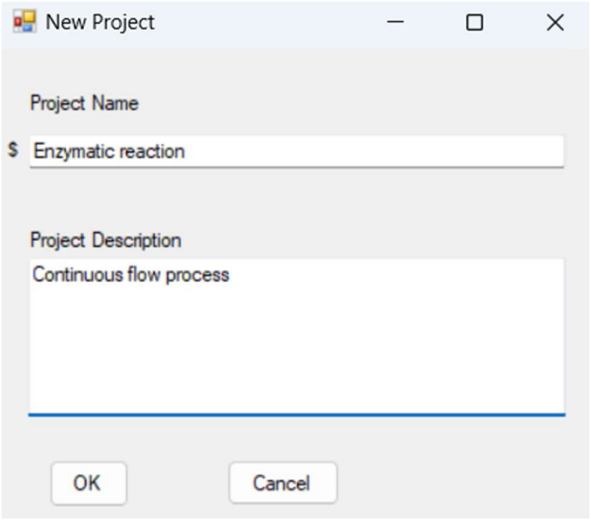



**Figure 3. Starting a new Project.**

Click **Ok** to proceed further.

Then input the data related to **Chemistry,** such as solvent, reactants, process temperature, and chemical reactions from the Edit input> Chemistry menu.

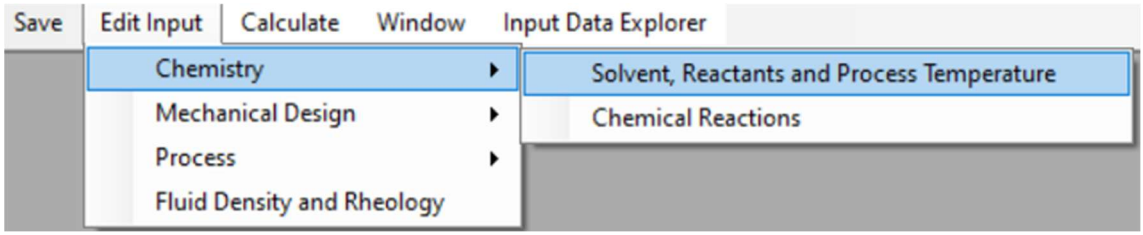



**Figure 4. Edit Input - Chemistry menu for Solvent, Reactants and Process temperature data**

Select **Solvent, Reactants and Process temperature**. A new window will appear where we can enter the corresponding data. All the reactants, product, enzyme, intermediates and byproducts along with their molecular weights and concentrations should be entered in the fields provided.

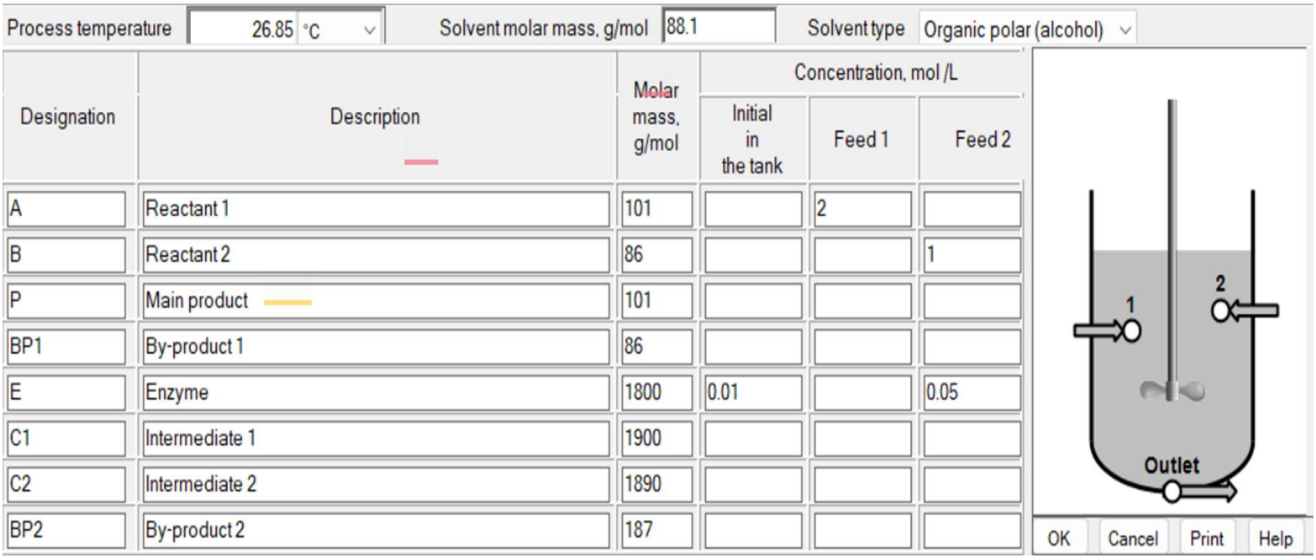



**Figure 5. Input the process temperature, solvent and reactants data**

Click **OK** to confirm, then navigate to the **Edit Input > Chemistry** menu and select the **Chemical Reactions** to enter the data.

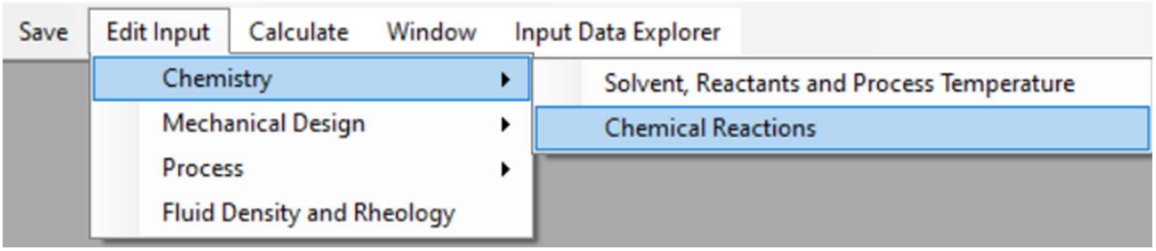



**Figure 6. Edit Input - Chemistry menu for Chemical reaction data**

The below window appears; Click '**Add**' option in any row to enter kinetics input data for a new chemical reaction, or **Edit** button in a row, which corresponds to a previously entered chemical reaction, in order to update kinetics input data for this reaction.

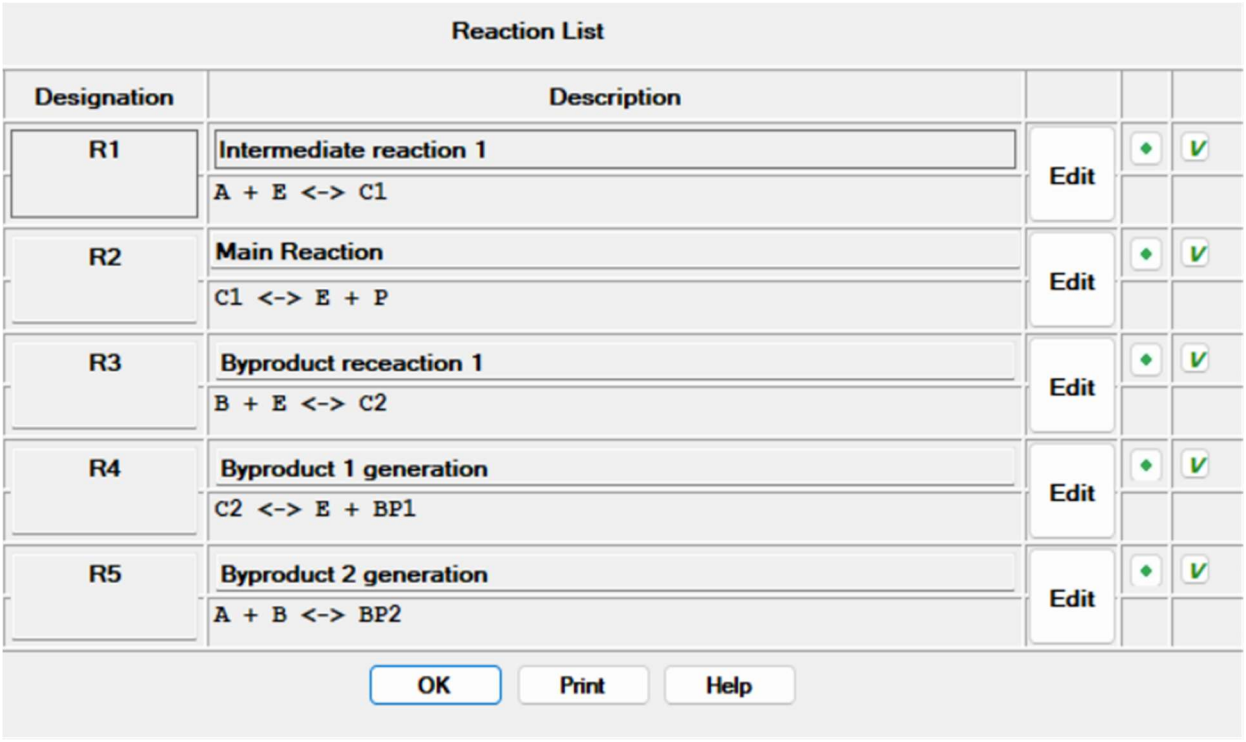



**Figure 7. Click Add/Edit option**

By clicking the **'Add'** option, the below window appears. Please note that all reactants listed in the **Solvent, Reactants and Process Temperature** section will appear in the chemical Equation window. Next, we need to enter the **forward reaction rate constant and reverse reaction rate constant** which is found through experiments.

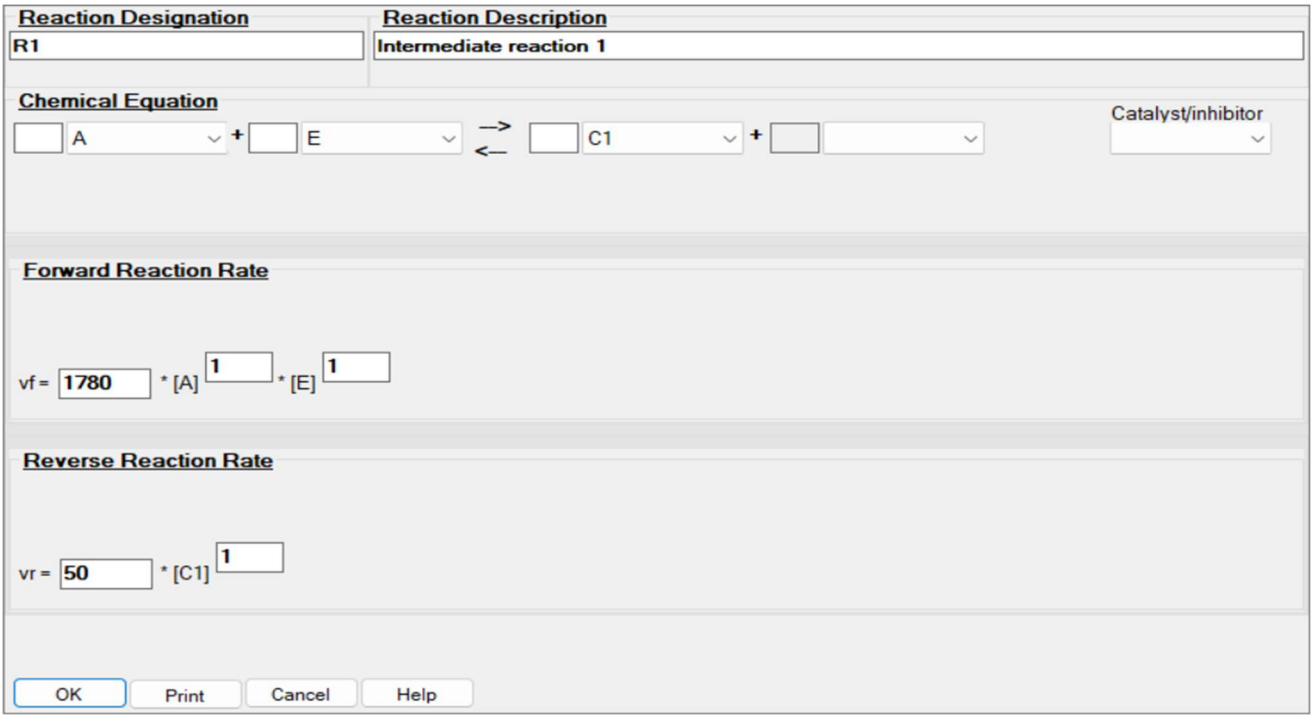



**Figure 8. Input the chemical reaction kinetics data for the Intermediate reaction 1**

Click **OK** to close the intermediate reaction 1 kinetics input window, then select **'Add'** in the second row to enter the main reaction details which is a irreversible reaction. Hence enter the reverse reaction rate constant as zero.

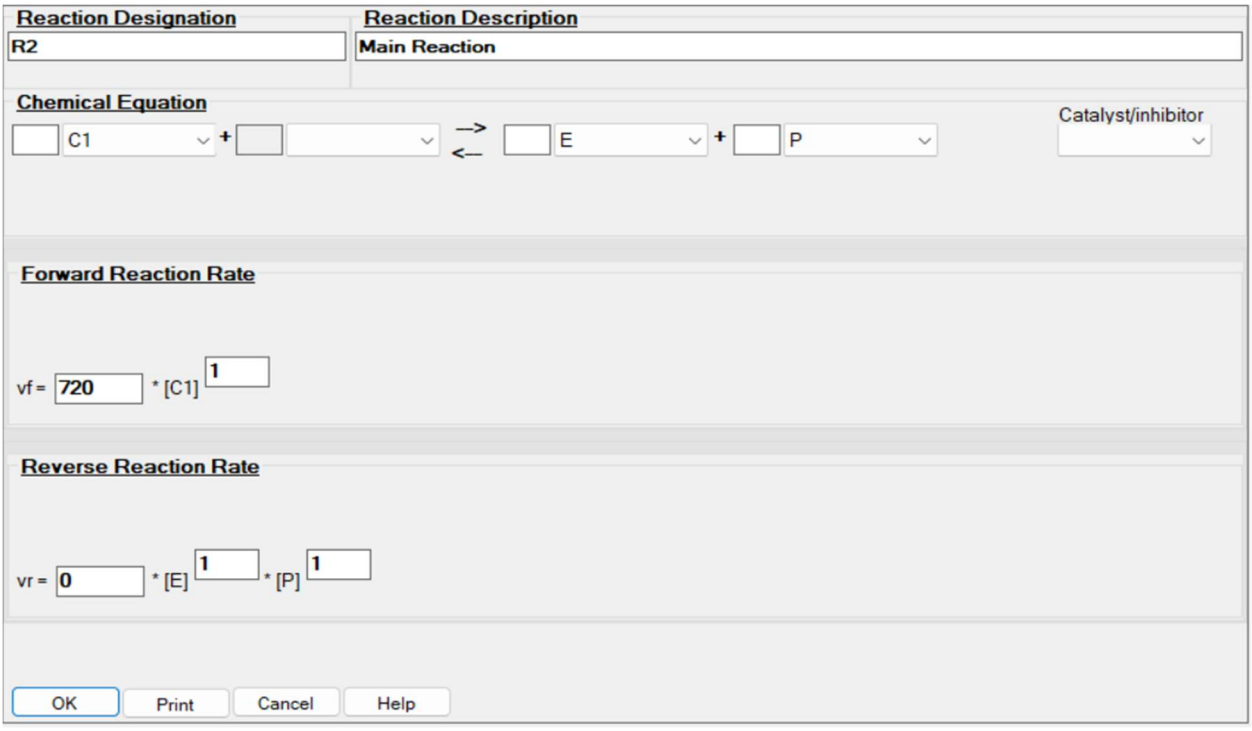



**Figure 9. Input the chemical reaction kinetics data for the main reaction**

Click **OK** to close the main reaction kinetics input window, then select **'Add'** in the third row to enter the reversible byproduct reaction 1 details ,and in the fourth row **Add** irreversible by product generation details.

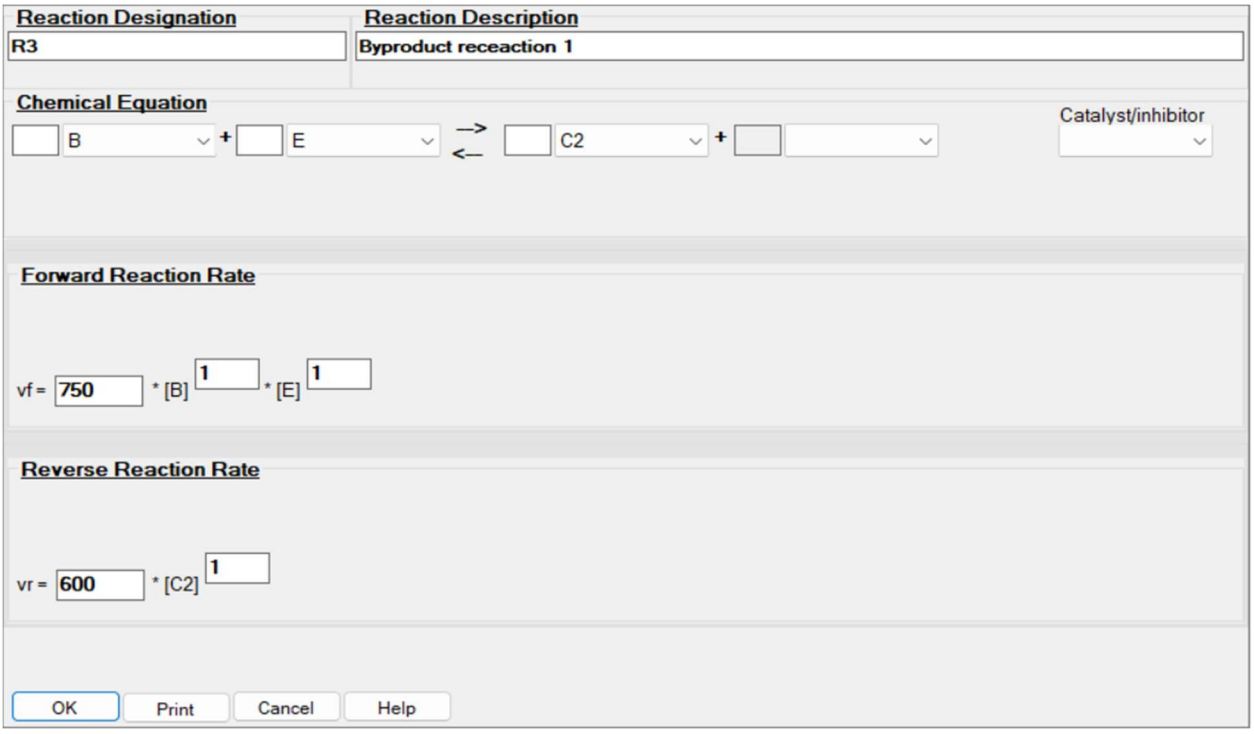



**Figure 10. Input the chemical reaction kinetics data for the byproduct reaction 1**

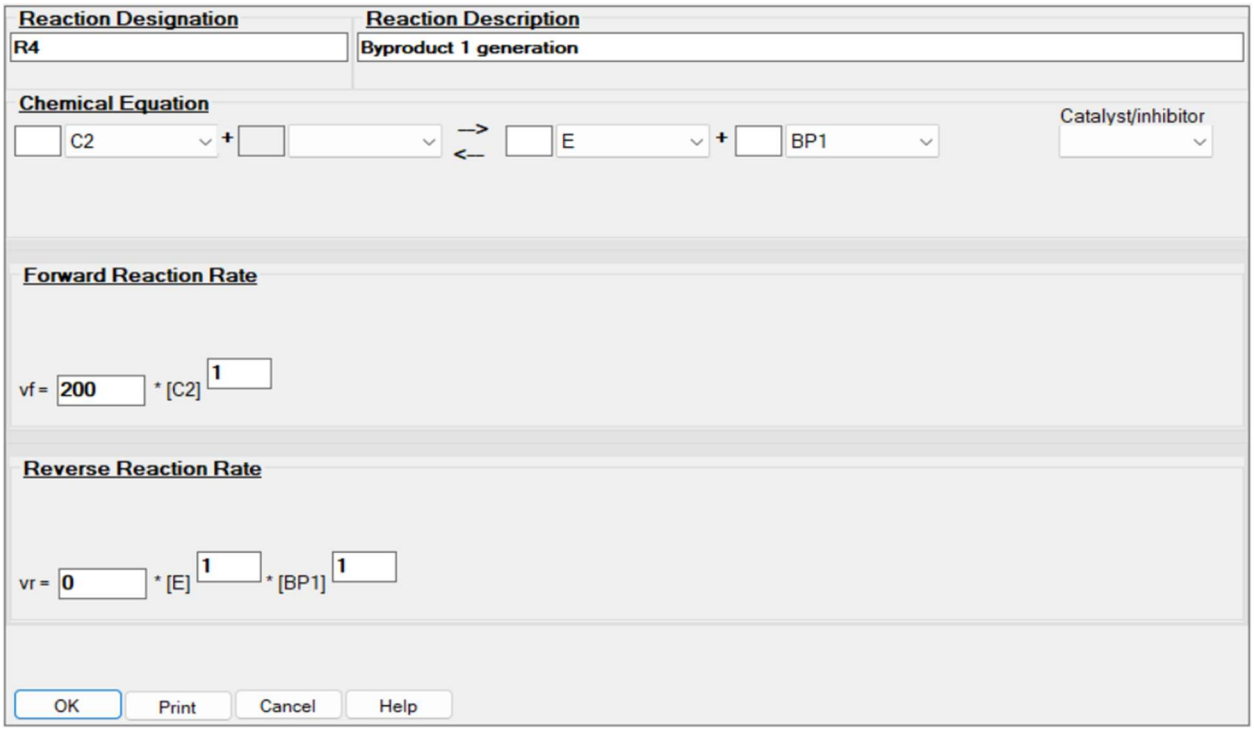



**Figure 11. Input the chemical reaction kinetics data for the byproduct 1 generation**

Click **OK** to close the byproduct 1 generation kinetics input window, then select **'Add'** in the fifth row to enter the irreversible byproduct 2 generation details.

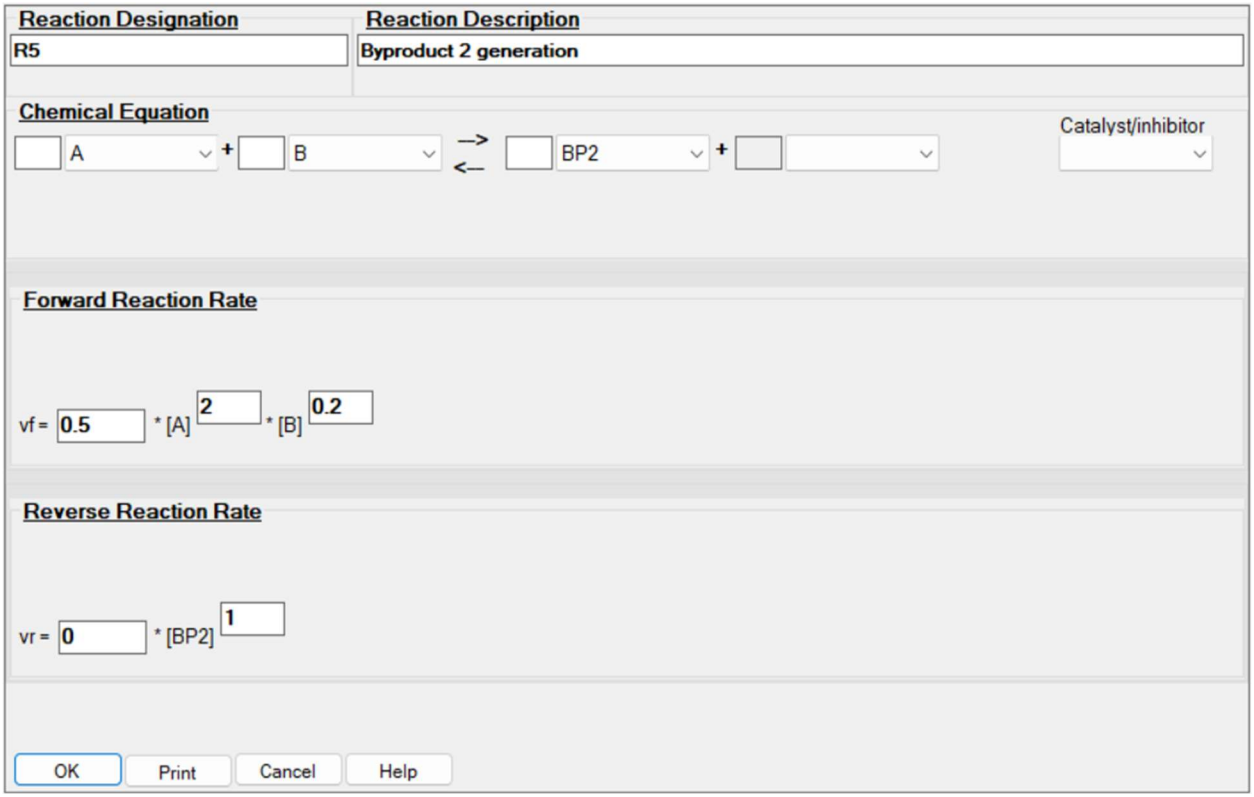



**Figure 12. Input the chemical reaction kinetics data for the byproduct 2 generation**

Press OK to close the byproduct 2 generation Kinetics Input Window. Go to the Edit input menu, then select the **Mechanical Design** option to enter the Tank, Baffles, Impellers and locations of inlets and outlets.

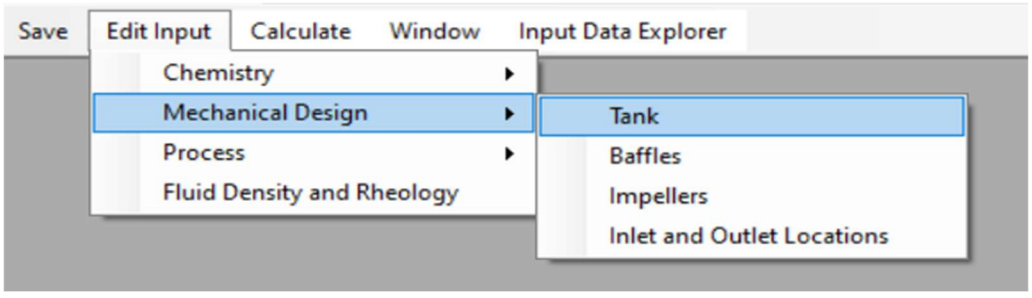



**Figure 13. Edit Input – Mechanical Design Menu**

Select the **Tank (Flat Bottom)** and enter the tank details i.e., tank inner diameter, tank height and fluid level. The system will automatically calculate the tank volume and fluid volume based on the provided parameters.

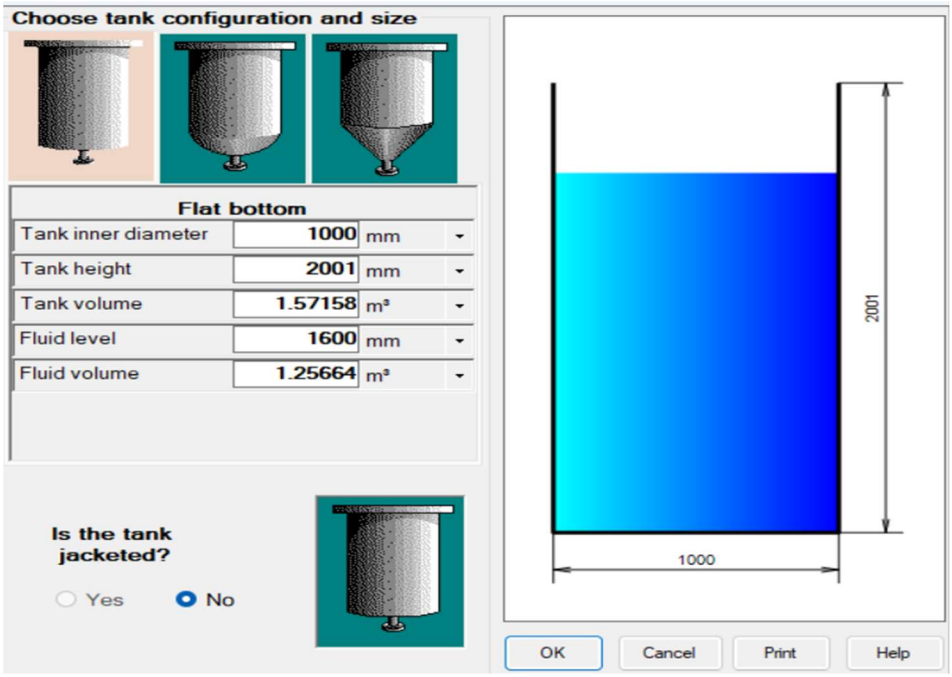



**Figure 14. Enter the tank details**

Choose the baffle type. Select **Flat Baffles** and enter the dimensions of the baffle.

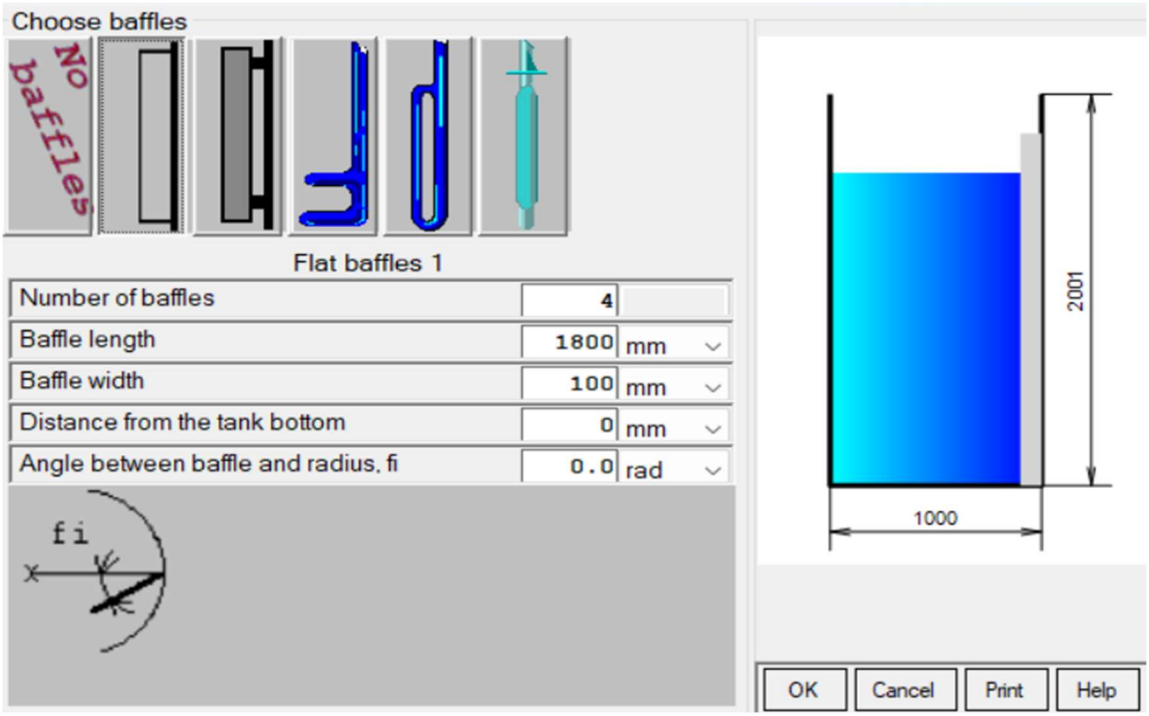



**Figure 15. Choose baffle type**

Select the **impeller type (3 stage - Paddle)** and enter the dimensions of the impeller.

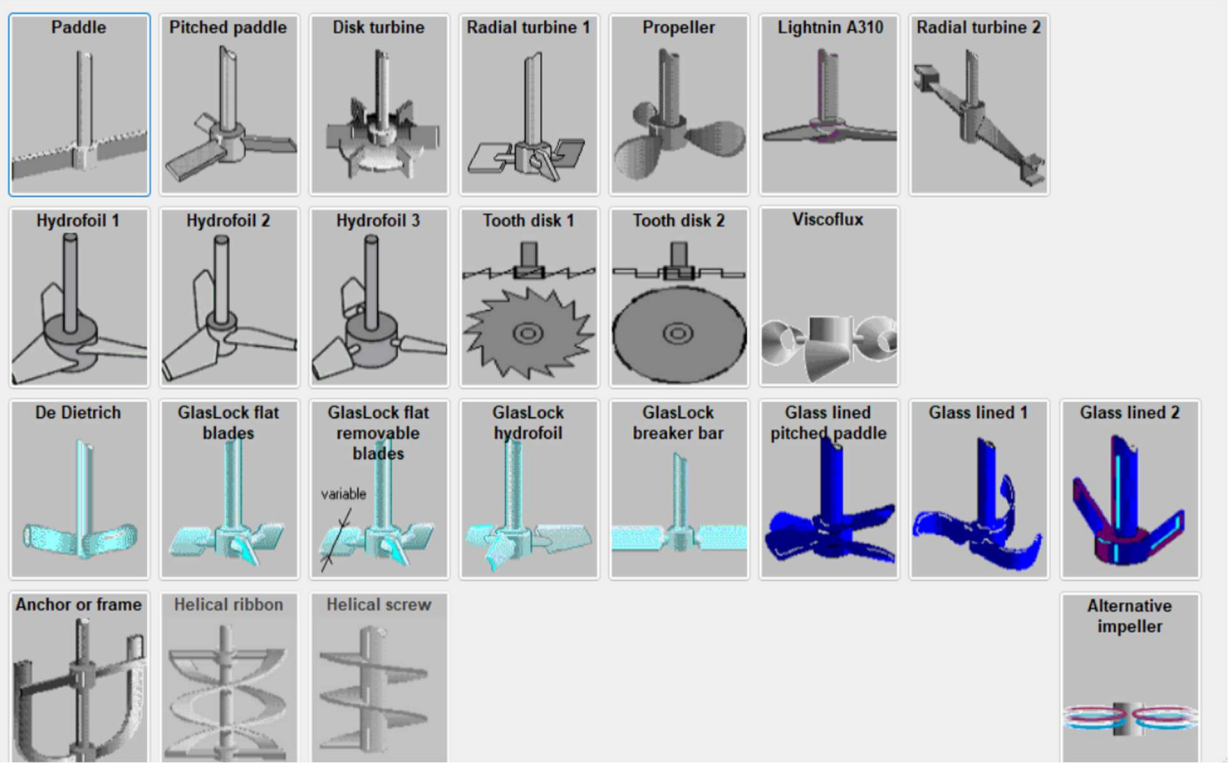



**Figure 16. Select the impeller type**

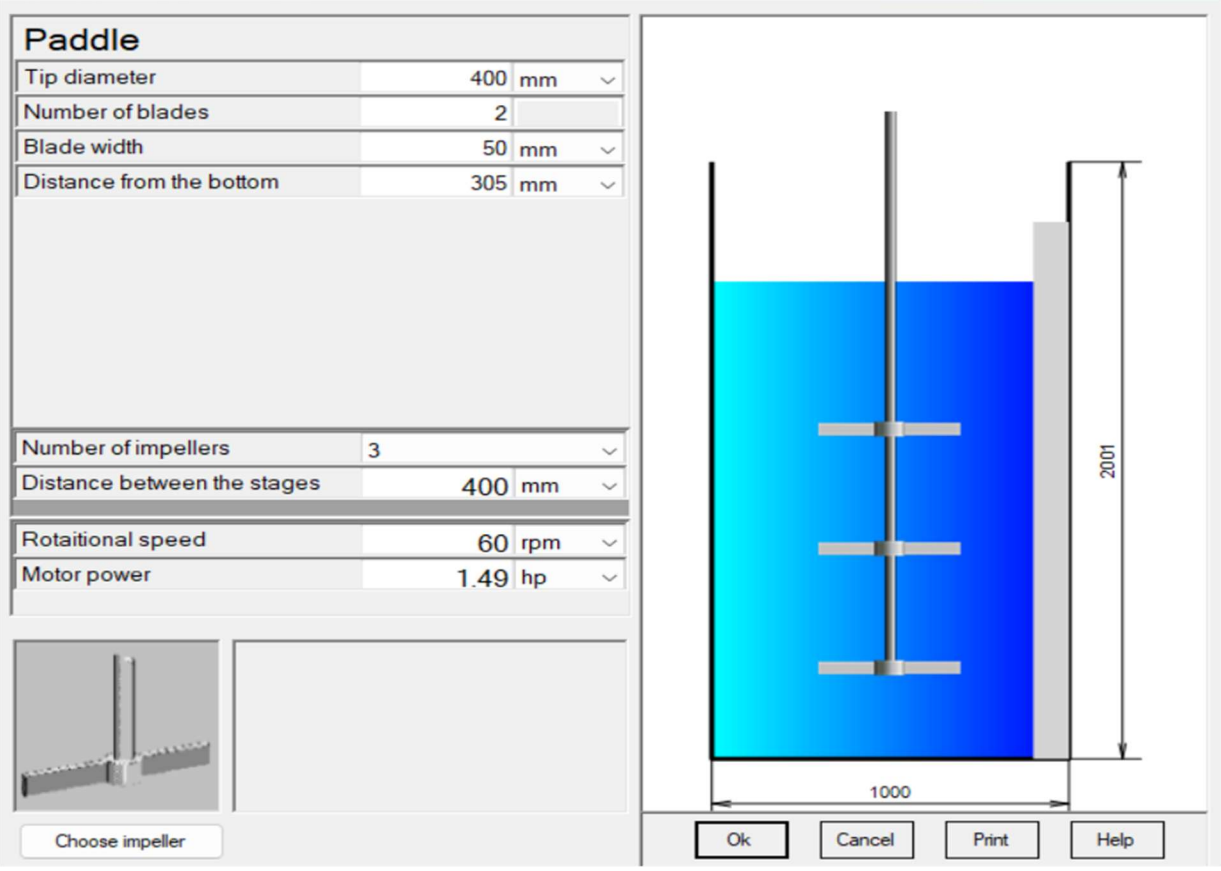



**Figure 17. Enter the impeller dimensions**

Select the **Inlet and Outlet positions** from the **mechanical design** option in the Edit menu.
**Inlet 1** is positioned at the top center of the reactor, along the shaft axis, at a height of 1500 mm from the base, ensuring uniform distribution of the feed throughout the reactor volume.
**Inlet 2** is located on the side of the reactor, near the bottom, at a radius of 500 mm and a height of 450 mm from the base, designed for controlled addition of reactants to enhance localized mixing.
**Outlet** is situated at the bottom center of the reactor (radius = 0 mm, height = 0 mm), allowing efficient removal of the processed stream while maintaining continuous flow conditions.

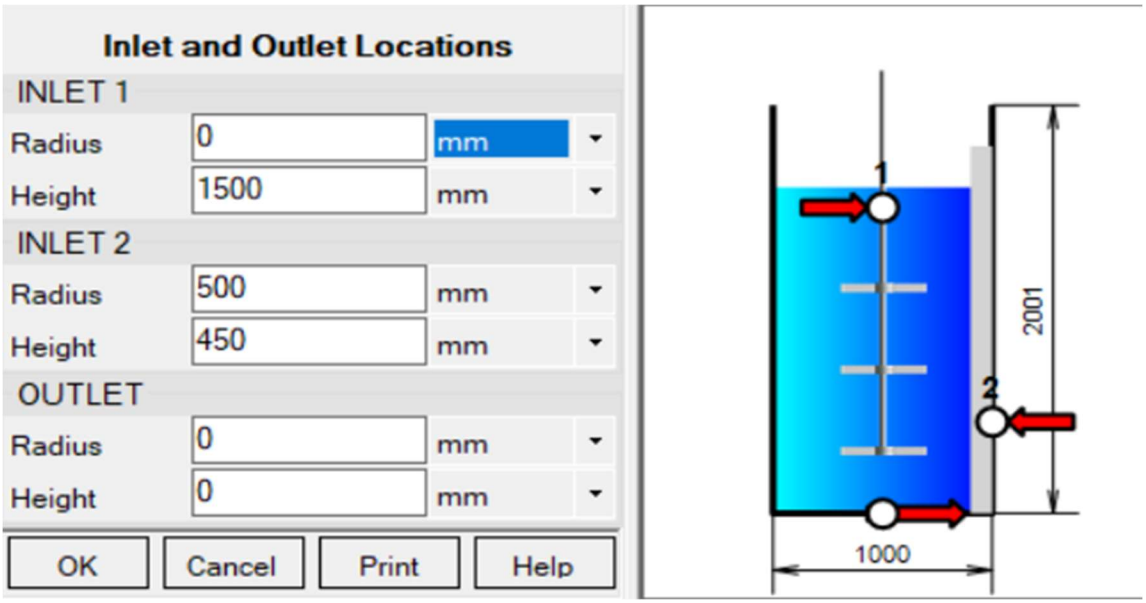



**Figure 18. Enter the Inlet and outlet positions**

Click OK to confirm and then select **Process** from the Edit Input menu.

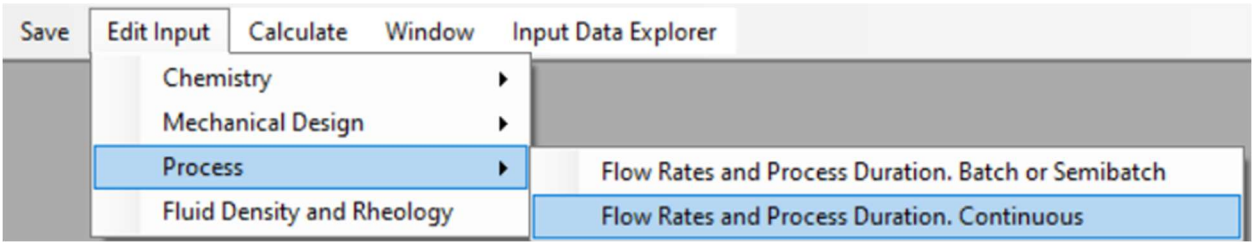



**Figure 19. Edit Input – Process menu**

Since ours is a continuous process, select the continuous option and enter the flow rate of reactants and the process duration in the window below.

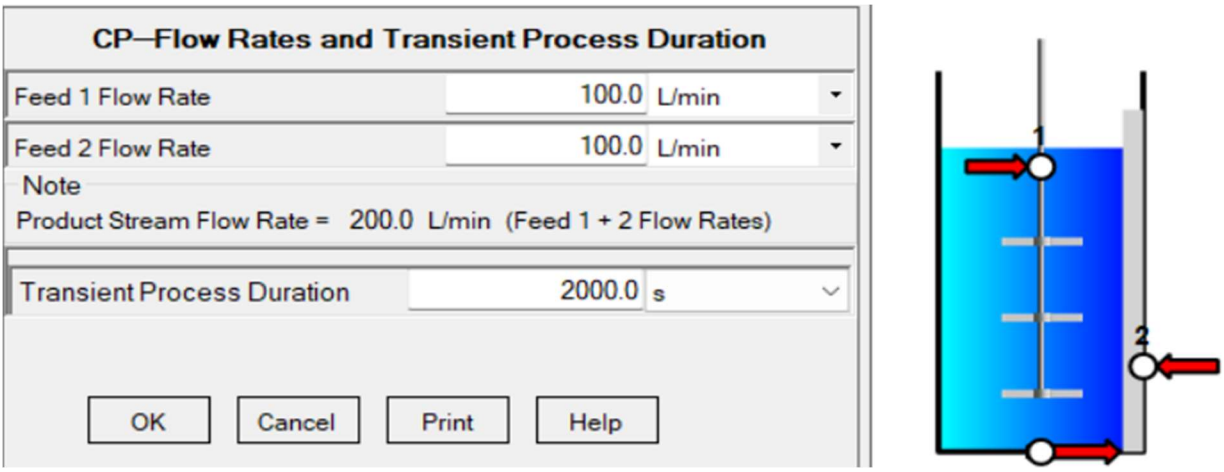



**Figure 20. Input the feed flow rate and process duration**

Click OK to confirm and then navigate to the Edit menu to further enter the fluid density and viscosity.

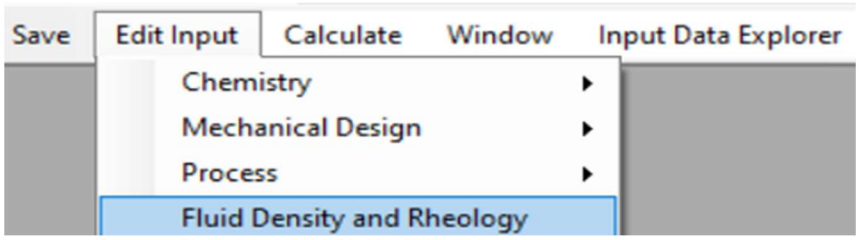



**Figure 21. Edit input – Fluid density and Rheology**

Enter the Average density and dynamic viscosity.

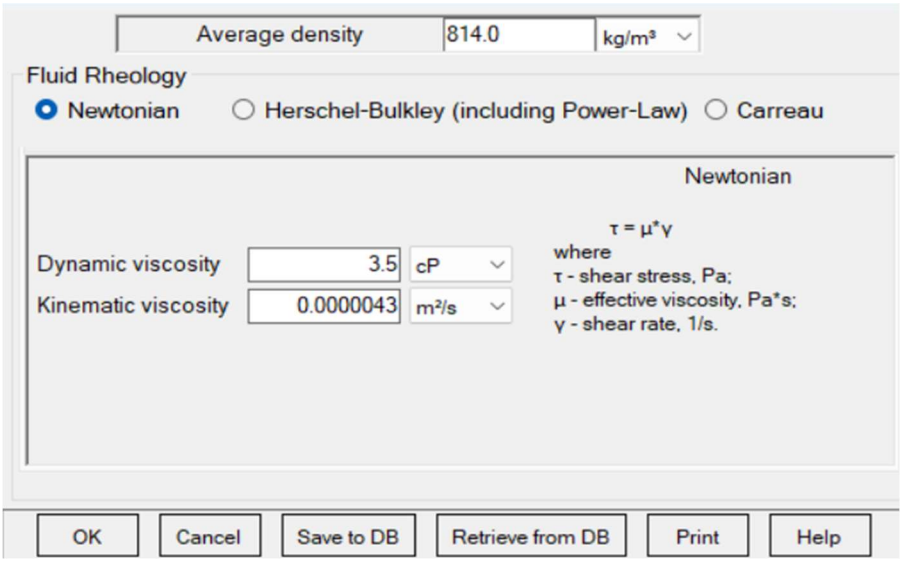



**Figure 22. Input Fluid density and Rheology data**

Click **OK** to confirm.

**Results of Mathematical Modelling**

Once the input parameters have been entered, navigate to the Calculate menu, then select Continuous flow Process > Final Parameters > Average Composition.

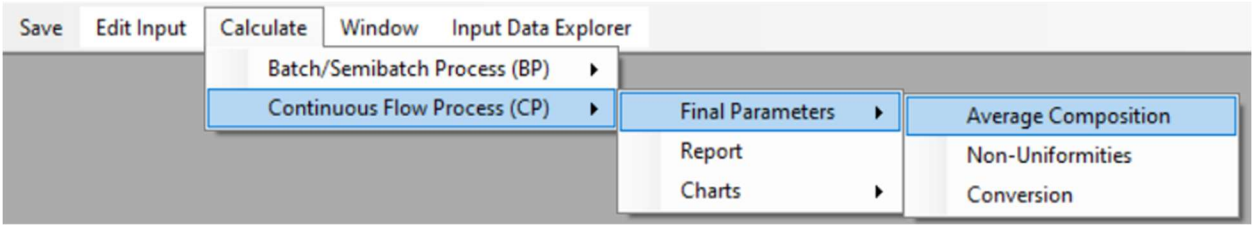



**Figure 23. Select Calculate Menu-Final Parameters**

Next, run the simulation in order to calculate the average composition, non-uniformities and conversion.

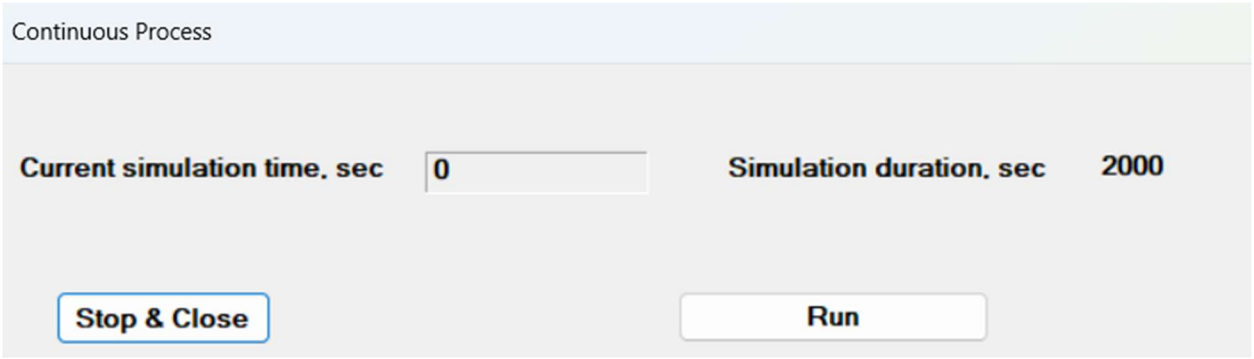



**Figure 24. Run the simulation**

The concentrations of the reactants, product, enzyme, intermediates and by-product (mol/L) in the tank and in the product stream are automatically calculated, taking into account both the actual reactor scenario and a reactor with ideal macromixing for ease of comparison, as presented in the window below:

**Continuous Flow Process—Average Concentrations, mol/L**

At the end of the transient process of requested duration

| | Reactant Designation | Actual Reactor—Tank | Actual Reactor—Product Stream | Reactor with Perfect Macromixing |
|---|---|---|---|---|
| ▶ | A | 0.9942 | 0.6648 | 0.5964 |
| | B | 0.1072 | 0.1929 | 0.1293 |
| | P | 0.01657 | 0.01731 | 0.02418 |
| | BP1 | 0.001394 | 0.001632 | 0.002503 |
| | E | 0.01067 | 0.01547 | 0.01444 |
| | C1 | 0.006823 | 0.008441 | 0.009587 |
| | C2 | 0.00058 | 0.001059 | 0.000898 |
| | BP2 | 0.2513 | 0.3027 | 0.3648 |
| * | | | | |

**Figure 25. Average concentration in the reactor mol/L**

Under Final Parameters> **Non-Uniformities** calculation, a window will appear where the local concentration standard deviation and the difference between the maximum and minimum local concentrations are calculated. The **local concentration standard deviation** is determined based on the concentration distribution throughout the bulk of the reactor. The **difference between the maximum and minimum local concentrations** represents the greatest variation in reactant concentration observed between any two points within the reactor.

**Continuous Flow Process—Concentration Non-Uniformities in Actual Reactor, mol/L**

At the end of the transient process of requested duration

| | Reactant Designation | Local Concentration Standard Deviation | Difference between the Maximum and Minimum Local Concentrations | Average Concentrations |
|---|---|---|---|---|
| ▶ | A | 0.2483 | 0.6372 | 0.9942 |
| | B | 0.07023 | 0.2007 | 0.1072 |
| | P | 0.000782 | 0.002487 | 0.01657 |
| | BP1 | 0.000169 | 0.000487 | 0.001394 |
| | E | 0.003853 | 0.01077 | 0.01067 |
| | C1 | 0.001134 | 0.003153 | 0.006823 |
| | C2 | 0.00032 | 0.000826 | 0.00058 |
| | BP2 | 0.03631 | 0.1023 | 0.2513 |
| * | | | | |

**Figure 26. Concentration Non-Uniformities in Actual Reactor, mol/L**

Next, navigate to Final Parameters> **Conversion** calculation, the following window will appear:

**Continuous Flow Process—Reactant Conversion**

At the end of the transient process of requested duration

| | Reactant Designation | Actual Reactor–Product Stream | Reactor with Perfect Macromixing |
|---|---|---|---|
| ▶ | A | 0.3352 | 0.4036 |
| | B | 0.6141 | 0.7414 |
| | P | | |
| | BP1 | | |
| | E | 0.3813 | 0.4225 |
| | C1 | | |
| | C2 | | |
| | BP2 | | |
| * | | | |

**Figure 27. Reactant conversion**

We can navigate to the Calculate menu>Continuous flow process>Charts to view the concentration versus time for each reactant and product as well as the conversion versus time for each reactant.

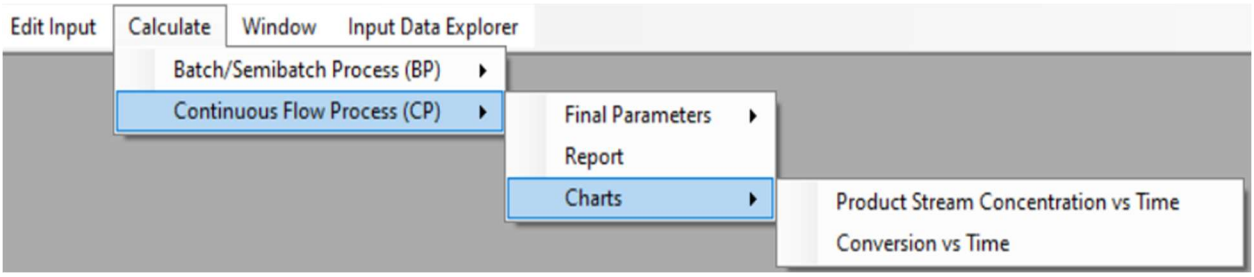



**Figure 28. Select Calculate Menu- Charts**

### Product Stream Concentration Vs time graph

The concentration versus time graphs for each reactant, product, enzyme, intermediates and by-product are presented below, considering both the actual reactor and the reactor with perfect macromixing.

### Reactant A

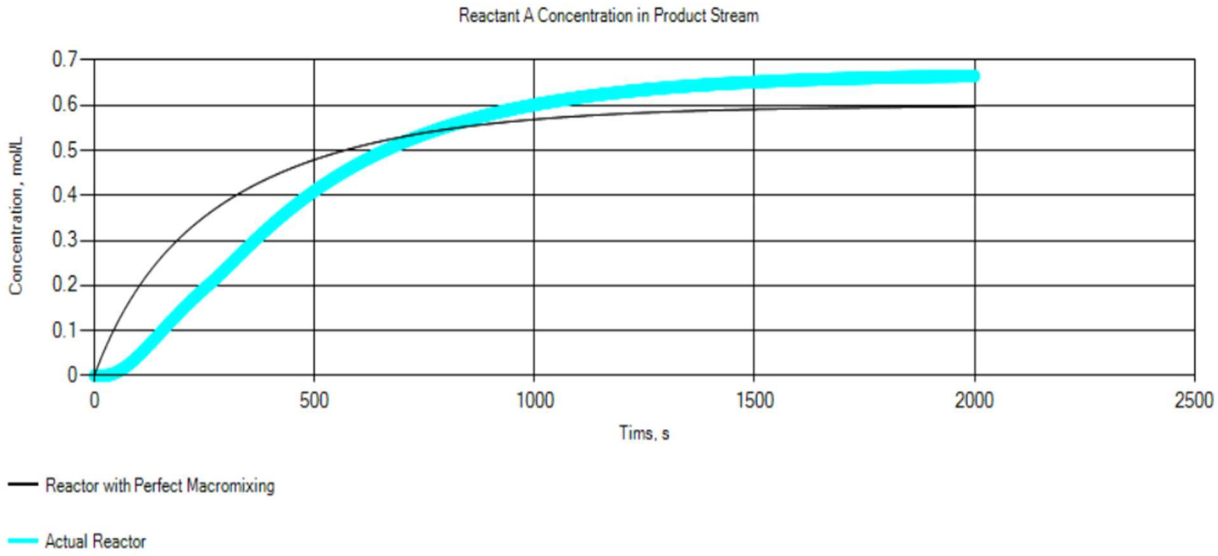



**Figure 29. Concentration Vs time graph– Reactant A**

This graph compares the concentration profile of Reactant A in the product stream for an ideal reactor with perfect macromixing and an actual reactor under continuous process flow conditions. In the actual reactor, the concentration gradually increases, taking approximately **2000 seconds** to stabilize at **0.66 mol/L**, whereas the perfect macromixing reactor reaches the

steady-state concentration much faster at **0.59 mol/L**, within about **1800 seconds**. This comparison highlights how local micro-mixing influences the behavior, reactant distribution, reaction kinetics and overall efficiency of the actual reactor.

**Reactant B**

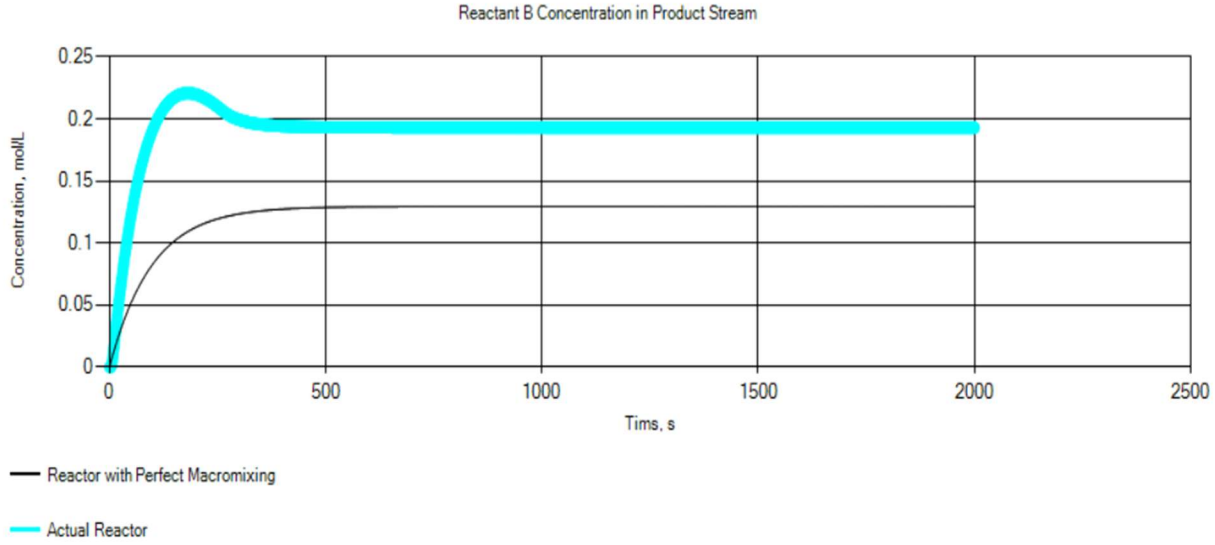



**Figure 30. Concentration Vs time graph – Reactant B**

In the actual reactor, the concentration of Reactant B initially peaks at approximately **0.22 mol/L** due to non-ideal mixing or localized accumulation, then gradually decreases, stabilizing at steady-state near **0.19 mol/L** after approximately **1000 seconds**. In contrast, the perfect macromixing reactor shows a smoother profile, reaching steady-state at the lower concentration of **0.13 mol/L** much earlier, within about **800 seconds**.

**Product P**

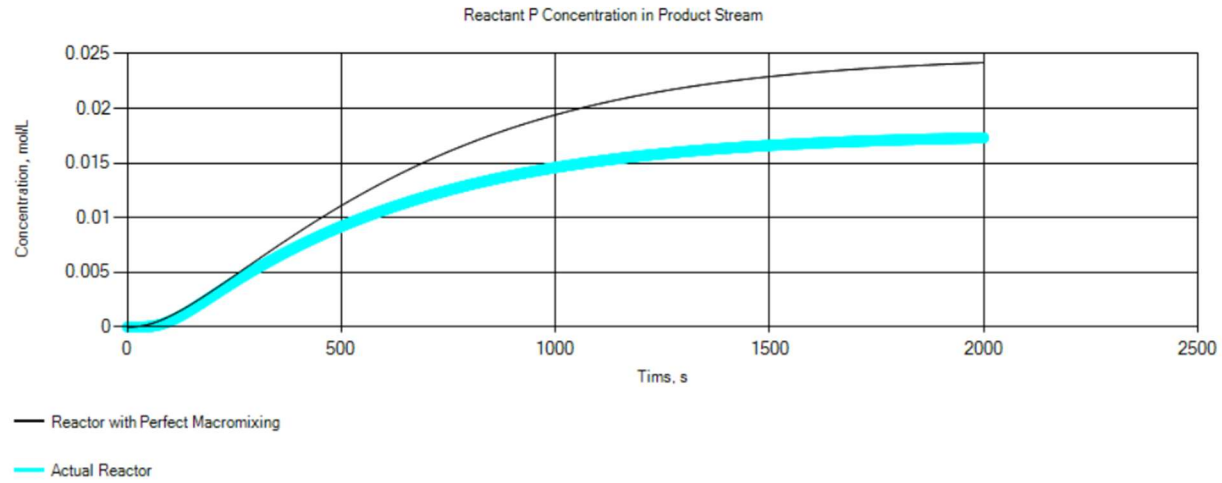



**Figure 31. Concentration Vs time graph – Product P**

In the actual reactor, the concentration gradually increases and stabilizes at approximately **0.017 mol/L** after **2000 seconds**. This slower rise and lower steady-state concentration reflect the effects of non-ideal mixing and localized concentration gradients, which limit reaction efficiency. In contrast, the reactor with perfect macromixing achieves a higher product concentration of **0.024 mol/L**, owing to uniform mixing and better reactant utilization. The difference between the two curves emphasizes the impact of mixing dynamics on product formation efficiency and reactor performance.

### Enzyme concentration

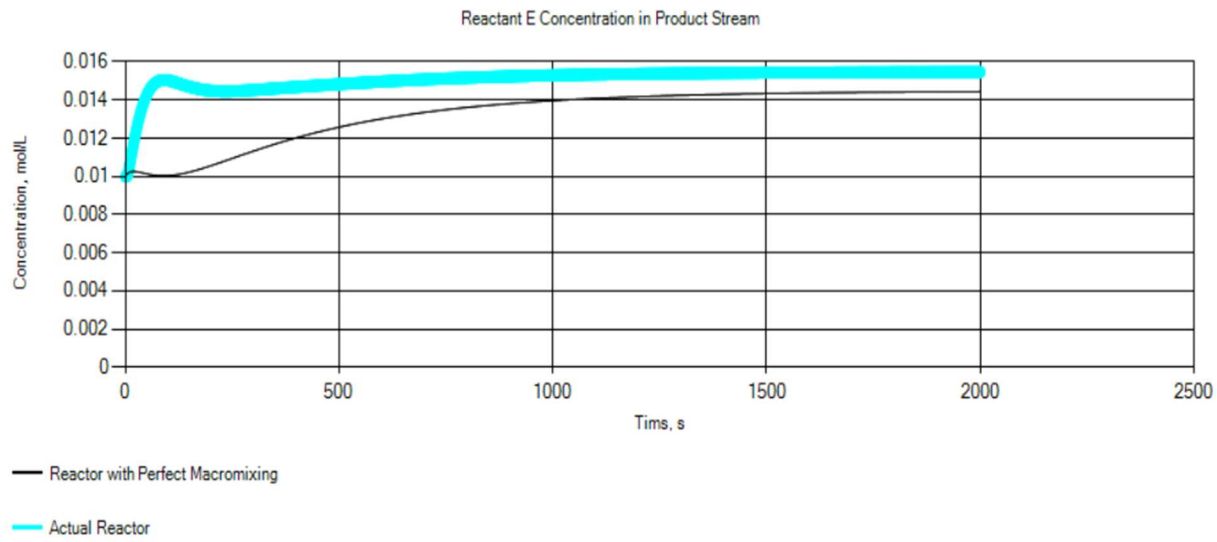



**Figure 32. Concentration Vs time graph – Enzyme**

In the actual reactor, the enzyme concentration rises quickly and stabilizes at approximately **0.015 mol/L** after **1000 seconds**, indicating localized accumulation due to non-ideal mixing. In contrast, the reactor with perfect macromixing shows a slower rise and stabilizes at a slightly lower concentration, **0.0144 mol/L**.

## By-product BP1 and BP2

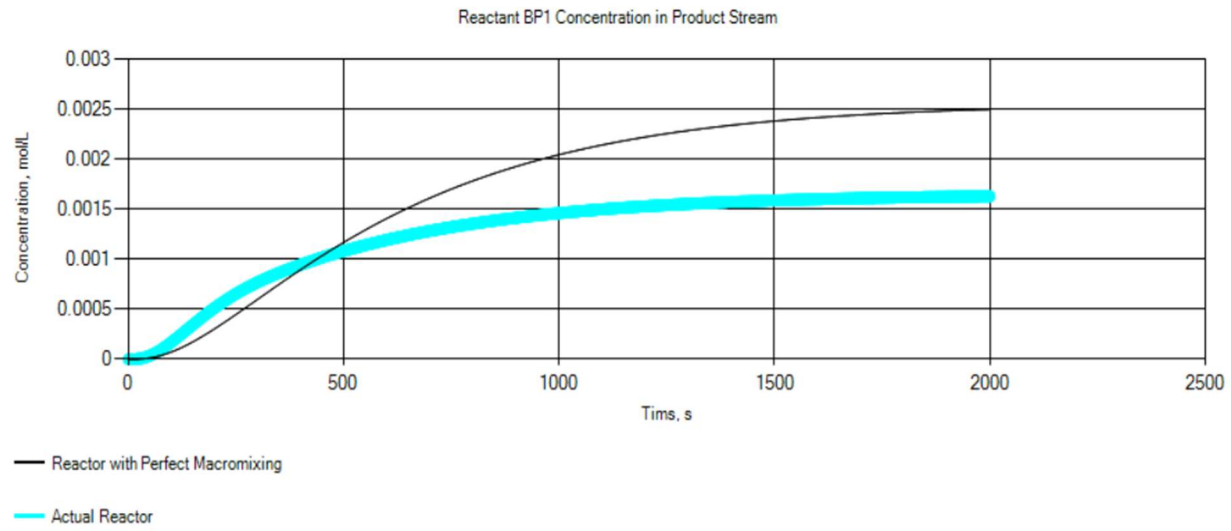



**Figure 33. Concentration Vs time graph – By-product 1**

In the Reactor with Perfect Macromixing, the BP1 concentration rises rapidly, reaching approximately **0.0025 mol/L** at around **2000 seconds**, where it stabilizes. In contrast, the Actual Reactor demonstrates slower kinetics, with the BP1 concentration leveling off at around **0.0016 mol/L** after approximately **2000 seconds**. The actual reactor shows a slower increase in BP concentration compared to the reactor with perfect macromixing. This suggests that the actual reactor achieves better control over by-product formation.

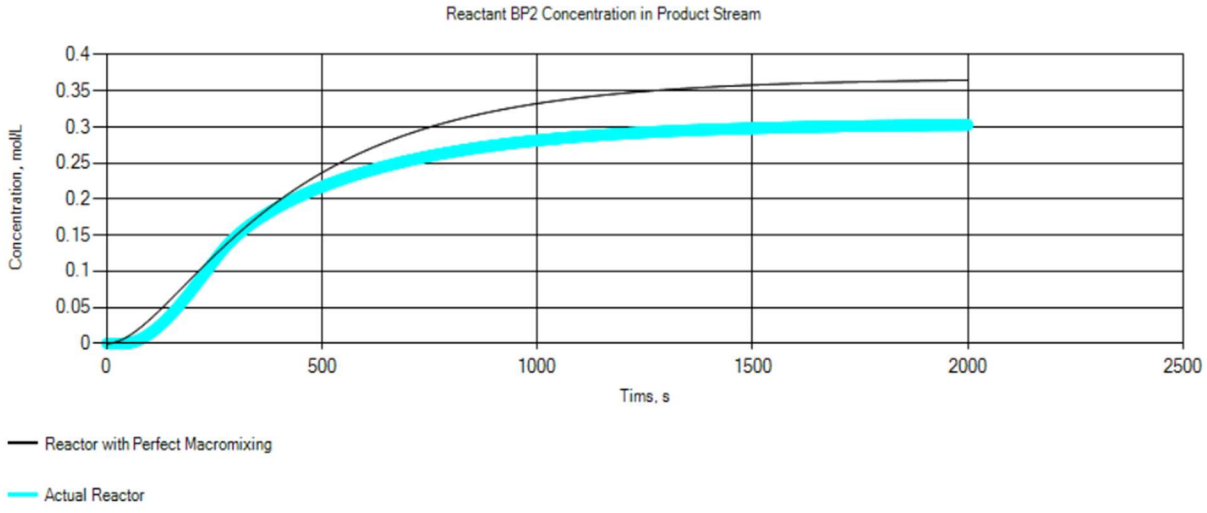



**Figure 34. Concentration Vs time graph – By-Product 2**

In the Reactor with Perfect Macromixing, the BP2 concentration rises quickly, reaching approximately **0.36 mol/L** at steady state after **2000 seconds**. In comparison, the Actual Reactor

stabilizes at a slightly lower concentration of around **0.3 mol/L**, indicating about ~**15%** reduction in BP2 concentration.

**Intermediates 1 and 2**

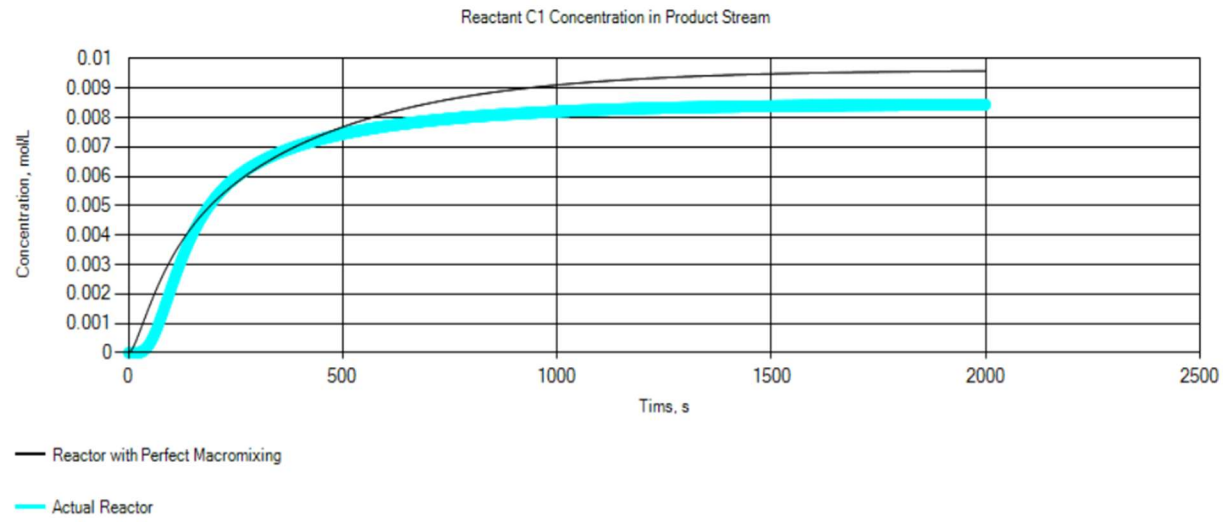



**Figure 35. Concentration Vs time graph – Intermediate 1**

The graph depicts the concentration of complex intermediate C1, which leads to the desired product, over time for an actual reactor and a Reactor with Perfect Macromixing. In the Reactor with Perfect Macromixing, the C1 concentration rapidly increases and stabilizes at approximately **0.0096 mol/L** after around **2000 seconds**, indicating efficient formation of the intermediate. In the actual reactor, the C1 concentration stabilizes slightly lower at about **0.0084 mol/L**. Enhancing micro-mixing could help achieve higher intermediate concentrations, thereby improving the yield of the desired product.

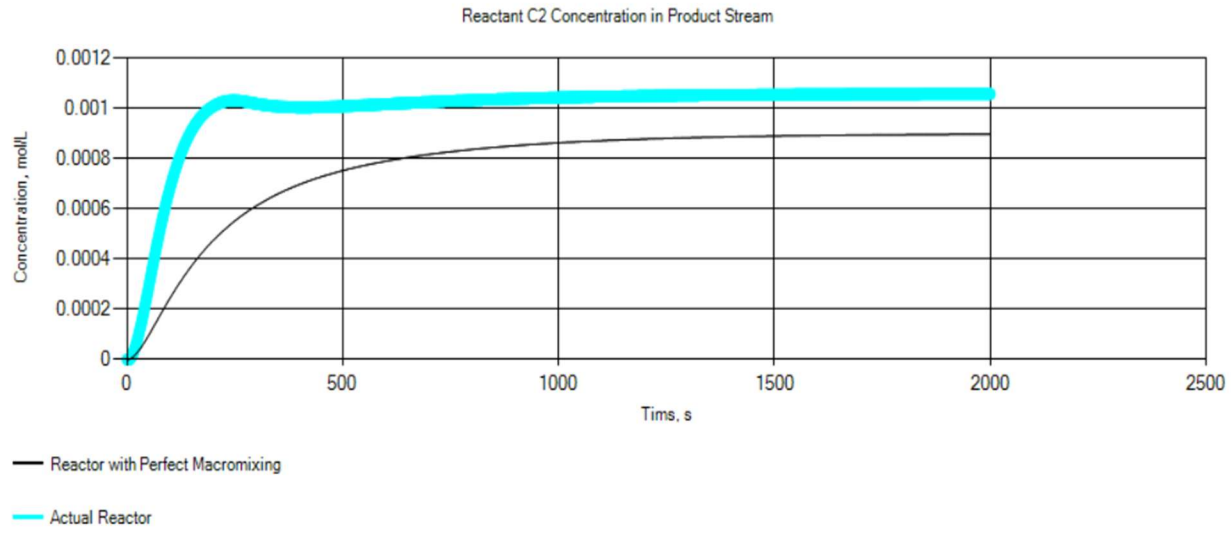


**Figure 36. Concentration Vs time graph – Intermediate 2**

The graph shows the concentration of complex intermediate C2, which contributes to undesired byproduct formation, over time for an Actual Reactor and a Reactor with Perfect Macromixing. In the Actual Reactor, C2 achieves a higher steady-state concentration of around **0.0012 mol/L**, while in the Reactor with Perfect Macromixing, it stabilizes at a lower value of approximately **0.0008 mol/L**.

## Conversion Vs time graphs

The conversion versus time graphs for each reactant are presented below, considering both the actual reactor and the reactor with perfect macromixing.

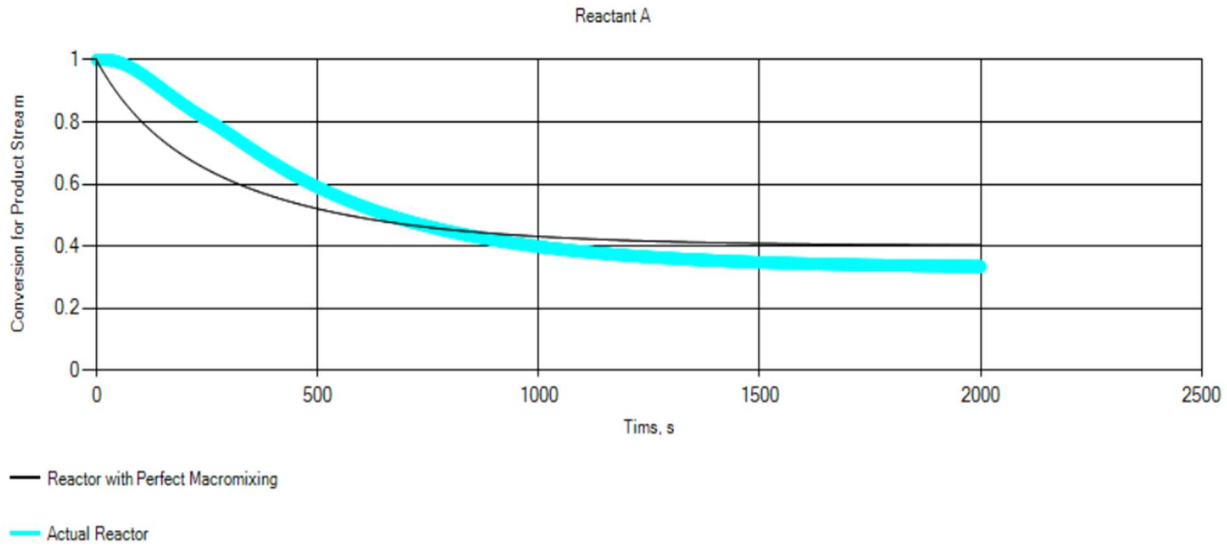



**Figure 37. Conversion Vs time graph – Reactant A**

In the actual reactor, slower conversion is observed initially due to imperfect mixing, which limits reactant distribution and reaction rates. However, at steady state, the conversion in the Actual Reactor levels off at approximately **33%**, which is lower compared to the Perfect Macromixing Reactor, which stabilizes at around **40%**. This difference suggests that imperfect mixing in the actual reactor may result in suboptimal utilization of Reactant A or its diversion into undesired pathways.

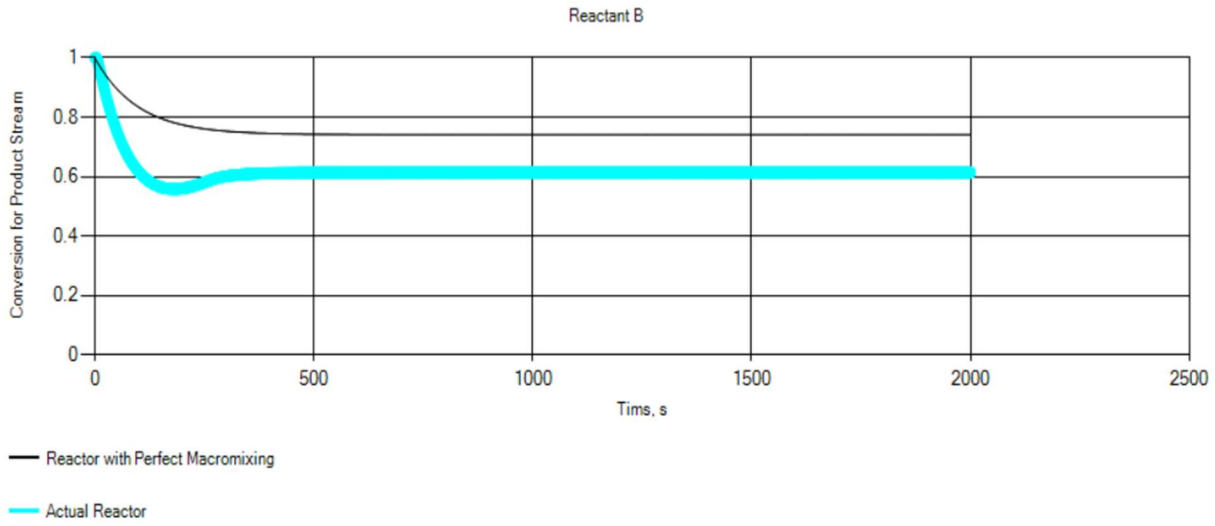



**Figure 38. Conversion Vs time graph – Reactant B**

Initially, the conversion in the actual reactor drops more rapidly, reaching a minimum around **58%** before stabilizing at approximately **61%.** In contrast, the Perfect Macromixing Reactor achieves a slightly higher steady-state conversion of around **74%.** This indicates that imperfect mixing conditions in the Actual Reactor may cause localized reaction inefficiencies or enhance undesired side reactions involving Reactant B.

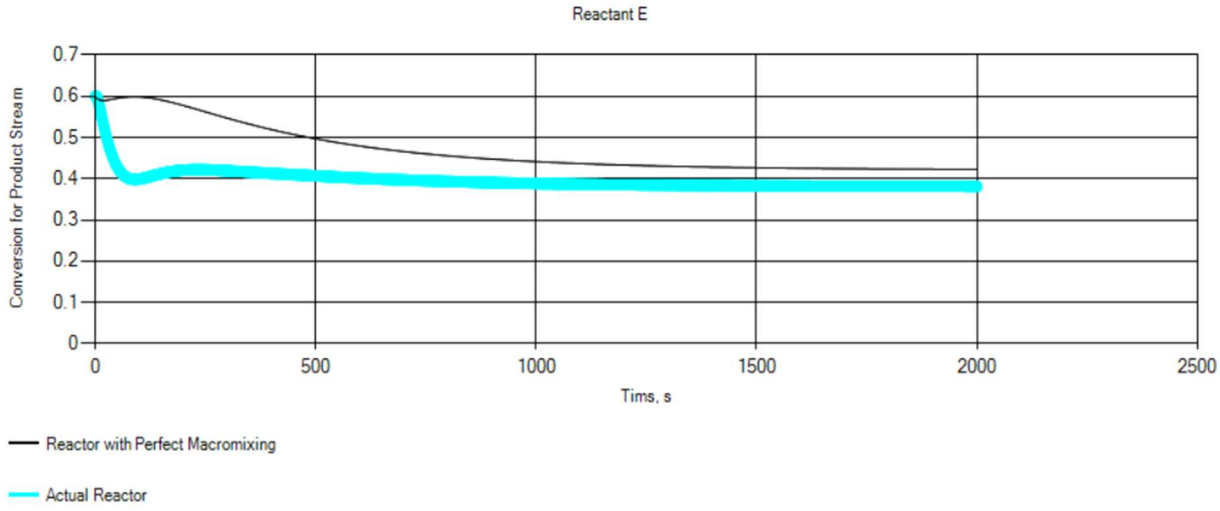



**Figure 39. Conversion Vs time graph – Enzyme E**

Initially, the enzyme conversion in the actual reactor drops more rapidly, reaching a minimum around **37%** before stabilizing near **38%.** In contrast, the reactor with Perfect Macromixing maintains a higher conversion of approximately **42%** at steady state.

**Results Overview:**
This study evaluates a 5-step reaction system involving Reactants A and B, an enzyme (E), desired intermediates (C1) and undesired intermediates (C2), and byproducts (BP1 and BP2) under **Actual Reactor** and **Perfect Macromixing Reactor** conditions.

1. **Reactant Conversion:**
   - **Reactant A**: The Actual Reactor exhibited lower conversion (**33%**) compared to the Perfect Macromixing Reactor (**40%**), suggesting limitations in mixing efficiency.
   - **Reactant B**: The Actual Reactor stabilized at a conversion of **61%,** lower than the ~74% observed in the Perfect Macromixing Reactor.
   - **Enzyme (E)**: The Actual Reactor showed a more significant initial drop in enzyme activity, stabilizing at ~**38%**, whereas the Perfect Macromixing Reactor retained **~42%** conversion.

2. **Intermediate Accumulation**
   - **C1 (Desired):** Lower accumulation in the Actual Reactor (0.0084 mol/L vs. 0.0096 mol/L).
   - **C2 (Undesired)**: Higher in the Actual Reactor (0.0012 mol/L vs. 0.0008 mol/L), contributing to byproduct formation.

3. **By Product formation**
   The Actual Reactor exhibited lower byproduct formation (BP1 and BP2) compared to the perfect macromixing reactor, despite the accumulation of undesired intermediates (C2). This is likely due to slower reaction kinetics or limited progression of secondary reactions in localized zones.

Overall, the actual reactor exhibited higher accumulation of undesired intermediates and byproducts due to localized reaction zones in comparison to the perfect macromixing reactor. This underscores the importance of optimizing reactor design to achieve better control over reaction kinetics and product formation.