VISIMIX CHEM
Continuous Flow Process: Main Reaction Vs By-Product Formation

- **VisiMix Chem** is designed for simulating the dynamics of stirred chemical reactors operating in turbulent flow regimes. It utilizes advanced VisiMix turbulent models to simulate all hydrodynamic mixing processes.
- Using tank design, agitator or rotor speed, fluid rheology and feed flow rates as input, these models support analysis of fluid dynamics variables, i.e., pressure, velocity, circulation flow rate and local turbulence characteristics (such as local energy dissipation, $\boldsymbol{\varepsilon}$, and the smallest scale of turbulence fluctuations, $\boldsymbol{\delta}$), which determine local macromixing and micromixing characteristics.
- VisiMix Chem calculations are conducted for actual chemical reactors where neither macromixing nor micromixing is ideal, and results of these calculations are compared in all output tables and charts against respective calculations conducted for a respective reactor with perfect macromixing.

Consider the following example, which includes both the main reaction and the side reaction leading to by-product formation.

Main reaction
A + B <-> P
By-product reaction
2 A + B <-> BP

Where ‘A’ and ‘B’ are reactants, ‘P’ is the main product and ‘BP’ is the by-product.

This project highlights the distinction between idealized perfect macro mixing and realistic mixing models in a **continuous process**, with a focus on two competing reactions where the side reaction exhibits a significantly higher rate constant than the main reaction.

Objective:

To determine the concentration of each reactant as a function of time and analyze the corresponding conversion rates, ultimately generating concentration versus time and conversion versus time graphs to illustrate the kinetics of the reaction in a continuous process.

Initial data:

Process temperature: 26.85 °C
Solvent: Water
Solvent molar mass: 18 g/mol

Reactant A:
Molecular weight= 48 g/mol
Initial feed 1 concentration in the tank= 1 mol/L
Inlet 1 flow rate = 100 L/min

Reactant B:
Molecular weight= 56 g/mol
Initial feed 2 concentration in the tank= 1 mol/L
Inlet 2 flow rate = 100 L/min

Main Product (P):
Molecular weight= 104 g/mol

By-product (BP):
Molecular weight= 152 g/mol

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

Baffles: No baffles

Impeller: Paddle
Tip diameter = 400 mm;
Number of blades = 2
Blade width = 80 mm
Distance from bottom = 305 mm.
Number of impellers= 1
Rotational speed = 30 rpm
Motor power = 1111 W

Fluid properties:
Average density= 997 kg/m^3
Dynamic viscosity= 0.89 cP (Newtonian fluid)

It is a continuous process. The process duration is 1200 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.

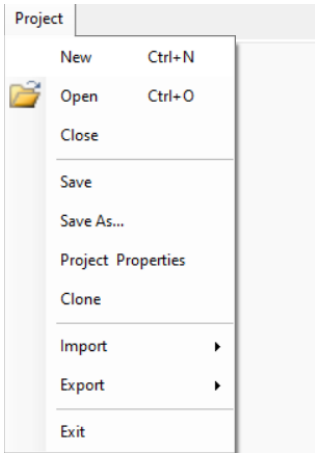

Figure 2. The Project sub-Menu.

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

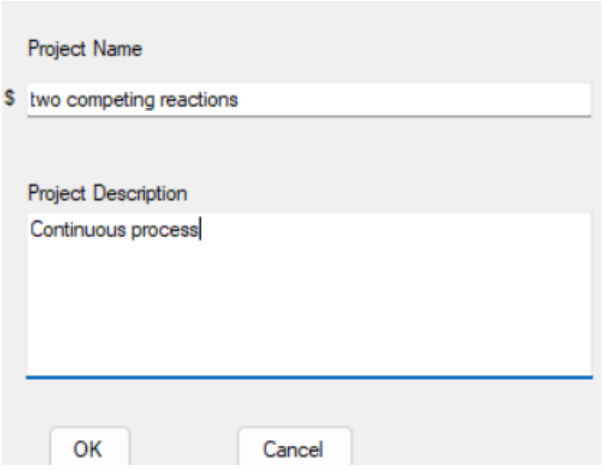

Figure 3. Starting a new Project.

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.

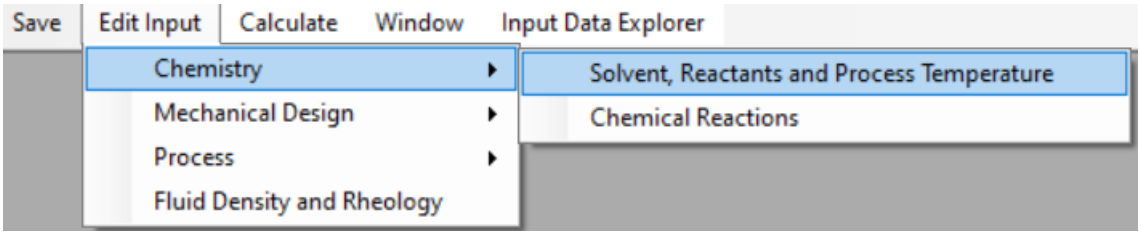

Figure 4. Edit Input - Chemistry menu for Solvent, Reactants and Process temperature data

Select **Solvent, Reactants and Process temperature**. A new window will appear where we can enter the corresponding data. All the reactants, products, catalysts (if applicable), and byproducts along with their molecular weights and concentrations should be entered in the fields provided. In our case, 'A' and 'B' are the reactants, 'P' is the main product, 'BP' is the by-product, and no catalyst is being used.

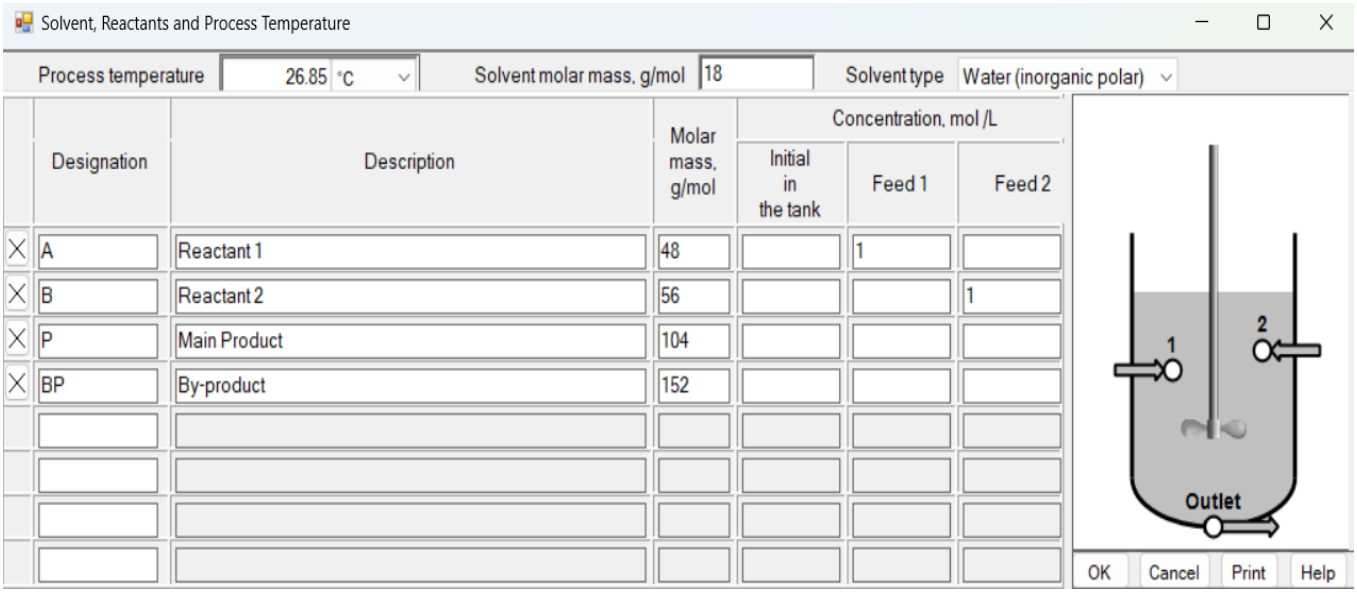

Figure 5. Input the process temperature, solvent and reactants data

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

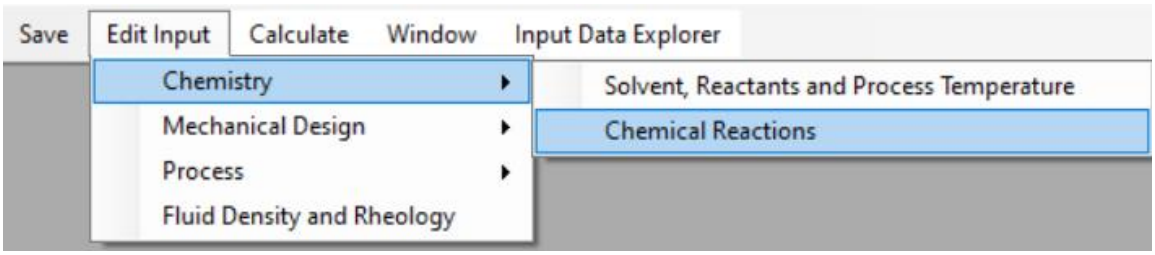

Figure 6. Edit Input - Chemistry menu for Chemical reaction data

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.

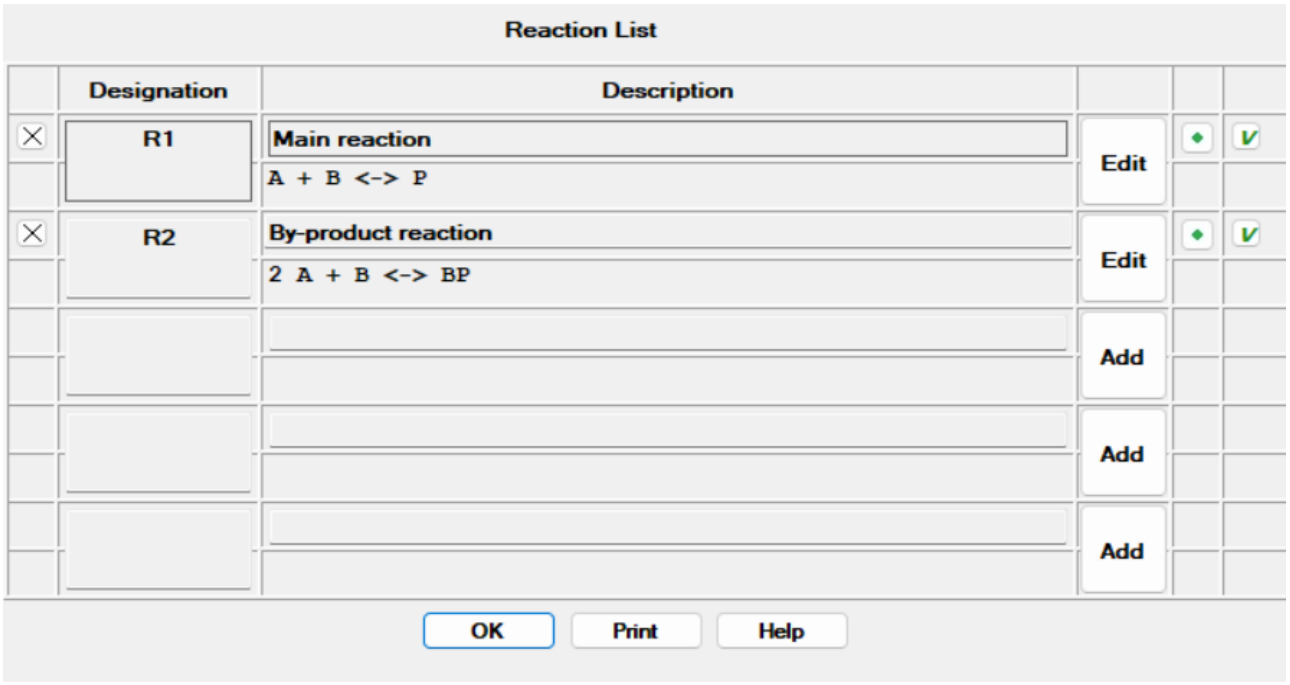

Figure 7. Click Add/Edit option

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. Since our reaction is not reversible**,** specify the reverse reaction constant as '0'. The reaction rate constant for the main reaction is higher than that of the side reaction. Start by entering the details for the main reaction.

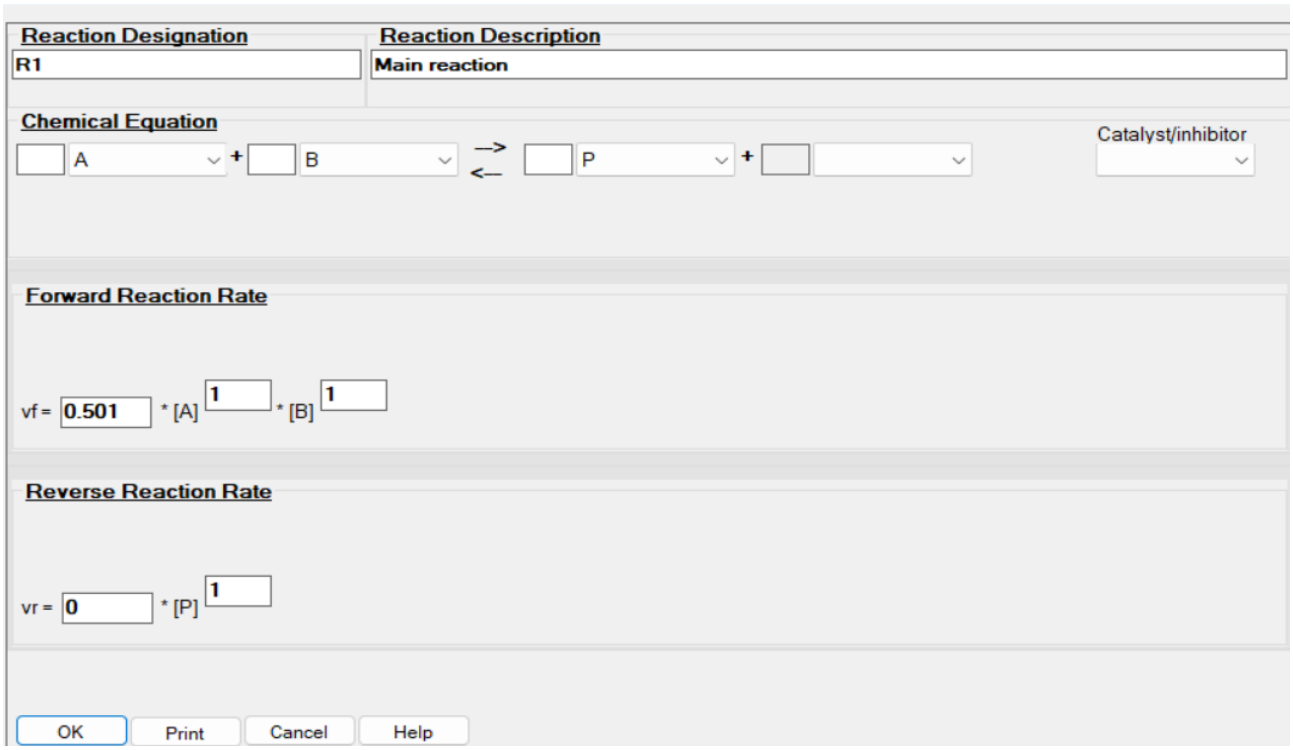

Figure 8. Input the chemical reaction kinetics data for the Main reaction

Click OK to close the main reaction kinetics input window, then select **'Add'** in the second row to enter the side reaction details.

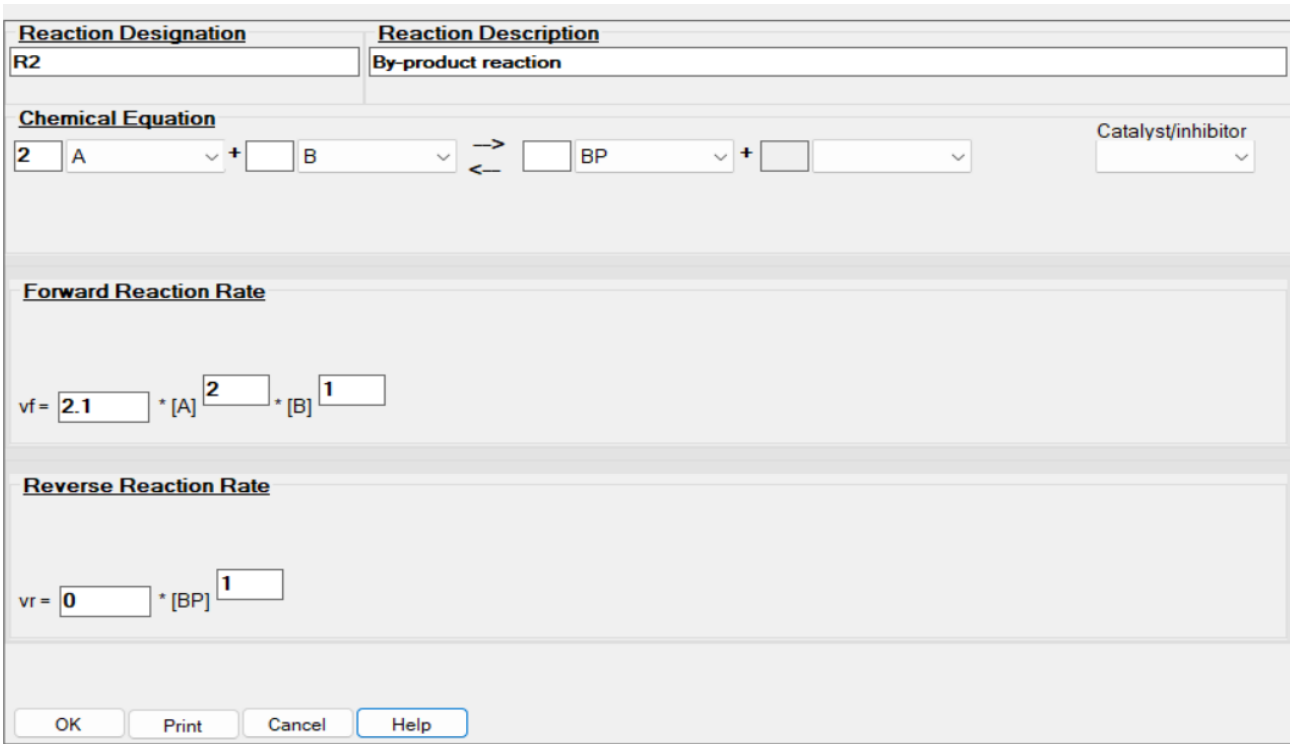

Figure 9. Input the chemical reaction kinetics data for the side reaction

Press OK to close 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.

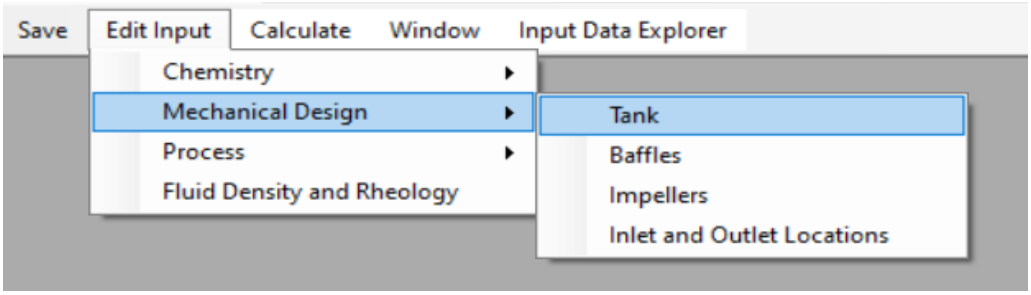

Figure 10. Edit Input – Mechanical Design Menu

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.

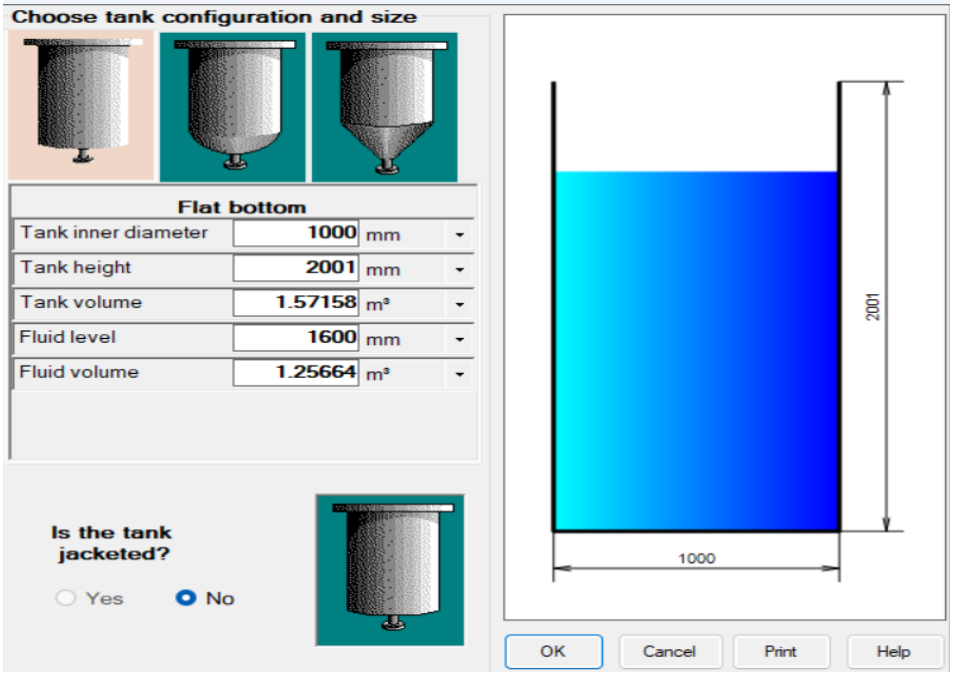

Figure 11. Enter the tank details

Choose the baffle type. In our case, we are not using any baffles. So please select ‘No baffles’.

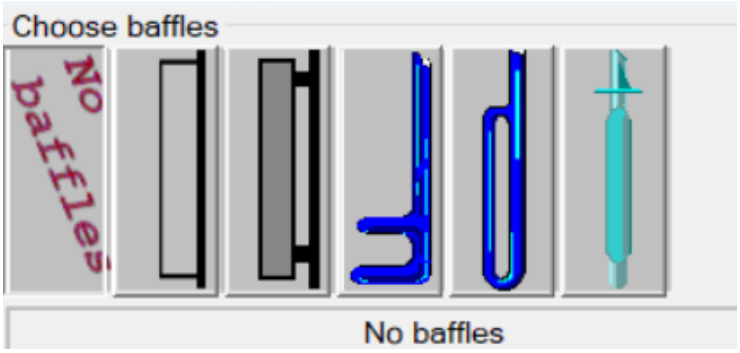

Figure 12. Choose baffle type

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

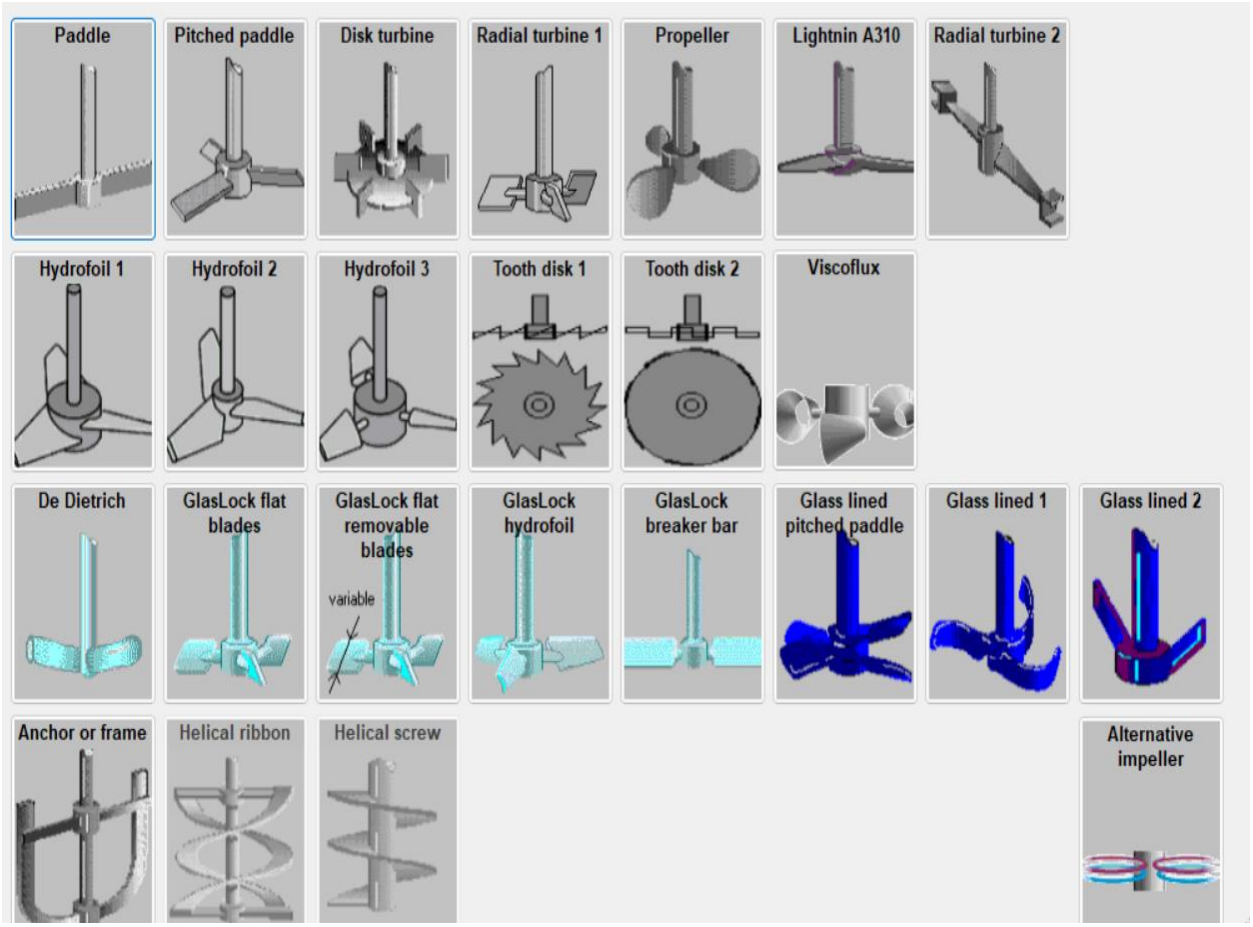

Figure 13. Select the impeller type

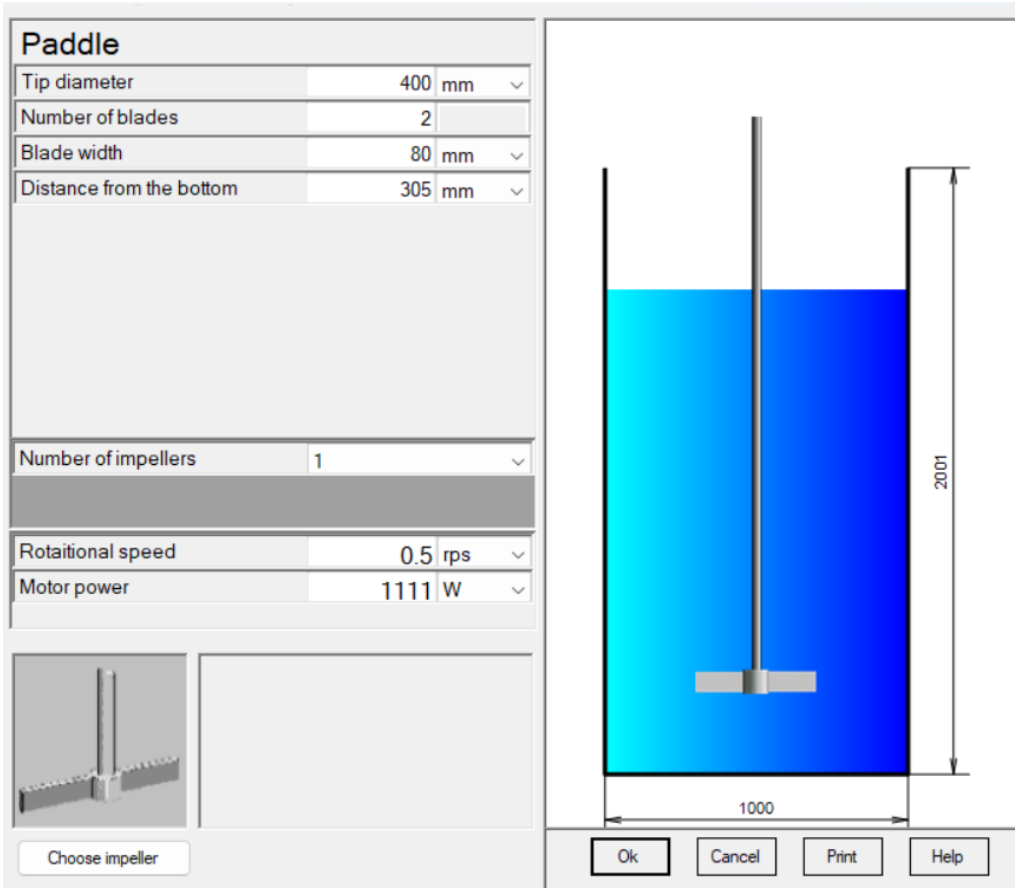

Figure 14. Enter the impeller dimensions

Select the **Inlet and Outlet positions** from the **mechanical design** option in the Edit menu.

Inlet 1 is located on the side of the reactor near the bottom at a radius of 500 mm and at a height of 500 mm from the base of the reactor.
Inlet 2 is positioned along the shaft near the top of the reactor at a radius of 500 mm and at a height of 1500 mm from the base of the reactor which delivers feed directly downward along the axis of the reactor, likely aiding in uniform distribution along the shaft.
Outlet is located at the side of the reactor near the top, at the same height as Inlet 2 (1500 mm from the base). It allows the continuous removal of the product stream as the process progresses, maintaining steady flow and ensuring the reactor operates under continuous conditions.

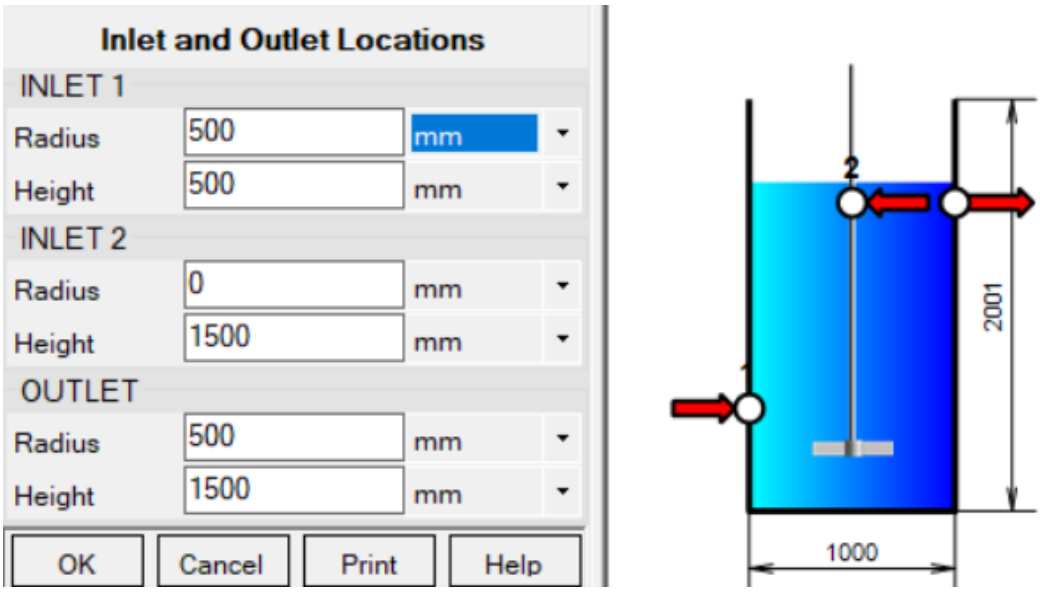

Figure 15. Enter the Inlet and outlet positions

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

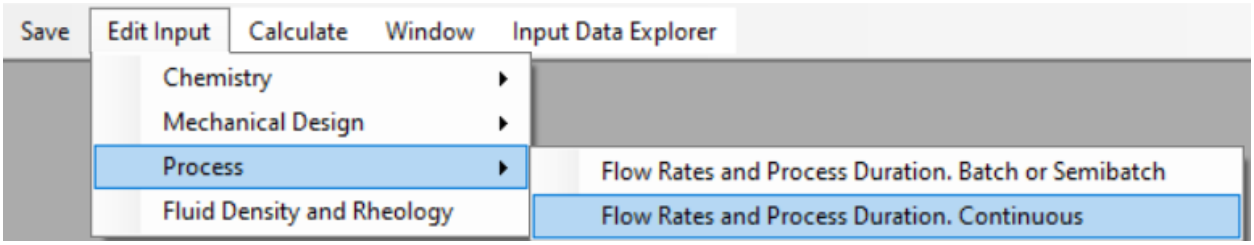

Figure 16. Edit Input – Process menu

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.

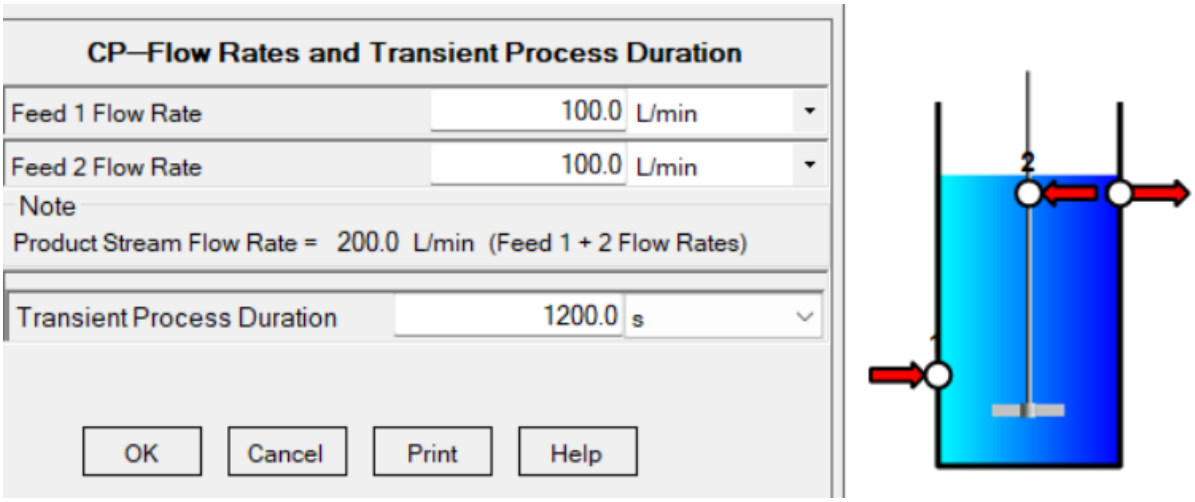

Figure 17. Input the feed flow rate and process duration

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

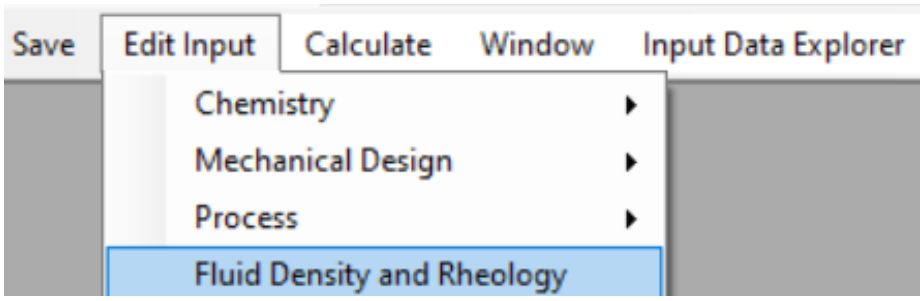

Figure 18. Edit input – Fluid density and Rheology

Enter the Average density and dynamic viscosity.

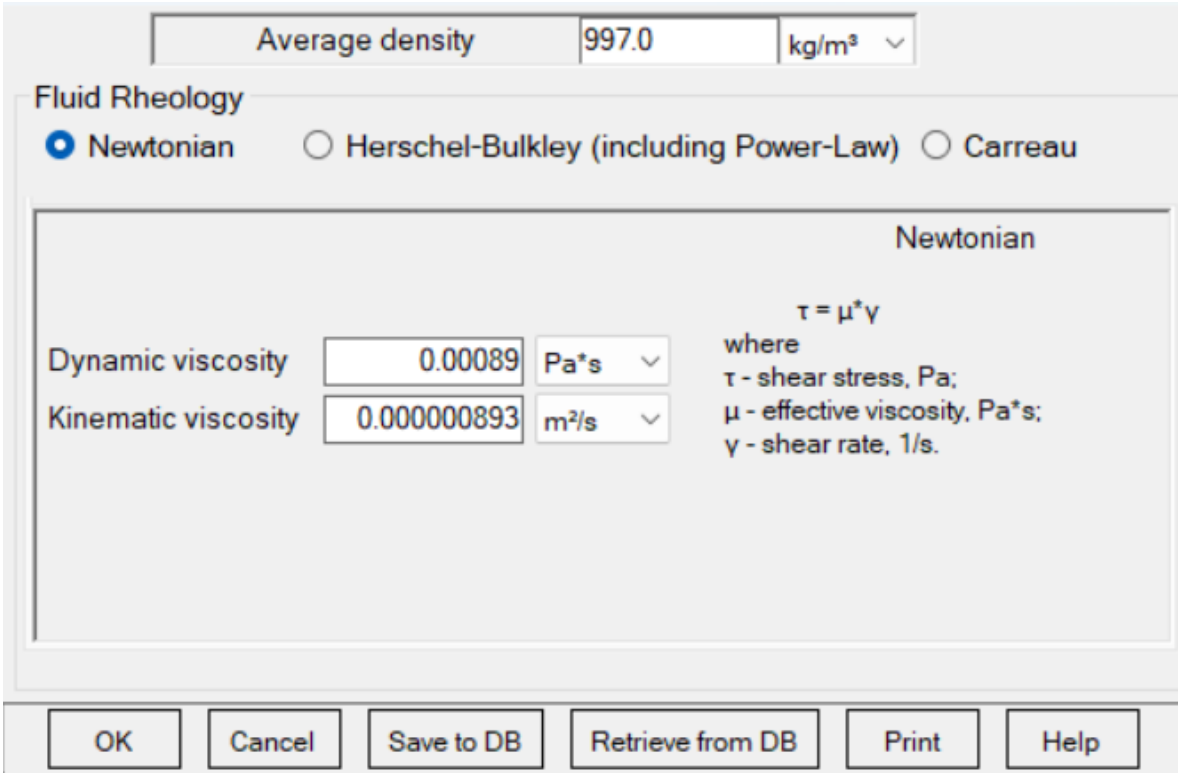

Figure 19. Input Fluid density and Rheology data

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.

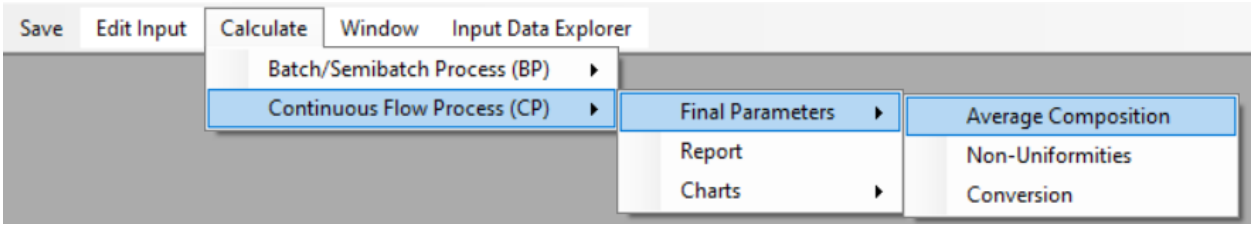

Figure 20. Select Calculate Menu-Final Parameters

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

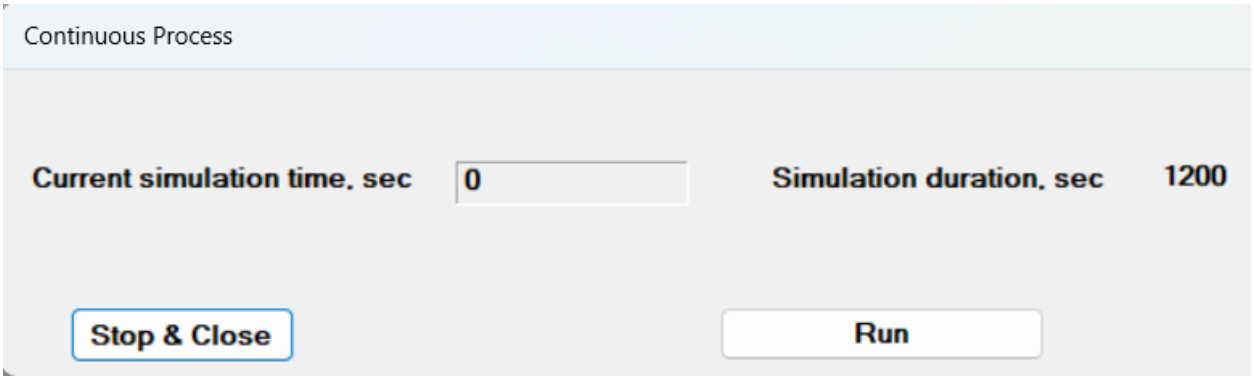

Figure 21. Run the simulation

The concentrations of the reactants, product 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 comparision, 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	0.06111	0.02271	0.02659
	B	0.04057	0.09434	0.07056
	P	0.3135	0.3112	0.3635
	BP	0.07421	0.07079	0.04396
*				

Figure 22. 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	0.02727	0.07621	0.06111
B	0.03324	0.1956	0.04057
P	0.006915	0.07615	0.3135
BP	0.00241	0.02171	0.07421

Figure 23. 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	0.9546	0.9468
B	0.8113	0.8589
P		
BP		

Figure 24. 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.

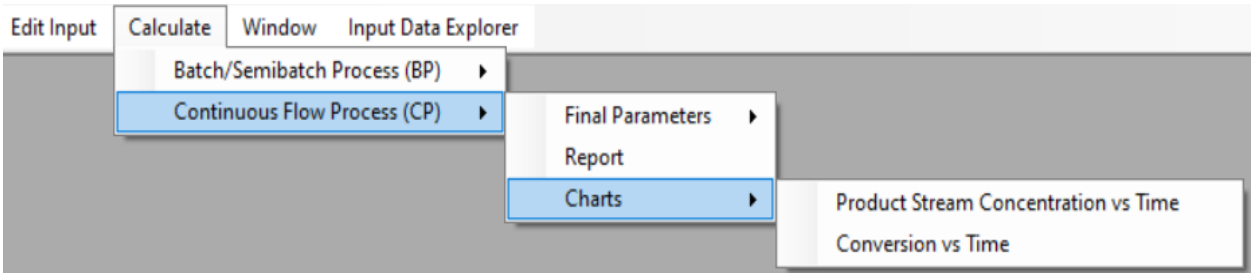

Figure 25. Select Calculate Menu- Charts

Product Stream Concentration Vs time graph

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

Reactant A

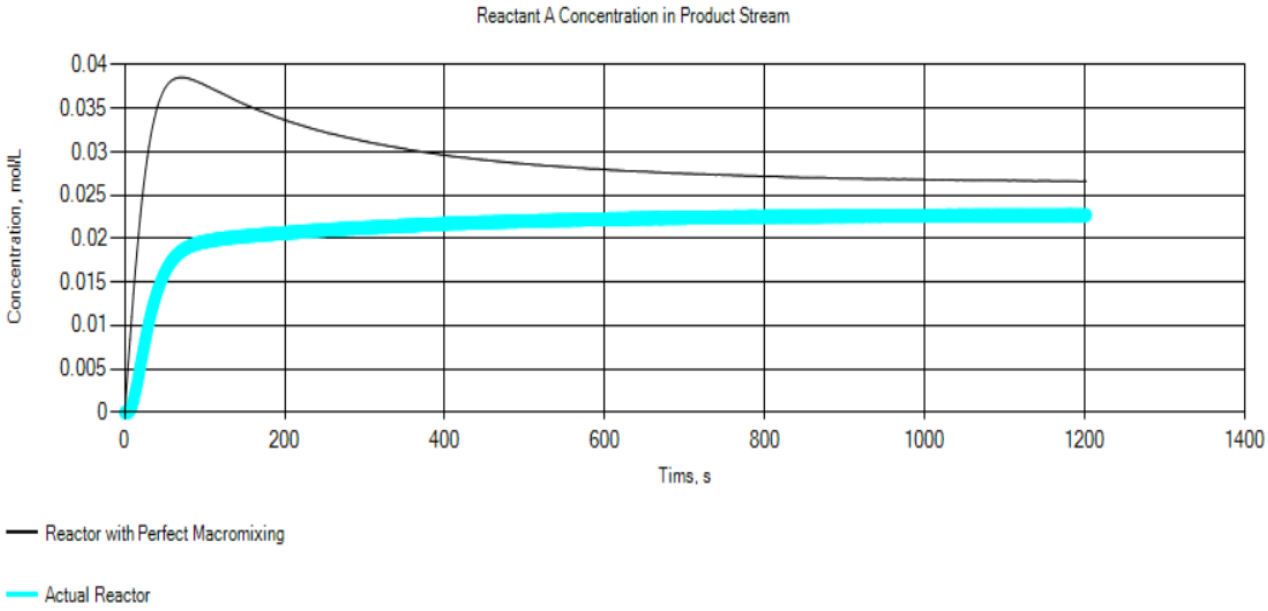

Figure 26. Concentration Vs time graph– Reactant A

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. The concentration of A starts at a high concentration and decreases over time as it is consumed in the reaction. In the actual reactor, influenced by real-world factors such as local micro mixing, the concentration stabilizes at 0.022 mol/L within 1000 seconds, compared to the ideal reactor, which achieves a concentration of 0.026 mol/L at 1000 seconds under perfect macromixing conditions. This comparison highlights how local micro-mixing influences the behavior, distribution, and overall efficiency of the actual reactor.

Reactant B

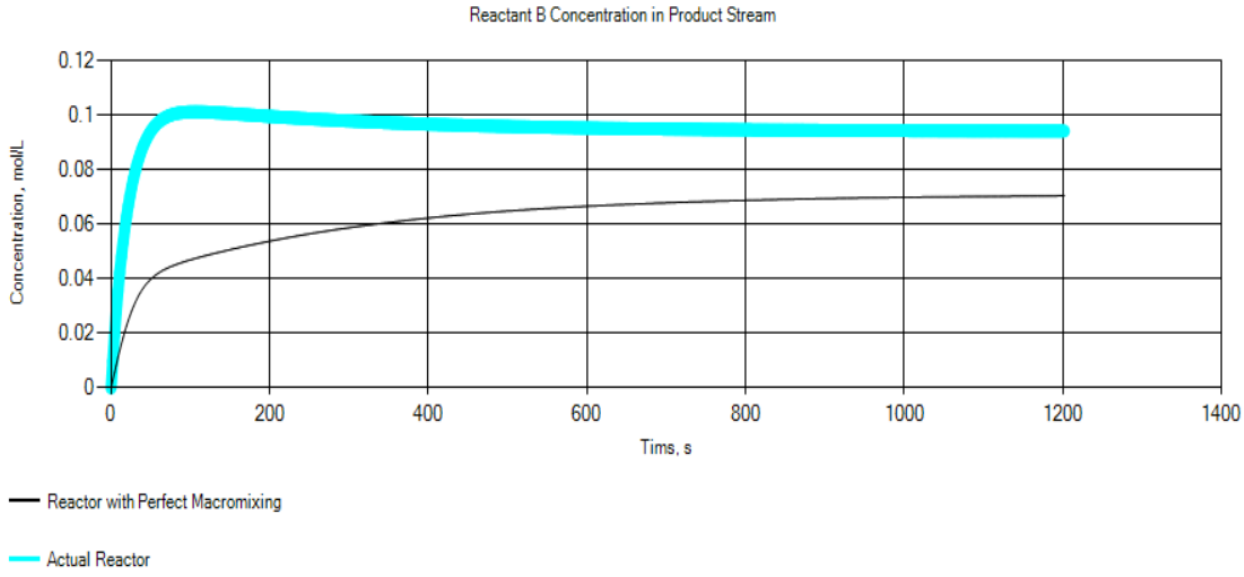

Figure 27. Concentration Vs time graph – Reactant B

The concentration of B in the actual reactor, influenced by real-world factors such as flow irregularities, stabilizes at 0.094 mol/L within 800 seconds. In comparison, the ideal reactor achieves a concentration of 0.07 mol/L at 800 seconds under perfect macromixing conditions.

Product P

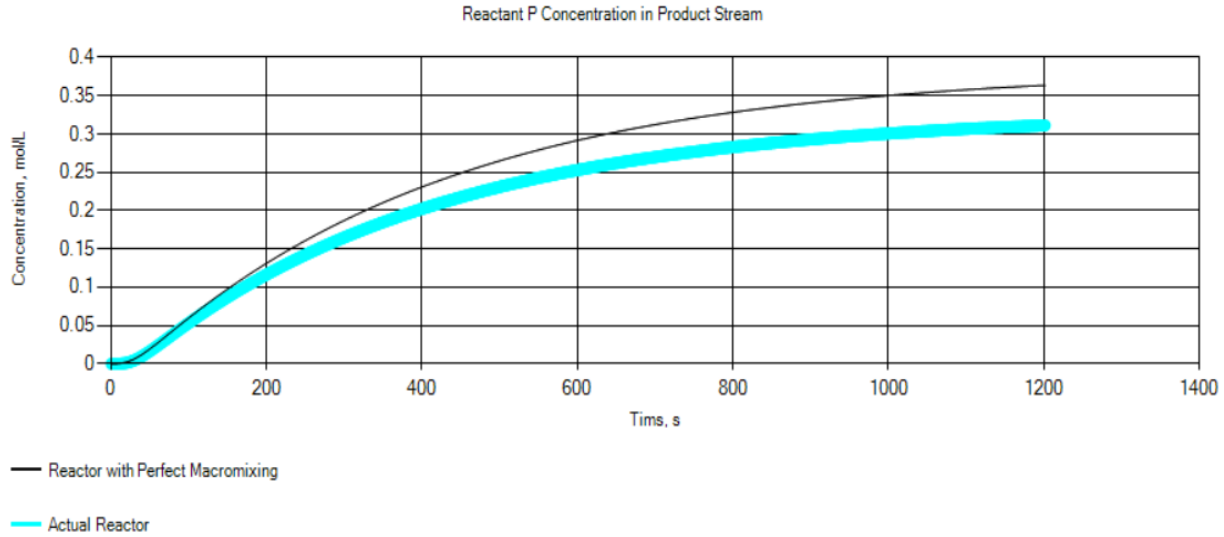

Figure 28. Concentration Vs time graph – Product P

The concentration of P in the actual reactor, influenced by real-world factors such as flow irregularities, stabilizes at 0.31 mol/L within 1200 seconds, compared to the ideal reactor, which achieves a concentration of 0.36 mol/L at 1200 seconds under perfect macromixing conditions.

By-product BP

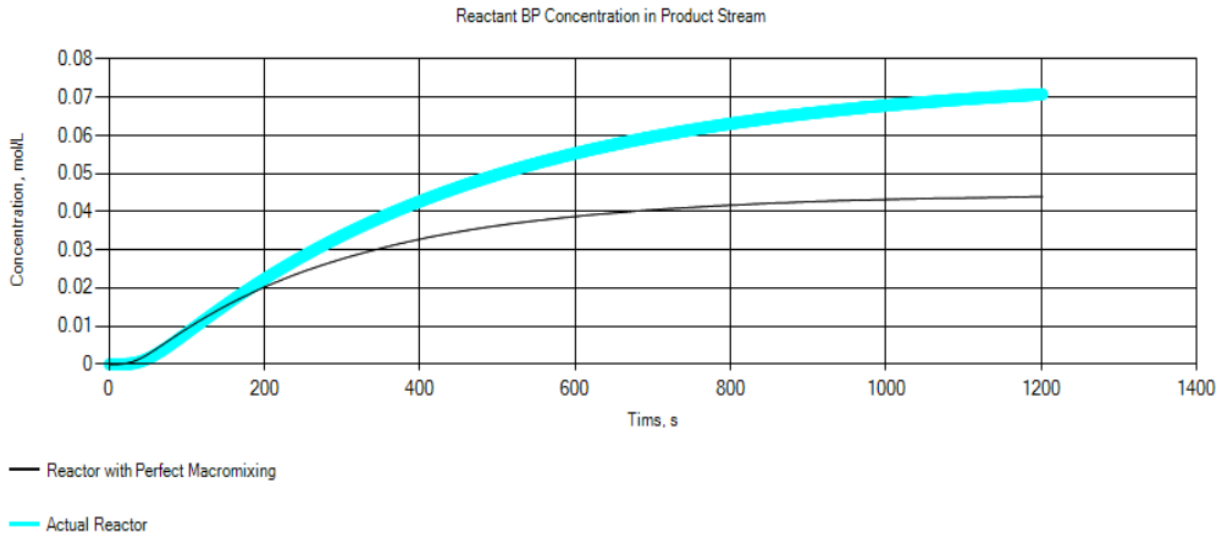

Figure 29. Concentration Vs time graph – By-Product

The concentration of BP in the actual reactor, influenced by real-world factors such as flow irregularities, stabilizes at 0.07 mol/L within 1200 seconds, compared to the ideal reactor, which achieves a concentration of 0.043 mol/L at 1200 seconds under perfect macromixing conditions.

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.

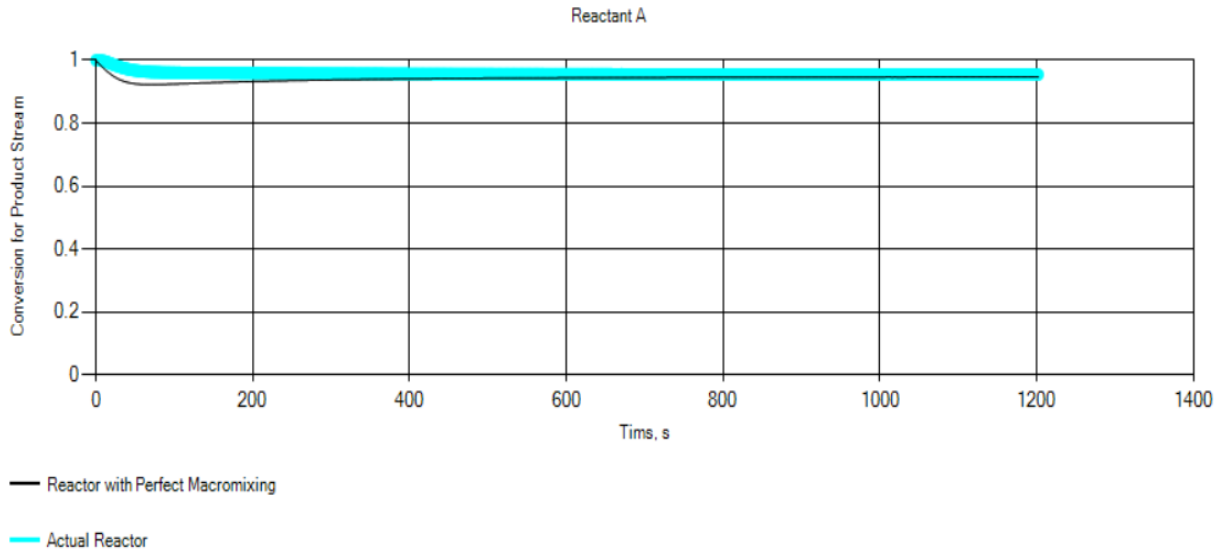

Figure 30. Conversion Vs time graph – Reactant A

The graph shows that initially, the conversion fluctuates slightly during the transient phase as the system stabilizes. Ultimately, Reactant A achieves a conversion of **0.95** in the actual reactor which is slightly higher than the ideal reactor's conversion **0.94**, demonstrating that the actual reactor effectively converts Reactant A, indicating efficient local micro-mixing and good mixing performance within the reactor system.

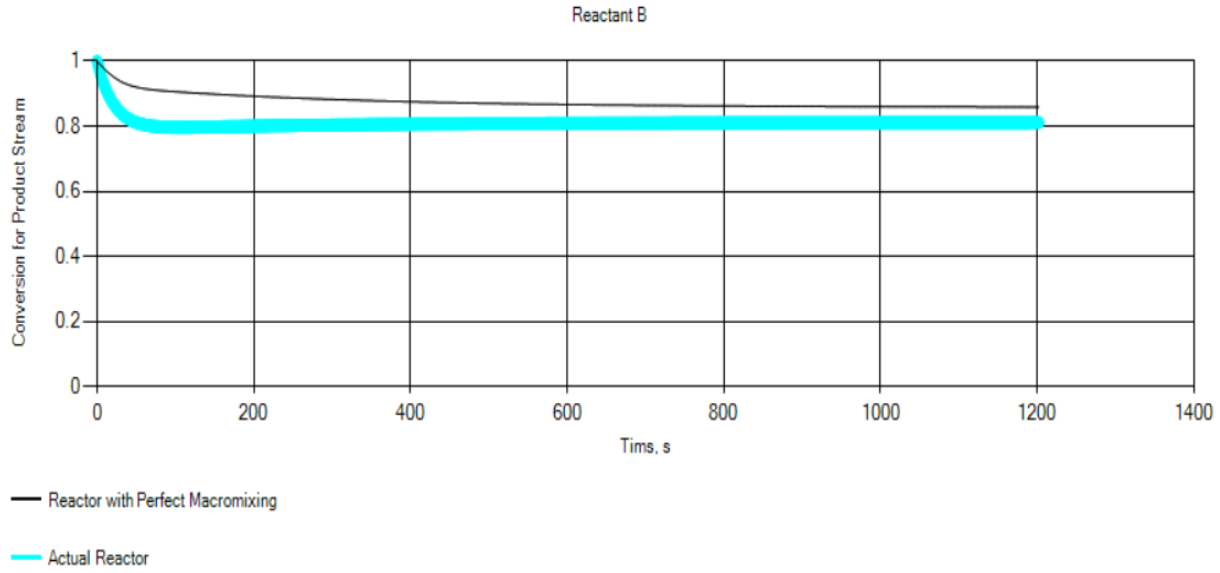

Figure 31. Conversion Vs time graph – Reactant B

This graph shows that Reactant B achieves a conversion of 0.81 in the actual reactor, which is lower than the 0.86 observed in the ideal reactor. This suggests that local micro-mixing effects in the actual reactor may impact reactant distribution and reduce its conversion efficiency compared to the ideal reactor.

Results Overview:

The investigation highlights the impact of the Feed 2 Inlet position, located near the top of the reactor and delivering feed downward along the axis without baffles, likely promoting uniform distribution along the shaft. Reactant A achieves a conversion of **0.95** in the actual reactor, slightly surpassing the ideal reactor's conversion of **0.94**, indicating effective performance, likely due to efficient local micro-mixing and effective utilization of reactants within the system. However, Reactant B achieves a lower conversion of **0.81** compared to the ideal reactor's **0.86**, likely due to non-uniform flow patterns, localized mixing zones, or dead zones hindering its efficiency.

Additionally, the by-product concentration in the actual reactor was measured at **0.07 mol/L,** reflecting a trade-off between optimizing main reaction performance and minimizing by-product formation. This analysis underscores the critical role of feed location in influencing product yield and by-product generation.