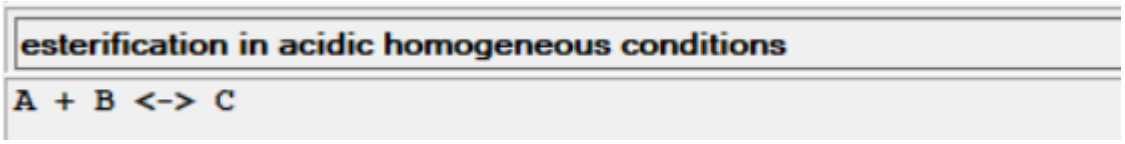
VISIMIX CHEM
Batch Reaction (Esterification)

- **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 Esterification reaction example:



This project highlights the significance of mixing intensity in facilitating rapid esterification in acidic reactions.

Methanol reacts with acetic acid in the presence of a water medium at 49 °C to give methyl acetate.

$CH_3OH + CH_3COOH \rightleftharpoons CH_3COOCH_3 + H_2O$
Methanol + Acetic Acid ⇌ Methyl Acetate + Water

One mole of methanol reacts with one mole of acetic acid to produce one mole of methyl acetate and one mole of water.

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.

Initial data:

Process temperature: 49 °C
Solvent: Water
Solvent molar mass: 18 g/mol

Methanol (A):
Molecular weight= 32 g/mol
Initial concentration in the tank= 1.2 mol/L

Acetic acid (B):
Molecular weight= 60 g/mol
Initial concentration in the tank= 1.2 mol/L

Methyl acetate (C):
Molecular weight= 74 g/mol

Tank: Flat Bottom
Inside diameter = 1000 mm;
Total tank height = 2000 mm;
Fluid level = 1600 mm;

Baffles: No baffles

Impeller: Paddle
Tip diameter = 500 mm;
Number of blades = 2
Blade width = 110 mm
Distance from bottom = 305 mm.
Number of impellers= 1
Rotational speed = 180 rpm
Motor power = 1119 W

Fluid properties:
Average density= 998.2 kg/m^3
Dynamic viscosity= 1 cP

It is a batch process.The process duration is 300 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.

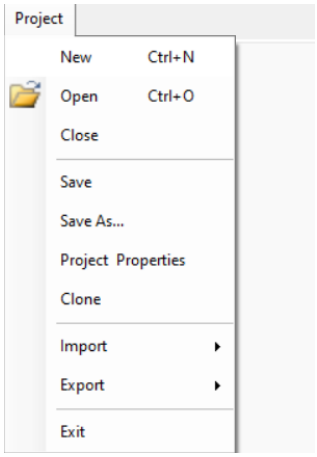


Figure 2. The Project sub-Menu.

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

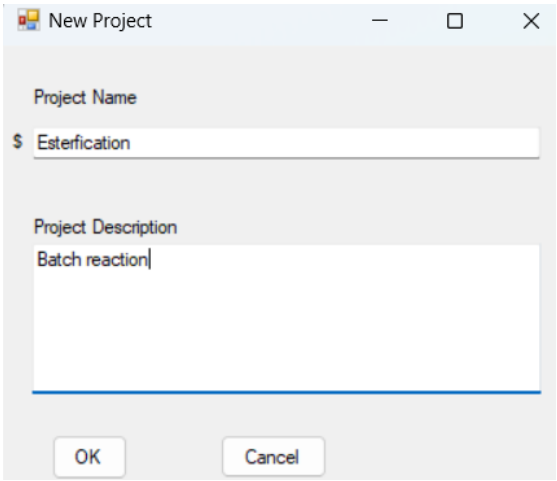


Figure 3. Starting a new Project.

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.

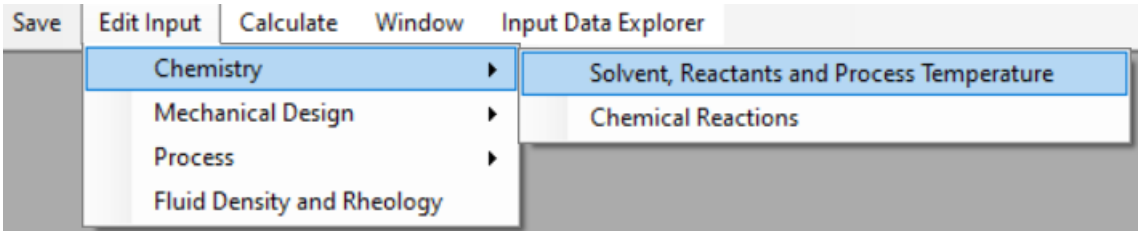


Figure 4. Edit Input - Chemistry menu for Solvent, Reactants and Process temperature data

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, 'C' is the product, and no catalyst is being used.

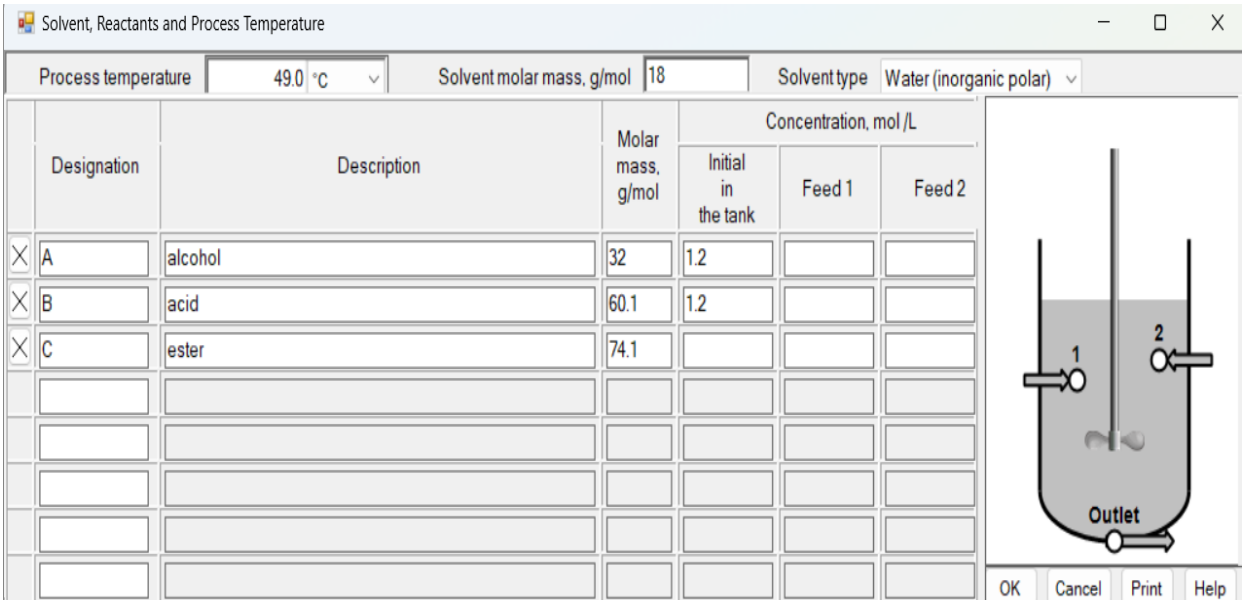


Figure 5. Input the process temperature, solvent and reactants data

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

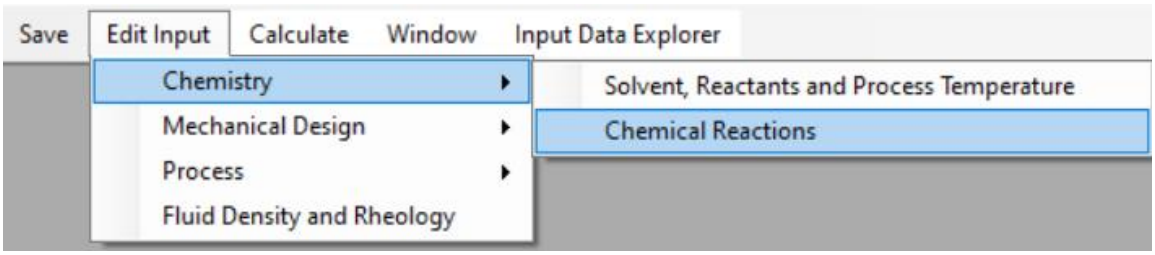


Figure 6. Edit Input - Chemistry menu for Chemical reaction data

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.

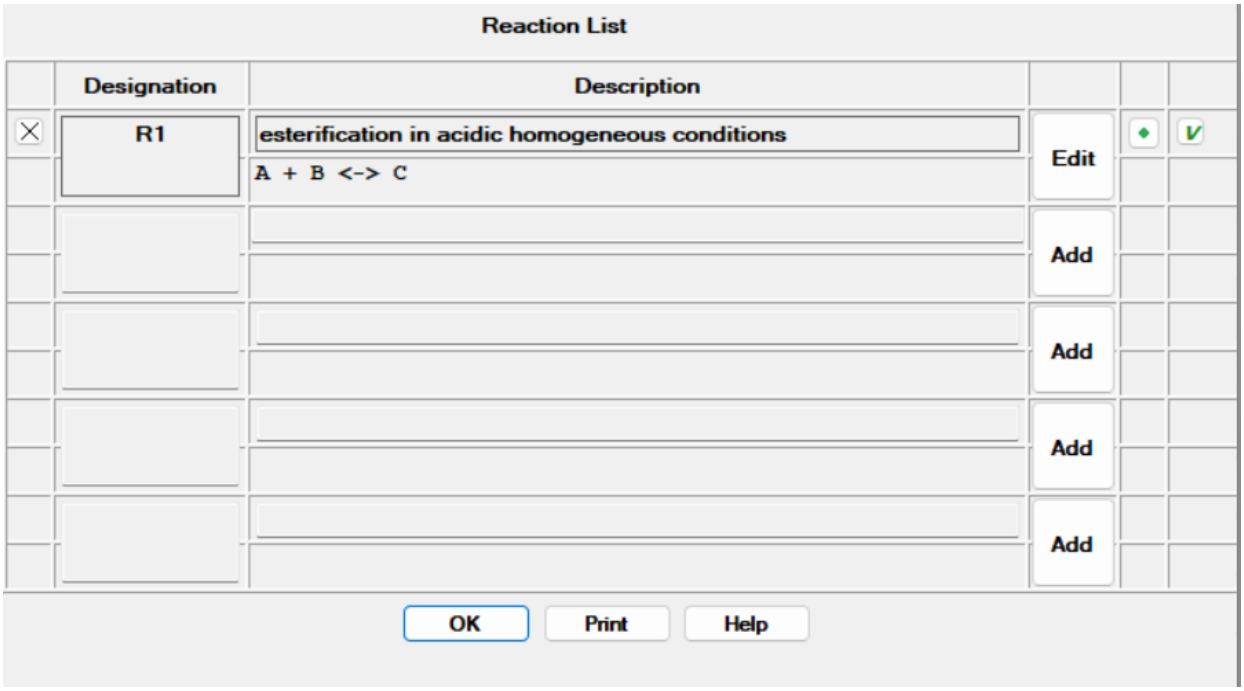


Figure 7. Click Add/Edit option

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.

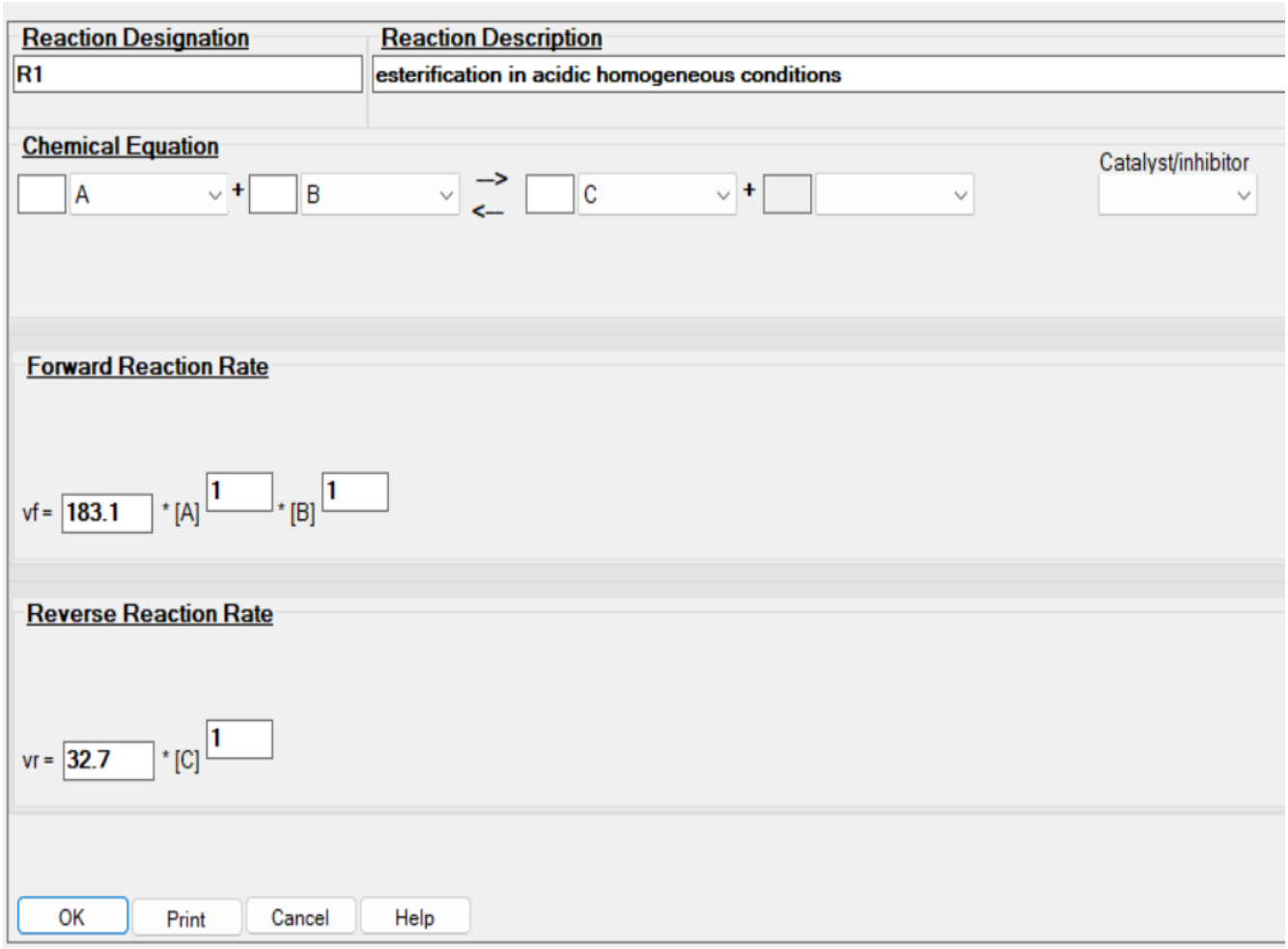


Figure 8. Input the chemical reaction kinetics data

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.

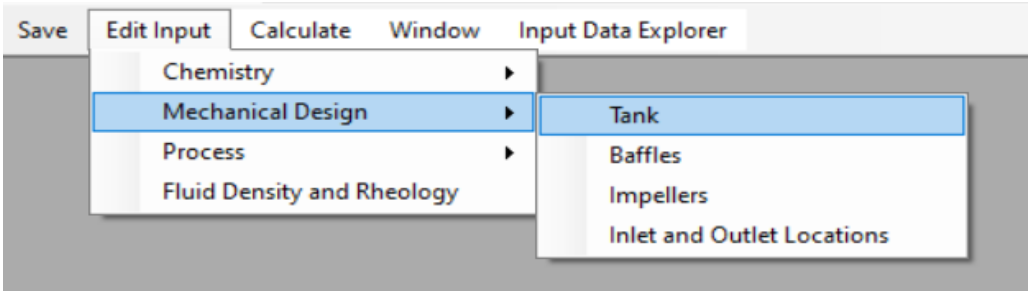


Figure 9. Edit Input – Mechanical Design Menu

Select the **Tank (Flat Bottom)** and enter the tank details i.e., tank inner diameter, tank height and fluid level.

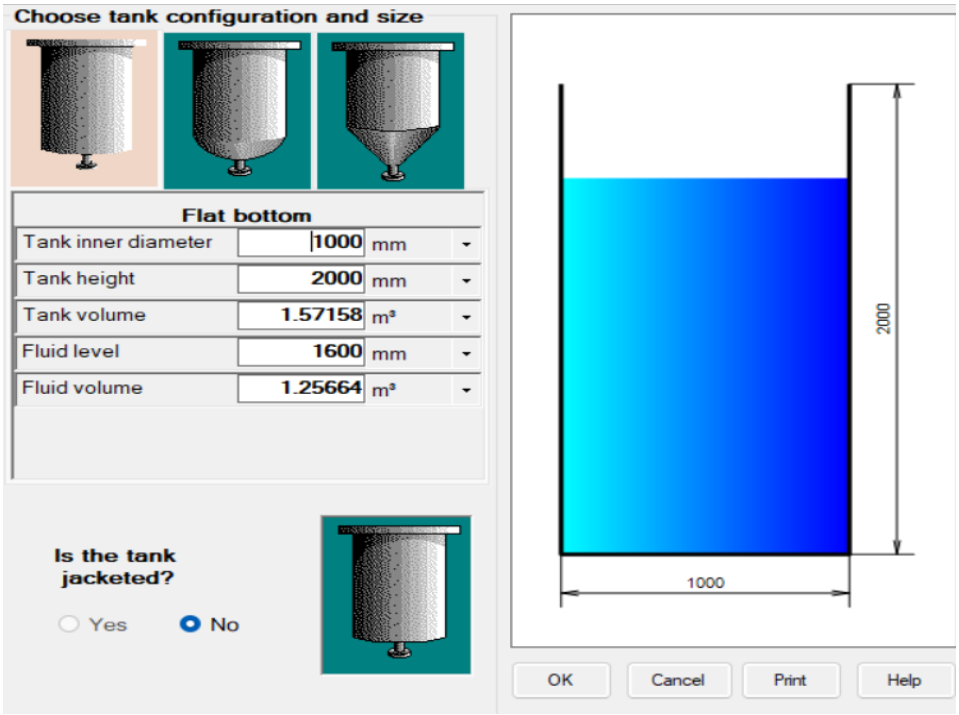


Figure 10. Enter the tank details

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

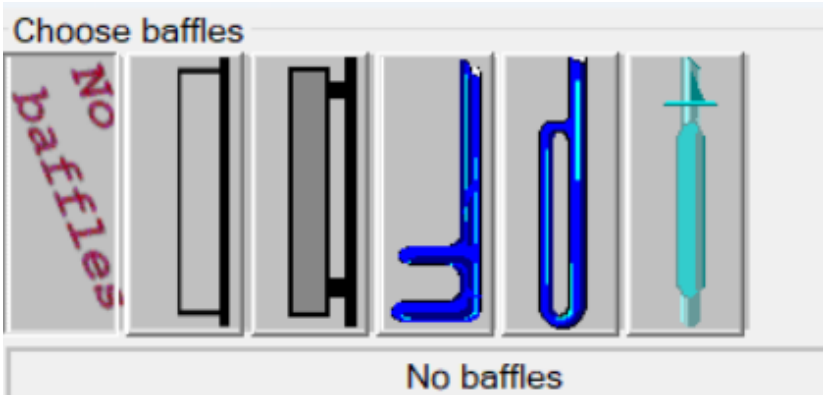


Figure 11. Choose baffle type

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

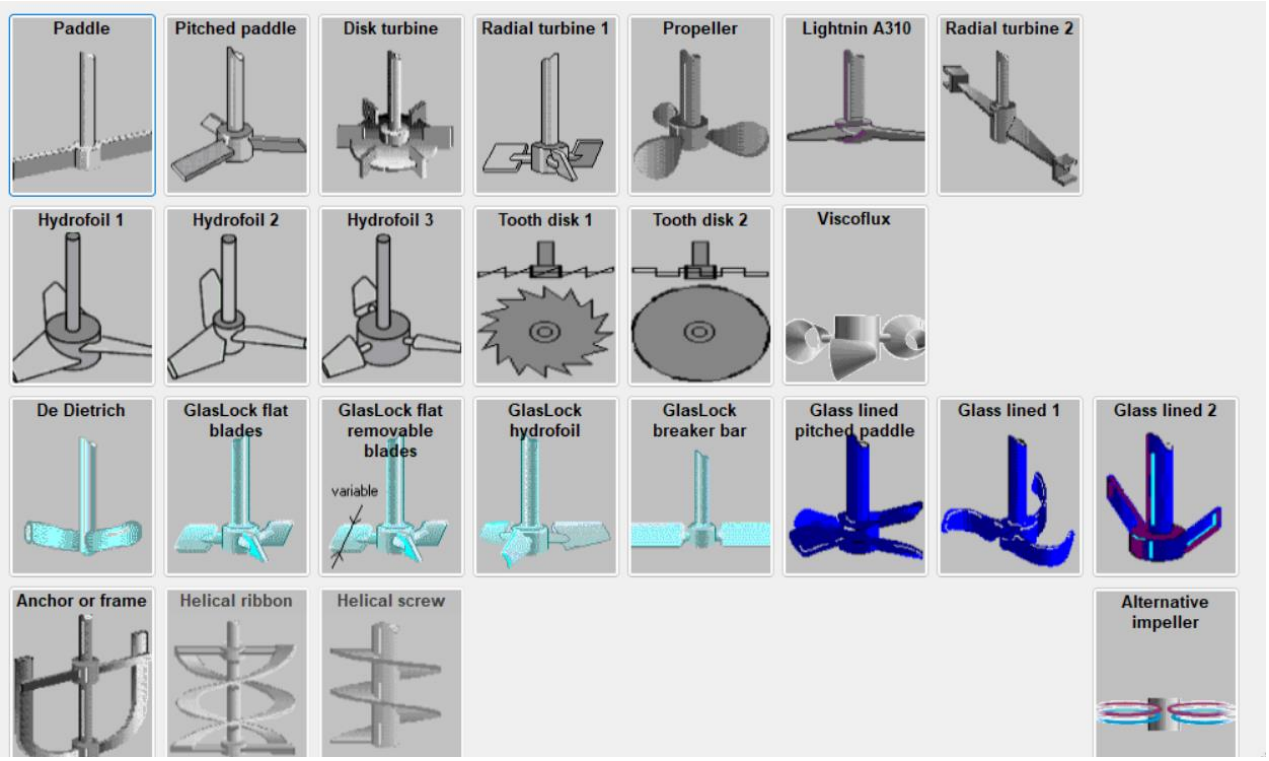


Figure 12. Select the impeller type

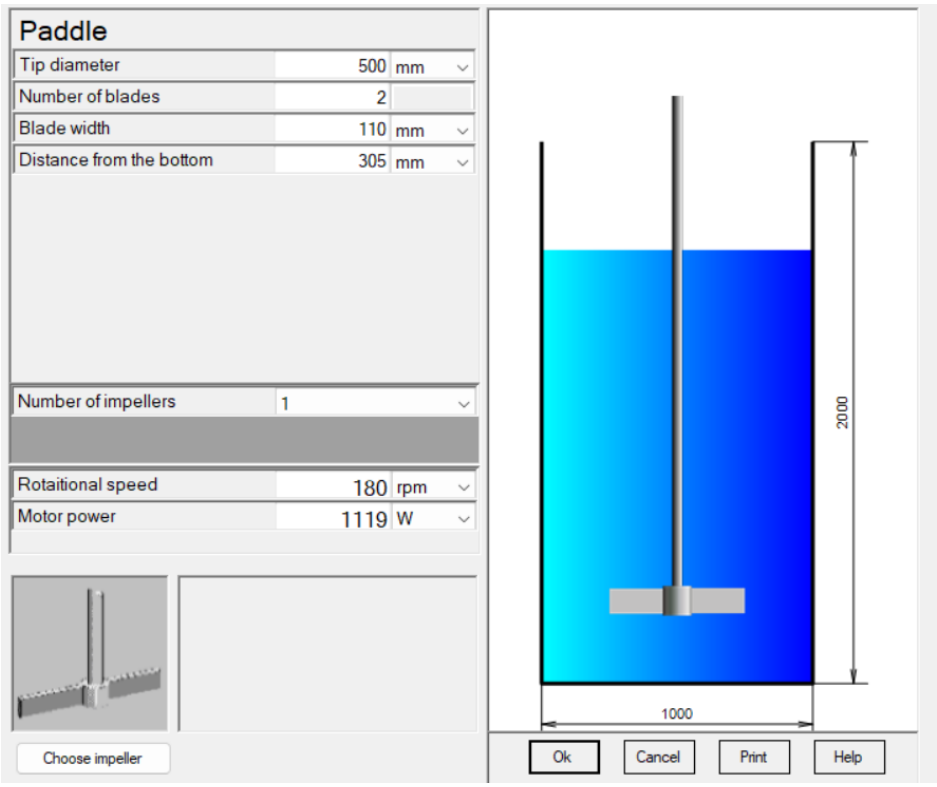


Figure 13. Enter the impeller dimensions

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

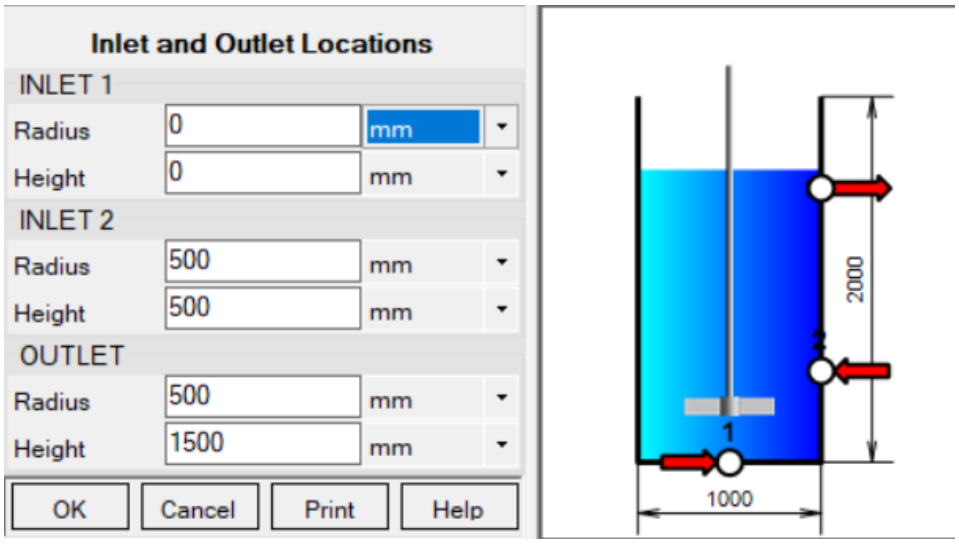


Figure 14. Enter the Inlet and outlet positions

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

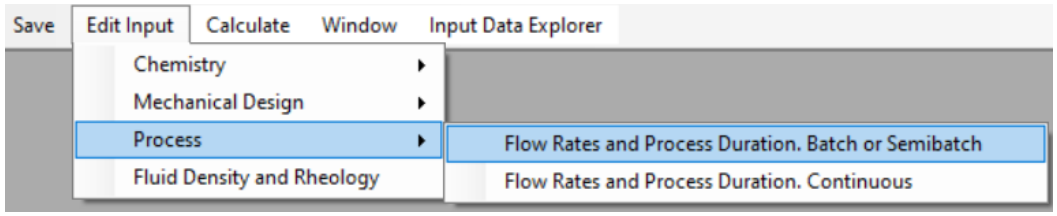


Figure 15. Edit Input – Process menu

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

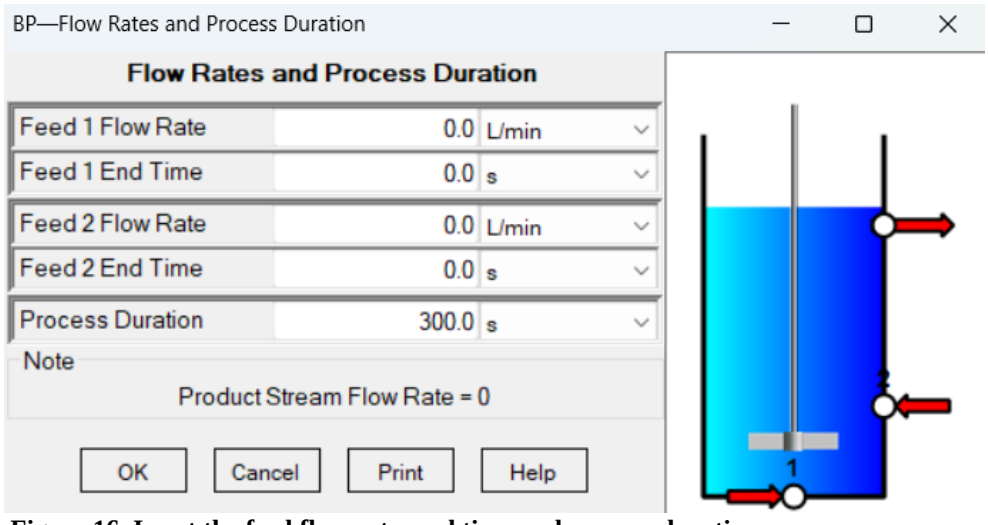


Figure 16. Input the feed flow rate, end time and process duration

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

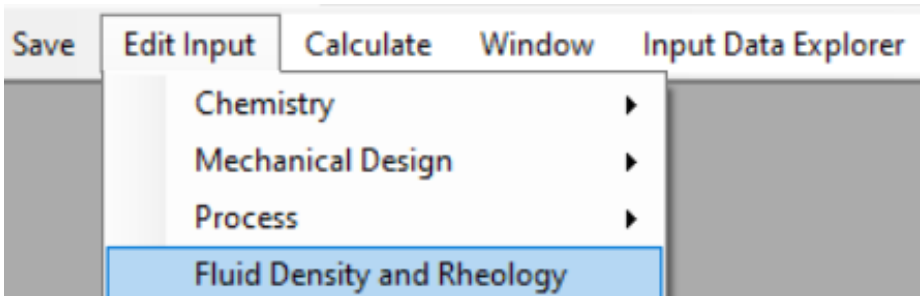


Figure 17. Edit input – Fluid density and Rheology

Enter the Average density and dynamic viscosity

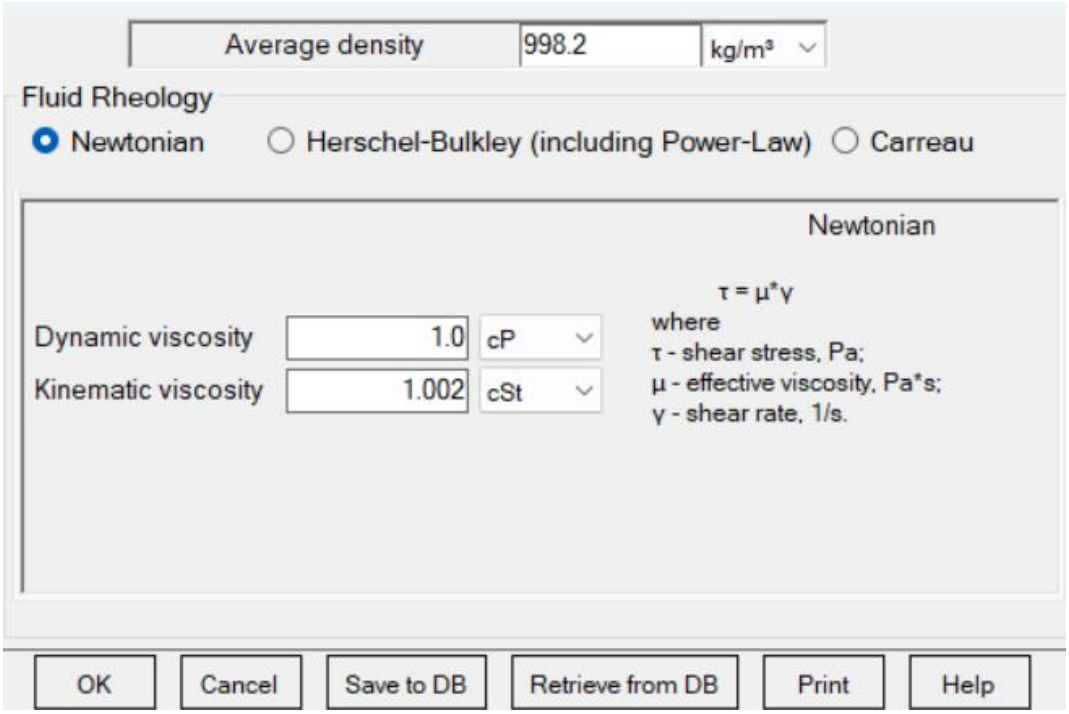


Figure 18. Input Fluid density and Rheology data

Results of Mathematical Modelling

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

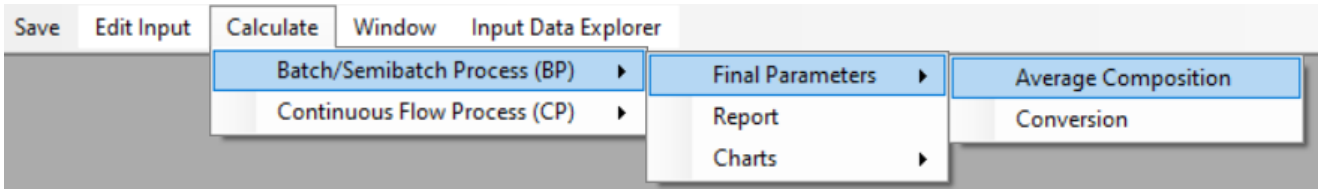


Figure 19. Select Calculate Menu-Final Parameters

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

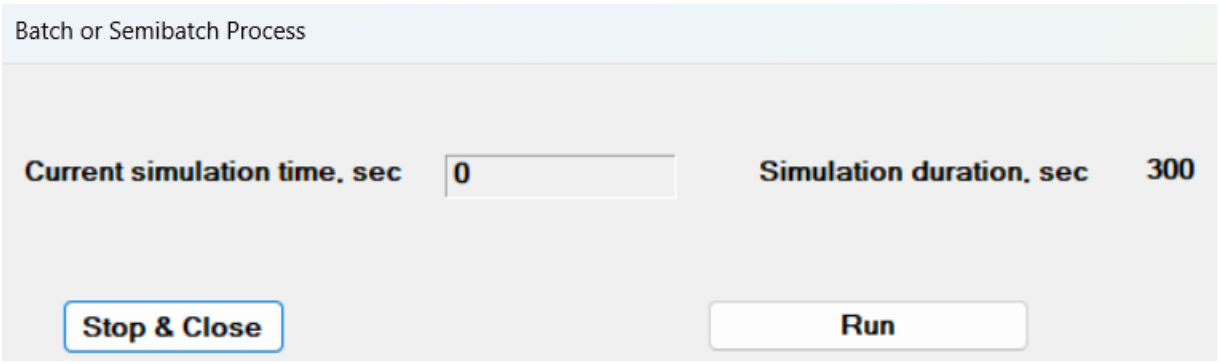
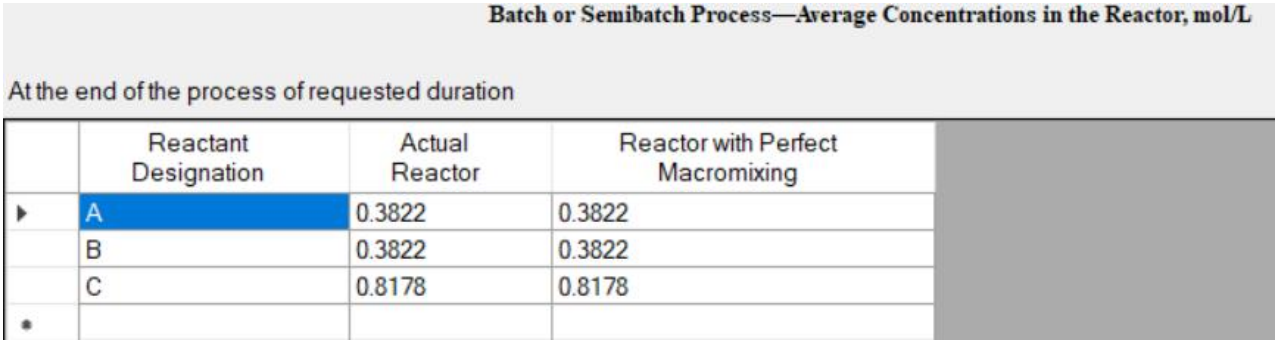


Figure 20. Run the simulation

The final concentrations of the reactants (mol/L) 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:



	Reactant Designation	Actual Reactor	Reactor with Perfect Macromixing
▸	A	0.3822	0.3822
	B	0.3822	0.3822
	C	0.8178	0.8178
*			

Figure 21. Average concentration in the reactor mol/L

If you navigate to the Conversion section under the Final Parameters> Conversion calculation, the following window will appear:

Batch or Semibatch Process—Reactant Conversion

At the end of the process of requested duration

	Reactant Designation	Actual Reactor	Reactor with Perfect Macromixing
▶	A	0.6815	0.6815
	B	0.6815	0.6815
	C		
*			

Figure 22. Reactant conversion

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

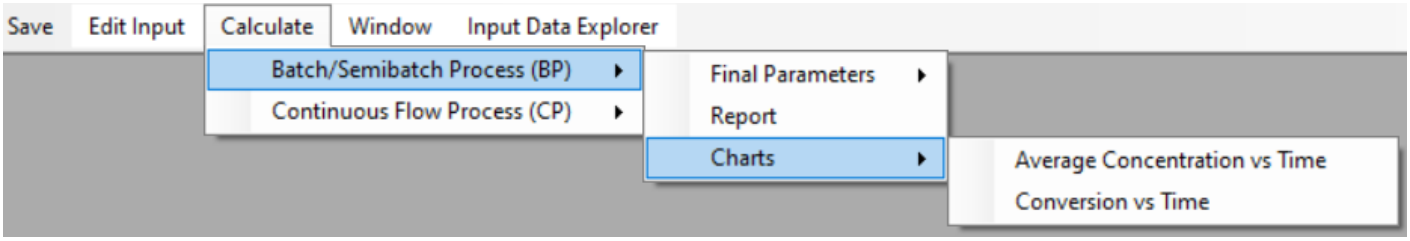


Figure 23. Select Calculate Menu- Charts

Concentration Vs time graph

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

Reactant A

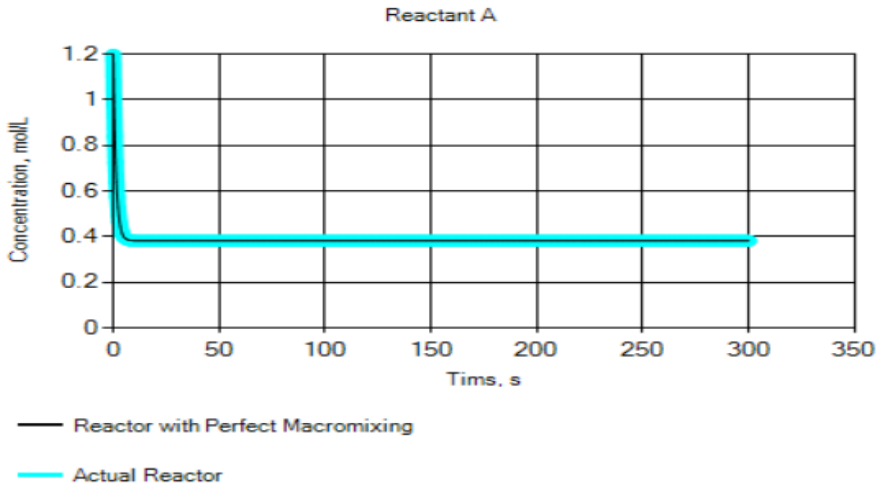


Figure 24. Concentration Vs time graph – Reactant A

Reactant B

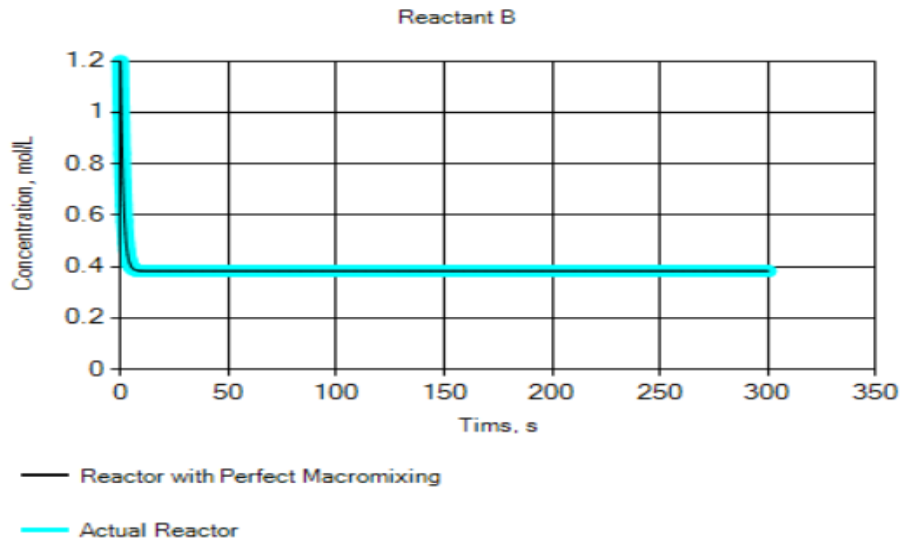


Figure 25. Concentration Vs time graph – Reactant B

Product C

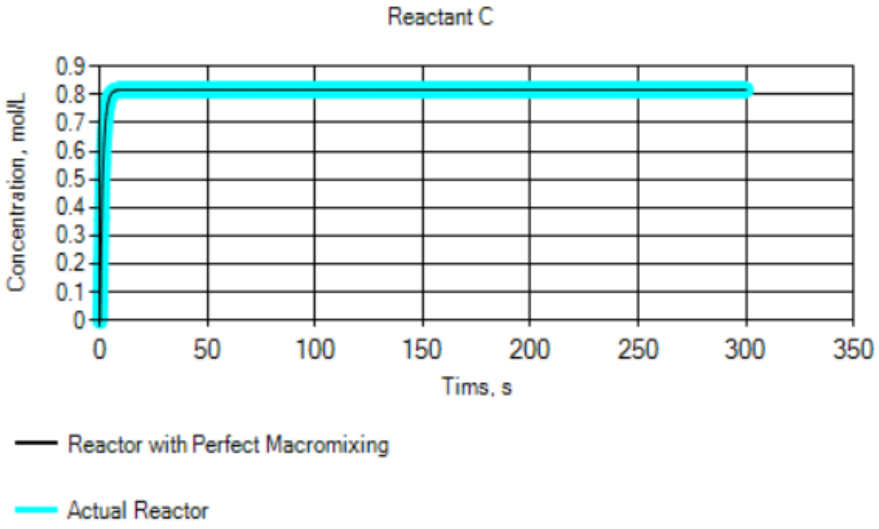


Figure 26. Concentration Vs time graph – Product C

Analysis of the concentration versus time graph reveals that the concentration of the reactant decreased from 1.2 mol/L to 0.38 mol/L over a period of 10 seconds. This significant decline in concentration underscores the rapid consumption of the reactant during the initial phase of the reaction, reflecting the effectiveness of the reaction conditions and the kinetics involved. The graph clearly illustrates the relationship between time and reactant concentration, highlighting the dynamics of the reaction."

Conversion Vs time graphs

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

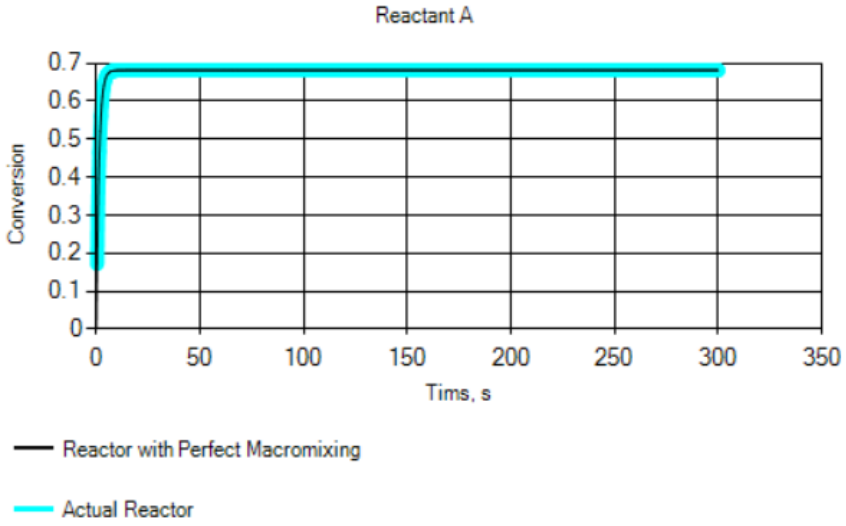


Figure 27. Conversion Vs time graph – Reactant A

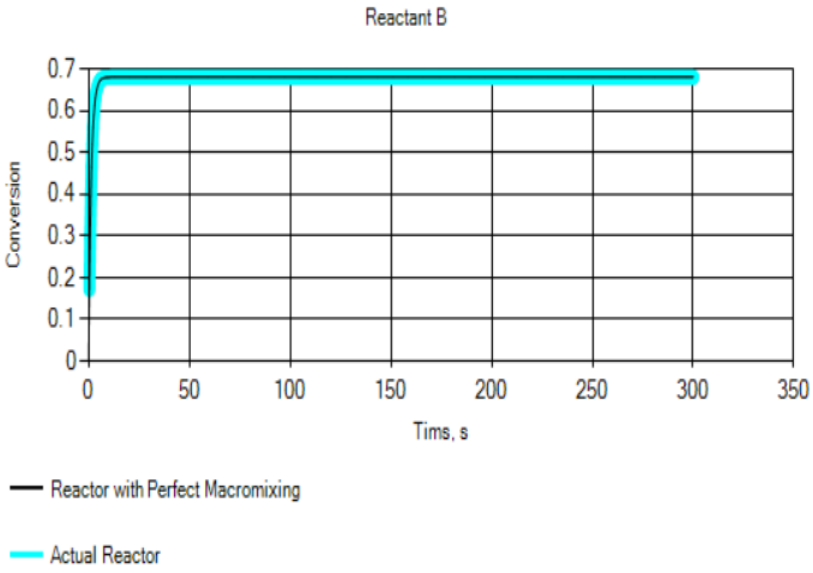


Figure 28. Conversion Vs time graph – Reactant B

Analysis of the conversion versus time graph indicates that an 68% conversion is achieved within a duration of 10 seconds. This rapid conversion illustrates the efficiency of the reaction process during its initial phase, emphasizing the effectiveness of the chosen reactants and operational conditions. The graph provides a clear representation of the relationship between time and conversion, demonstrating the swift transformation of reactants into products.

Results Overview:

This report presents an investigation of the batch esterification reaction using water as the solvent. The concentration of each reactant was systematically monitored, resulting in a maximum conversion of 68%. Notably, the concentration of reactant A decreased from 1.2 mol/L to 0.38 mol/L over a period of 10 seconds.

These results highlight the effectiveness of water as a solvent in facilitating the esterification process, demonstrating significant reactant conversion in a relatively short time. This study provides important insights into the dynamics of esterification reactions and sets the stage for further exploration of different solvents to optimize reaction conditions.