VISIMIX CHEM
Continuous Flow Process: Effect of Feed Location on Reaction & By-Product Formation

Previous study overview (Demo Project 2.1):

The previous report, titled **Continuous Flow Process: Main Reaction vs By-Product Formation**, investigated the performance of a reactor with **Inlet 2 (Reactant B)** positioned near the **top of the reactor**, delivering feed downward along the reactor axis, **without the use of baffles**. In this configuration, Reactant A achieved 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.

Current study overview:

The current study focuses on investigating the continuous flow process with a modified feed inlet location for Reactant B. In this configuration, Inlet 2 is positioned near the **bottom** of the reactor at a radius of 500 mm and a height of 120 mm from the base, **without the use of baffles**. The placement of the feed inlet plays a critical role in determining the mixing efficiency, reactant distribution, and overall reaction performance. By comparing the results from this new feed location with those from the previous study, this analysis evaluates the impact of the bottom feed position on reactant conversion, by-product formation, and process yield. The findings will provide valuable insights into how adjusting the feed inlet position influences conversion rates and reactor behavior in continuous flow processes.

Objective:

This report aims to analyze the impact of varying the Feed 2 (Reactant B) inlet position on the performance of a continuous process.

The Solution:

To update the location of **Inlet 2** (Reactant B), navigate to the Edit Input>Mechanical Design>Inlet and Outlet locations section.

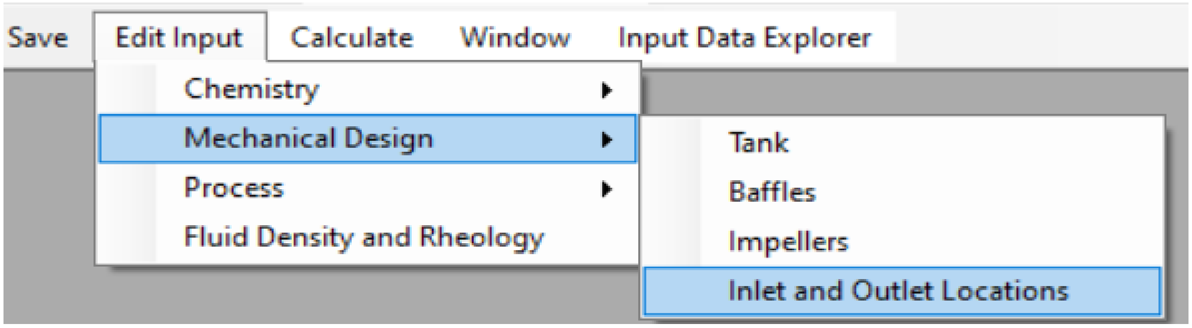

Figure 1. Edit Input – Mechanical Design menu for Inlet Location

The location of inlet 2 for Reactant B needs to be updated to position it near the bottom of the reactor, with a radius of 500 mm and a height of 120 mm from the base. This configuration will allow the feed to be delivered tangentially, promoting effective mixing and interaction with the existing reactor contents, which will enhance the overall reactor performance.

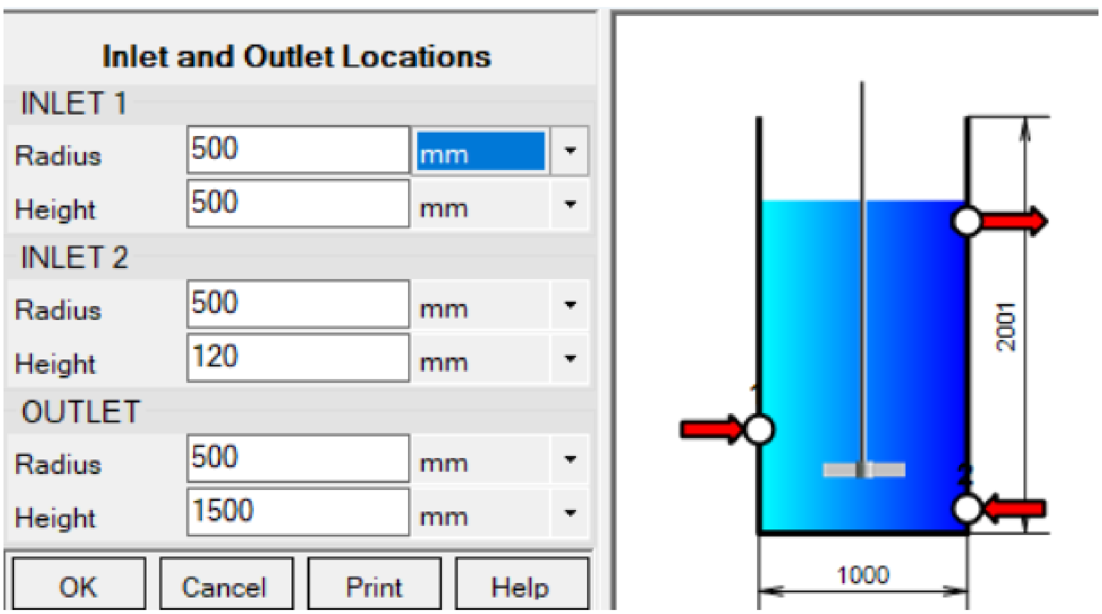

Figure 2. Update the Inlet 2 location

RESULTS:

Next, navigate to the **Calculate** menu, then select Continuous Process > Final Parameters > Average Composition, and run the simulation. Once the simulation is complete, return to the Calculate menu and select Continuous Process > Final Parameters > Average Composition again. This will provide the composition values, taking into account both the actual reactor conditions and perfect macromixing.

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	0.02339	0.01299	0.02663
B	0.08724	0.06291	0.07053
P	0.3536	0.3693	0.3636
BP	0.0493	0.05049	0.0439

Figure 3. Average concentration in the reactor mol/L

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

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	0.007199	0.02187	0.02339
B	0.0249	0.0749	0.08724
P	0.0136	0.03976	0.3536
BP	0.001164	0.003566	0.0493

Figure 4. 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	0.974	0.9467
B	0.8742	0.8589
P		
BP		

Figure 5. 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.

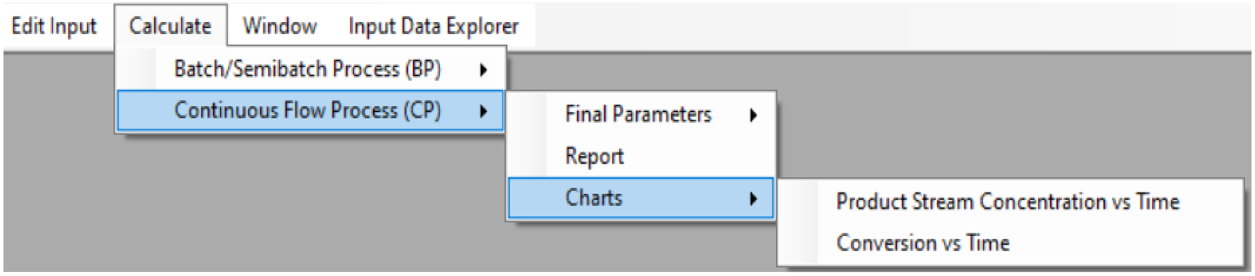

Figure 6. Select Calculate Menu- Charts

Product Stream Concentration Vs time graph in Product Stream

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

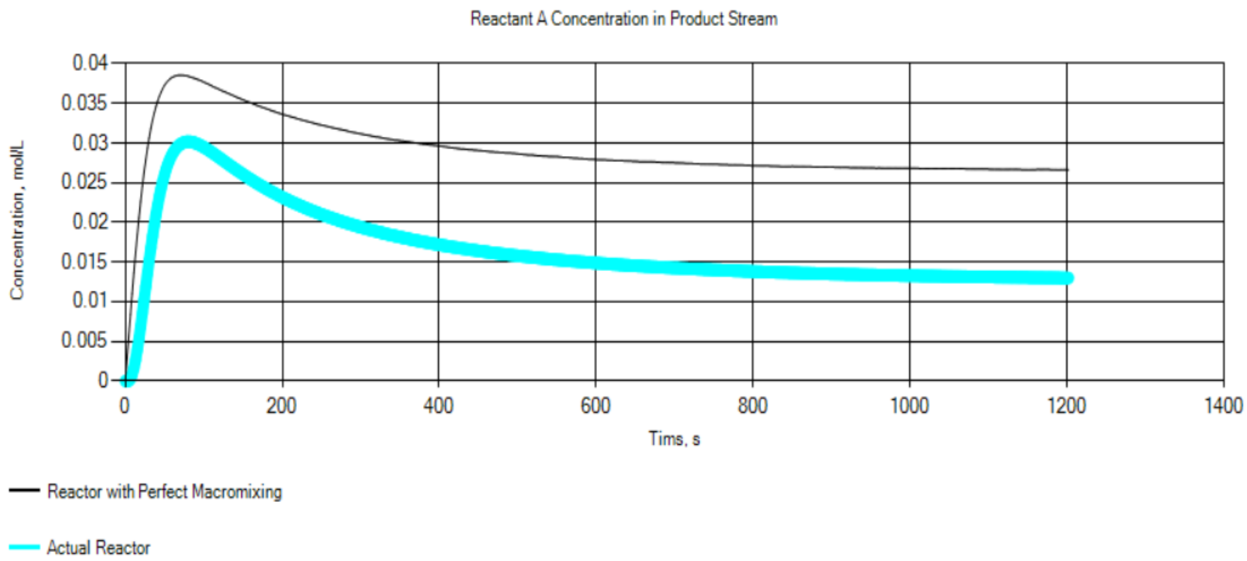

Figure 7. Concentration Vs time graph – Reactant A

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, influenced by real-world factors such as local micro mixing, the concentration stabilizes at 0.012 mol/L within 1000 seconds. In contrast, the ideal reactor achieves a higher concentration of 0.026 mol/L at 1000 seconds under perfect macromixing conditions.

Reactant B

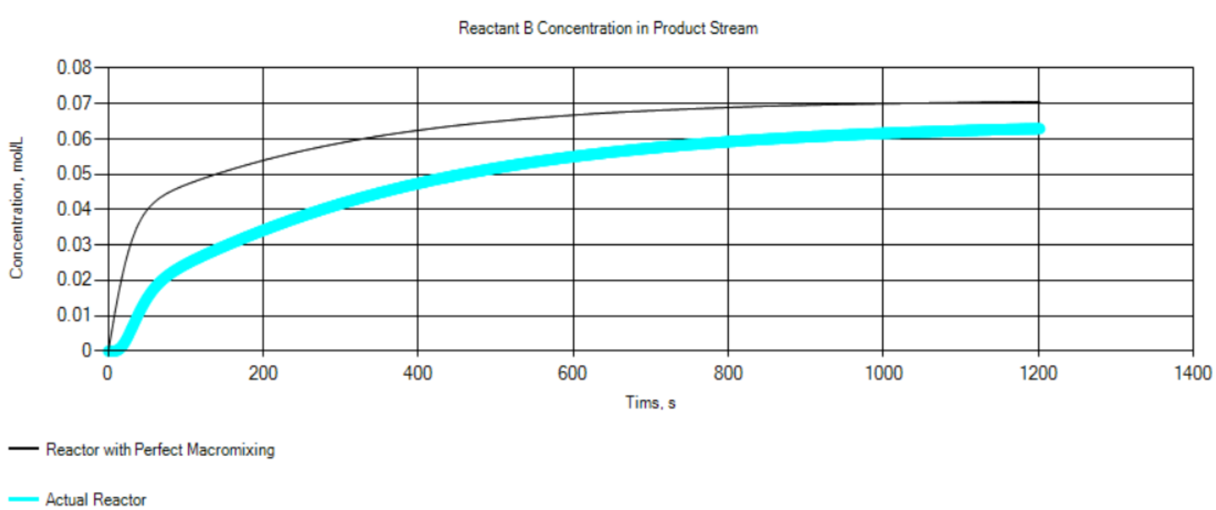

Figure 8. Concentration Vs time graph – Reactant B

The concentration of Reactant B in the actual reactor, affected by real-world factors such as local micro mixing, stabilizes at 0.063 mol/L within 1100 seconds. In comparison, the ideal reactor, operating under perfect macromixing conditions, achieves a concentration of 0.07 mol/L at 1000 seconds.

Product P

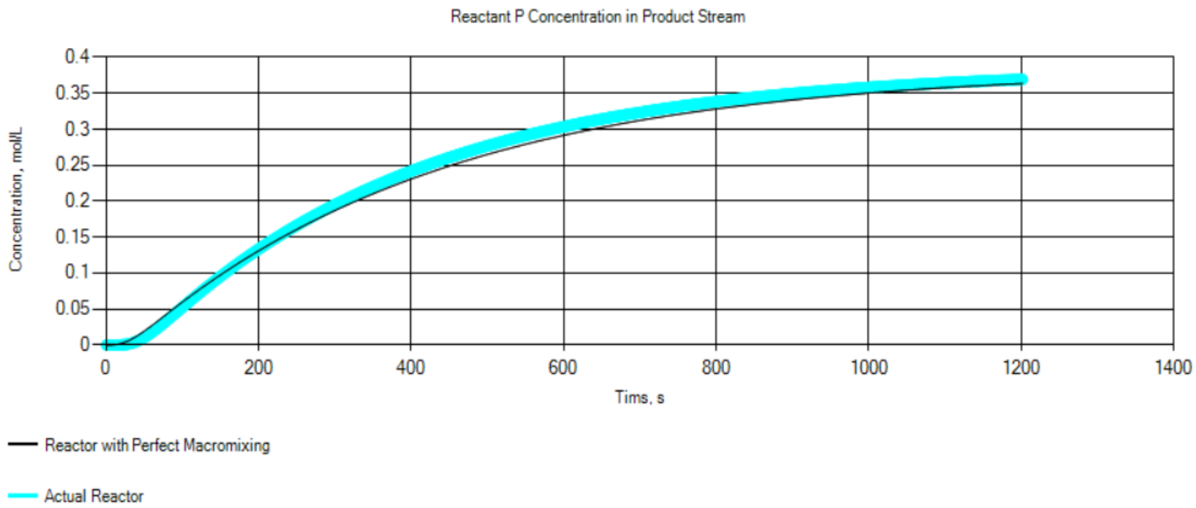

Figure 9. Concentration Vs time graph – Product P

The concentration of P in the actual reactor, influenced by real-world factors such as local micro mixing, stabilizes at 0.369 mol/L within 1200 seconds, slightly exceeding the concentration of 0.363 mol/L achieved by the ideal reactor under perfect macromixing conditions at the same time.

By-product BP

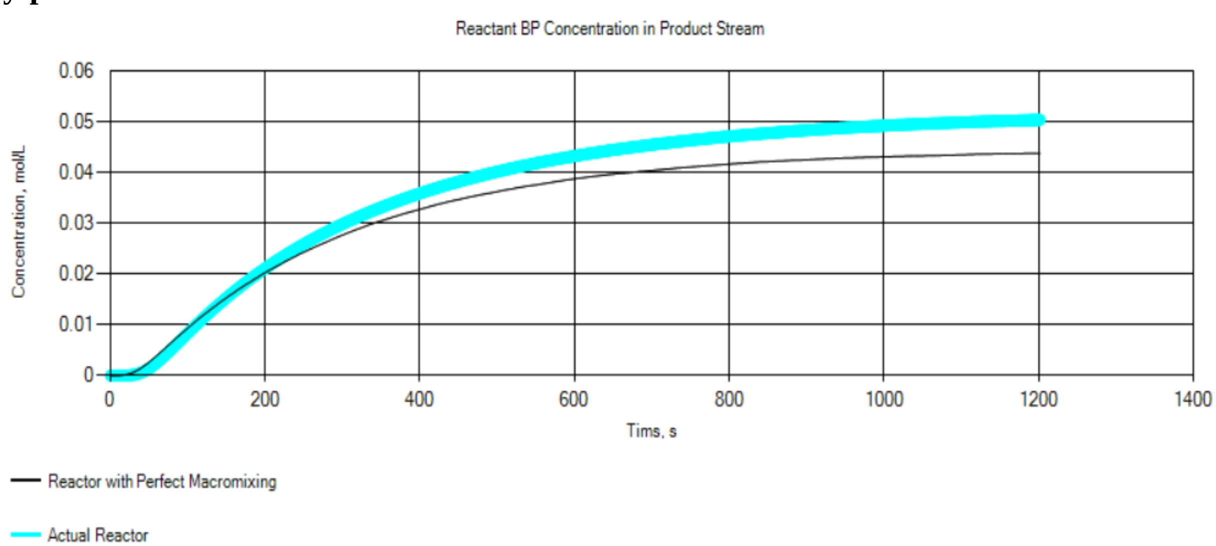

Figure 10. Concentration Vs time graph – By-Product

The concentration of the by-product in the actual reactor, impacted by real-world factors such as flow irregularities, stabilizes at 0.05 mol/L within 1200 seconds, whereas the ideal reactor, operating under perfect macromixing conditions, achieves a concentration of 0.04 mol/L at the same time.

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.

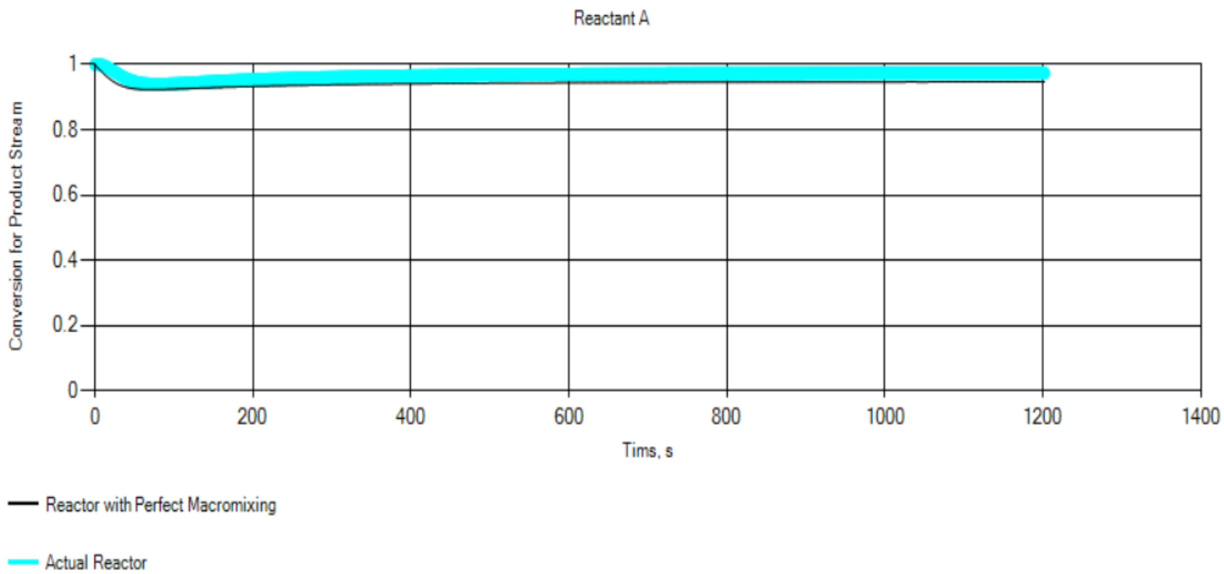

Figure 11. Conversion Vs time graph – Reactant A

The graph shows that initially, the conversion fluctuates slightly during the transient phase as the system stabilizes. Ultimately, Reactant A achieves a conversion of 0.97 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.

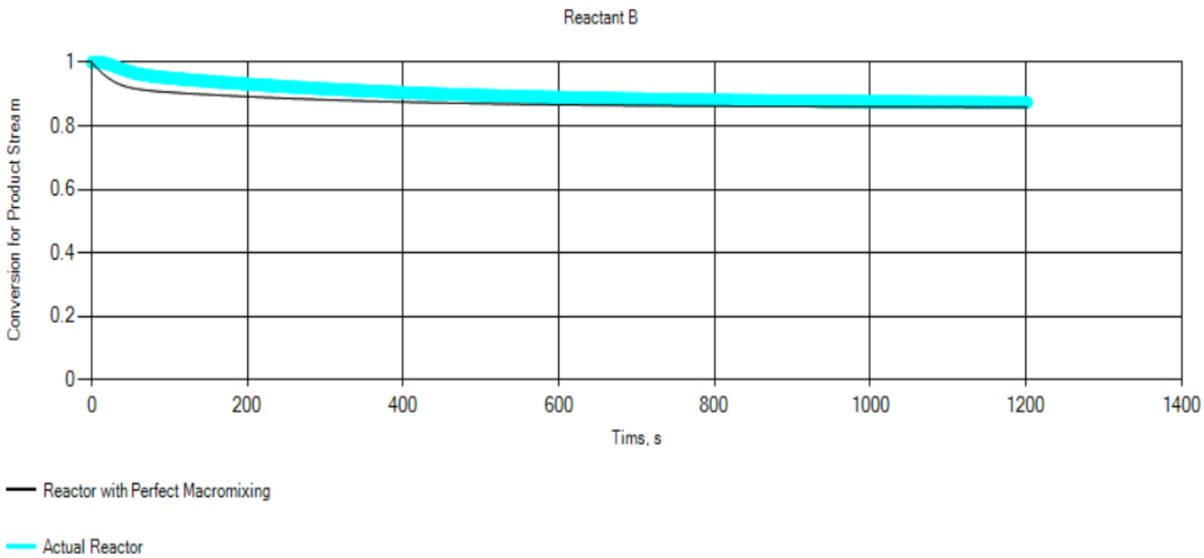

Figure 12. Conversion Vs time graph – Reactant B

This graph shows that Reactant B achieves a conversion of 0.87 in the actual reactor, which is higher than the 0.86 observed in the ideal reactor demonstrating that the actual reactor effectively converts Reactant B.

Results Overview:

The current study evaluates the impact of relocating the feed inlet to the bottom of the reactor, positioned at a radius of 500 mm and a height of 120 mm from the base, compared to the previous configuration with the inlet near the top. Reactant A achieved a conversion of **0.97** in the actual reactor, surpassing both the ideal reactor's **0.94** and the previous study's **0.95**, demonstrating improved performance. Similarly, Reactant B exhibited enhanced conversion, achieving **0.87** in the actual reactor compared to the ideal reactor's **0.86,** and outperforming the prior setup, where the actual conversion was only **0.81**.

Furthermore, the by-product concentration was significantly reduced to **0.05 mol/L**, compared to **0.07 mol/L** in the earlier configuration, reflecting improved selectivity. These findings underscore the critical role of feed inlet positioning in optimizing reactor performance, with the bottom placement proving more effective in balancing conversion efficiency and by-product minimization. This highlights the importance of strategic design adjustments in enhancing overall process efficiency.