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

Previous study overview (Demo Project 2.2):

The previous report, titled Continuous Flow Process: Effect of Feed Location on reaction & by-Product Formation, investigated the performance of a reactor with **Inlet 2 (Reactant B)** positioned near the **bottom of the tank at a radius of 500 mm and a height of 120 mm from the base without the use of baffles**. In this configuration, Reactant A achieves a conversion of **0.97** in the actual reactor, slightly surpassing the ideal reactor's conversion of **0.94**. This indicates effective performance, likely influenced by enhanced local micro-mixing at the feed location, which promotes efficient reactant dispersion and reaction kinetics. Similarly, Reactant B achieved a conversion of **0.87** in the actual reactor, which is higher than the ideal reactor's conversion of **0.86**. The by-product concentration in the actual reactor was measured at **0.05 mol/L**, reflecting a trade-off between optimizing main reaction performance and minimizing by-product formation.

Current study overview:

This report investigates the continuous flow process with the addition of three baffles, which are essential for improving mixing efficiency and overall reactor performance. Baffles disrupt vortex formation, ensuring better radial mixing and uniform distribution of reactants throughout the reactor. Their incorporation helps minimize flow irregularities and non-idealities, creating more consistent reaction conditions and enhancing kinetic performance. This study evaluates the impact of baffles in combination with the bottom feed inlet position, focusing on metrics such as reactant conversion, by-product formation, and yield. By comparing these results to the previous study without baffles, this analysis highlights the significant role of baffles in optimizing efficiency and selectivity in continuous flow processes.

Objective:

This report aims to analyze the impact of incorporating baffles into the reactor design on the performance of a continuous flow process, focusing on improving mixing efficiency, reactant conversion, and by-product formation.

The Solution:

To update the baffle details , navigate to the **Edit Input>Mechanical Design>Baffles** section.

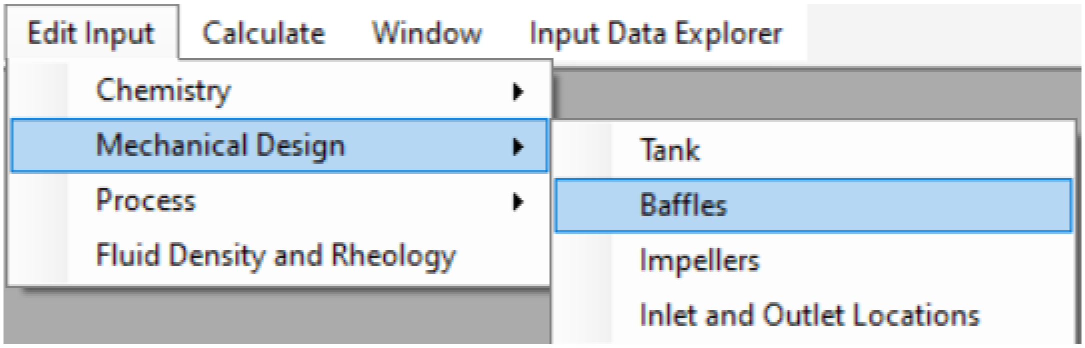


Figure 1. Edit Input – Mechanical Design menu for Baffle details

Select **Flat Baffle** and input the baffle details.

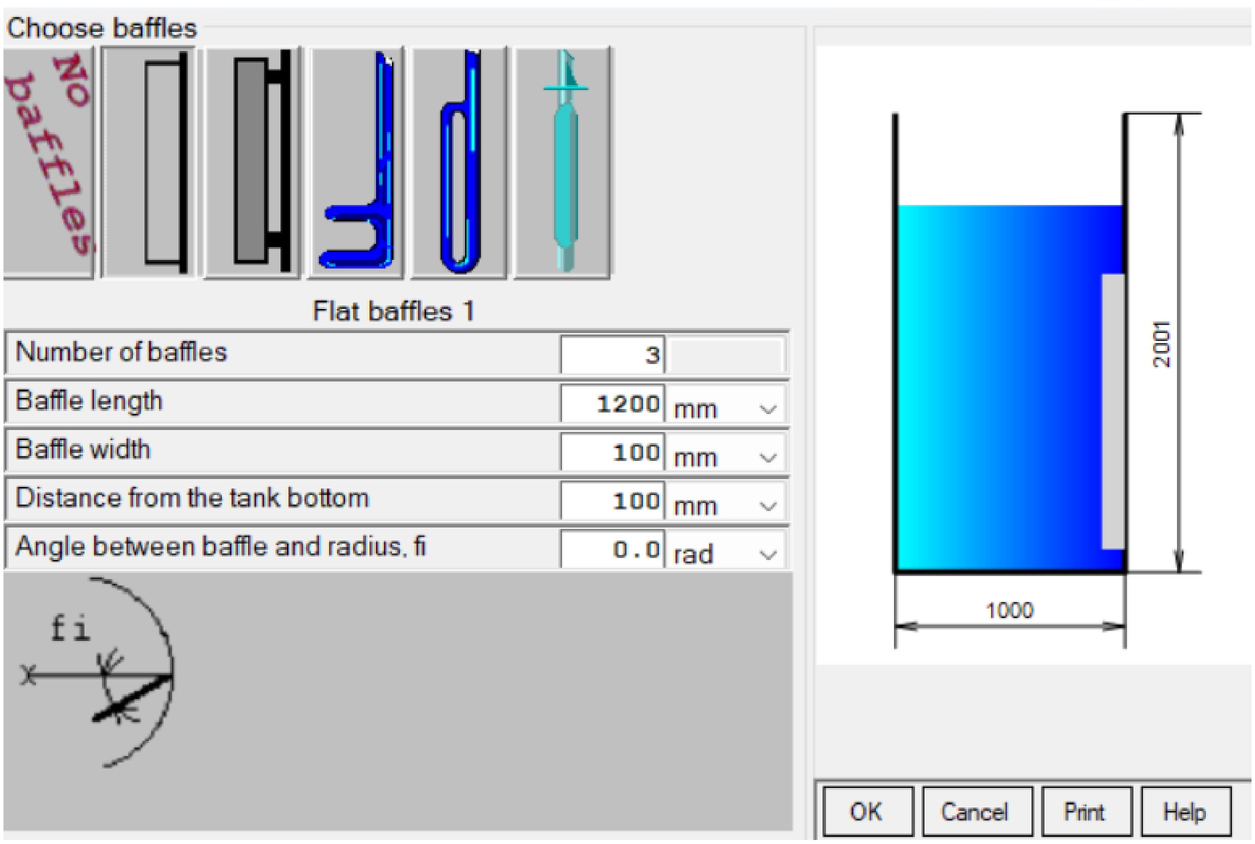


Figure 2. Input the baffle details

Click OK to confirm.

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	0.01733	0.003927	0.02799
B	0.1445	0.06603	0.07202
P	0.3227	0.3584	0.3632
BP	0.05896	0.06415	0.04403

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:

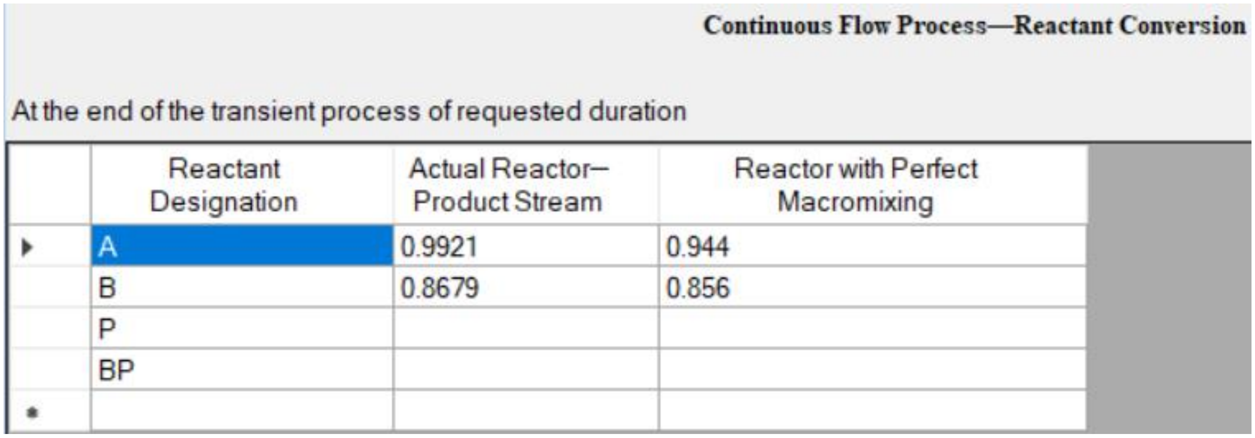
Continuous Flow Process—Concentration Non-Uniformities in Actual Reactor, mol/L

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	0.01832	0.09381	0.01733
B	0.1056	0.3125	0.1445
P	0.0398	0.12	0.3227
BP	0.007338	0.02129	0.05896

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	0.9921	0.944
B	0.8679	0.856
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.

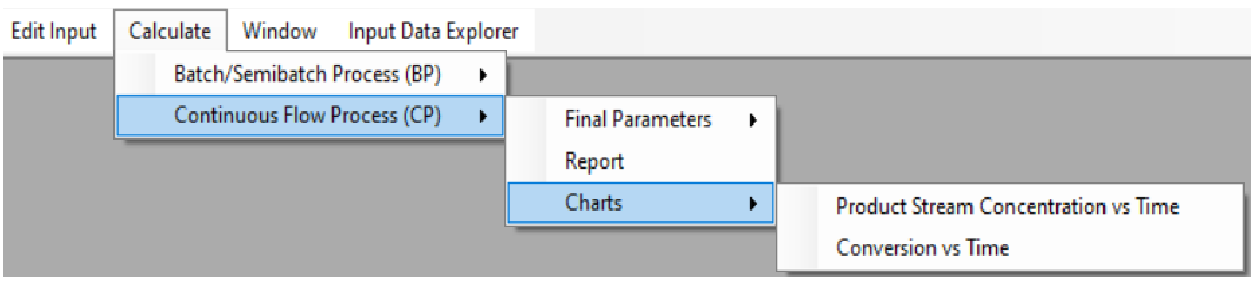


Figure 6. Select Calculate Menu- Charts

Product stream Concentration Vs time graph

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

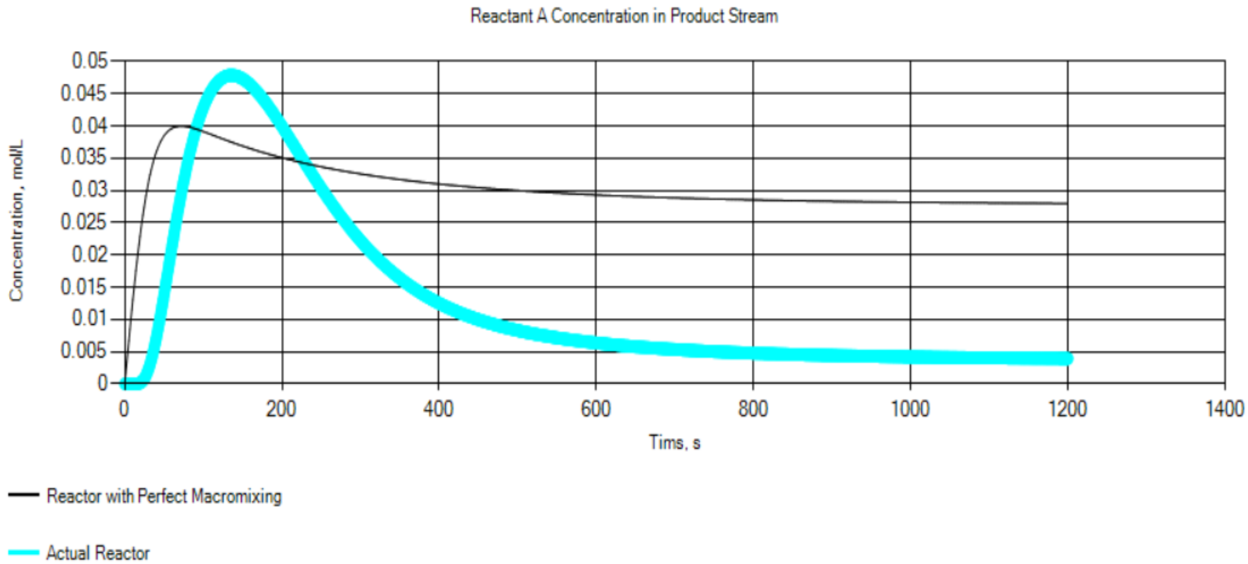


Figure 7. Concentration Vs time graph – Reactant A

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 0.0039 mol/L within 1200 seconds. In contrast, the ideal reactor achieves a concentration of 0.027 mol/L at 1200 seconds under perfect macromixing conditions. This comparison underscores the impact of local micro-mixing effects on the behavior, distribution, and efficiency of the actual reactor.

Reactant B

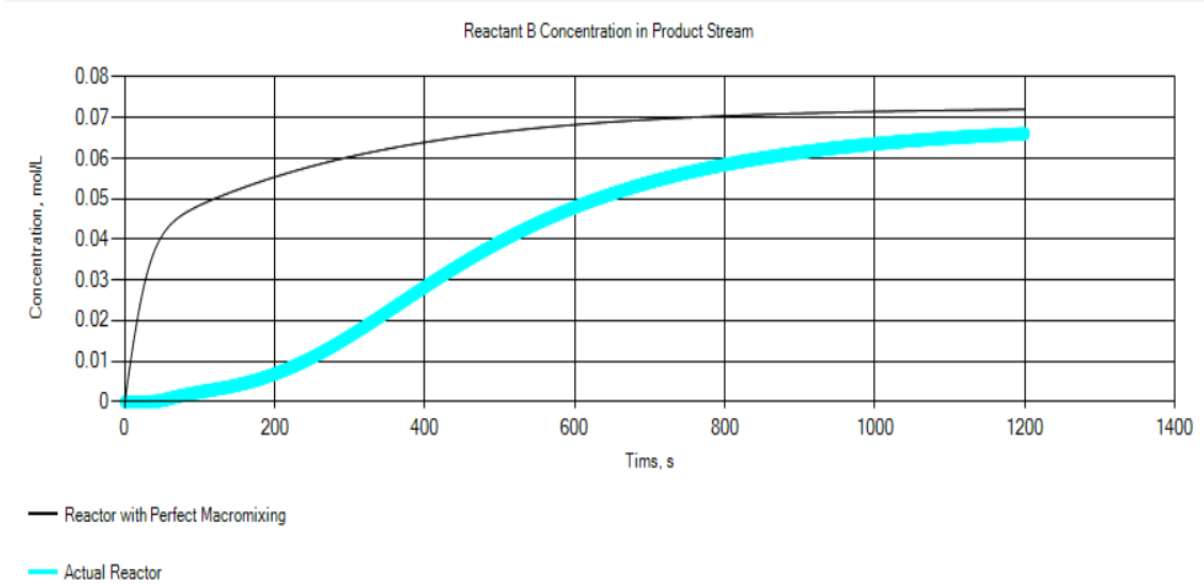


Figure 8. Concentration Vs time graph – Reactant B

The concentration of Reactant B in the actual reactor, affected by real-world factors such as local micro mixing, stabilizes at 0.066 mol/L within 1200 seconds.
In comparison, the ideal reactor, operating under perfect macromixing conditions, achieves a concentration of 0.072 mol/L at 1200 seconds.

Product P

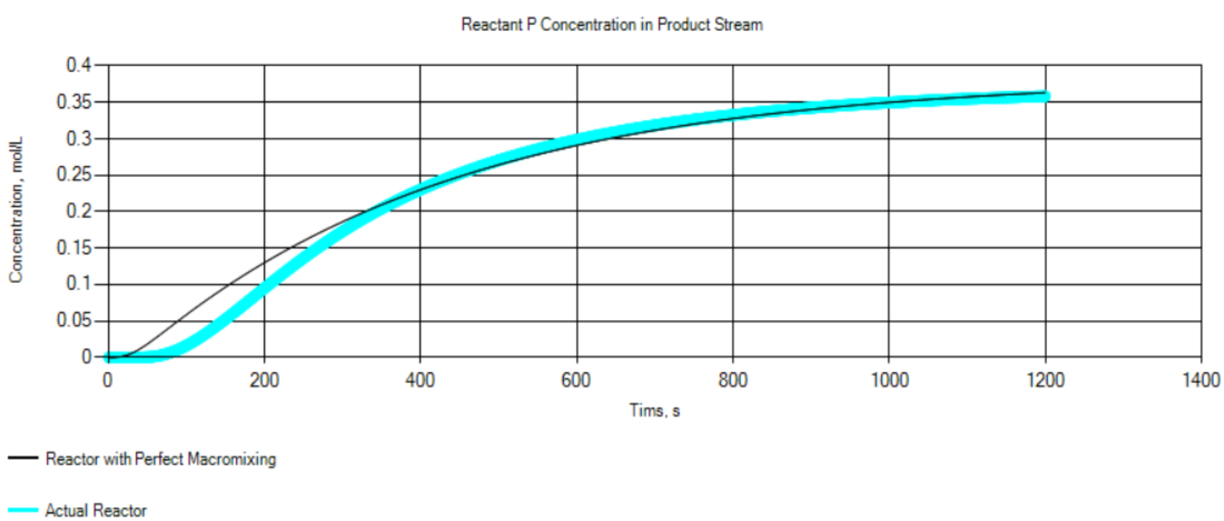


Figure 9. Concentration Vs time graph – Product P

The concentration of P in the actual reactor stabilizes at 0.358 mol/L within 1200 seconds, which is slightly lower than the 0.363 mol/L observed in the ideal reactor under perfect macromixing conditions.

By-product BP

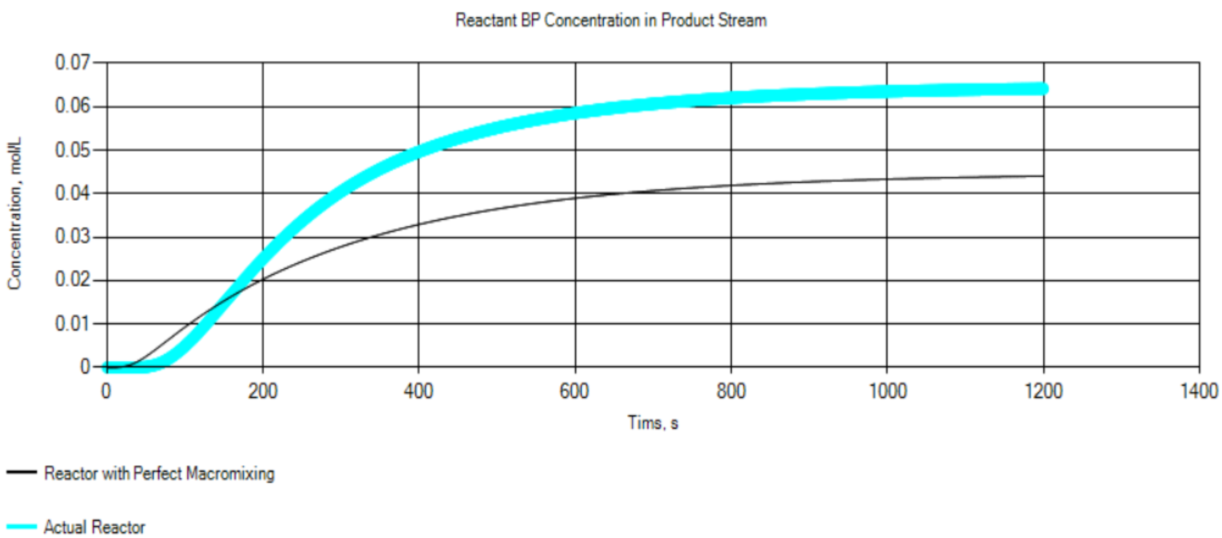


Figure 10. Concentration Vs time graph – By-Product

The concentration of the by-product in the actual reactor stabilizes at 0.064 mol/L within 1200 seconds, whereas the ideal reactor, operating under perfect macromixing conditions, achieves a concentration of 0.044 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.

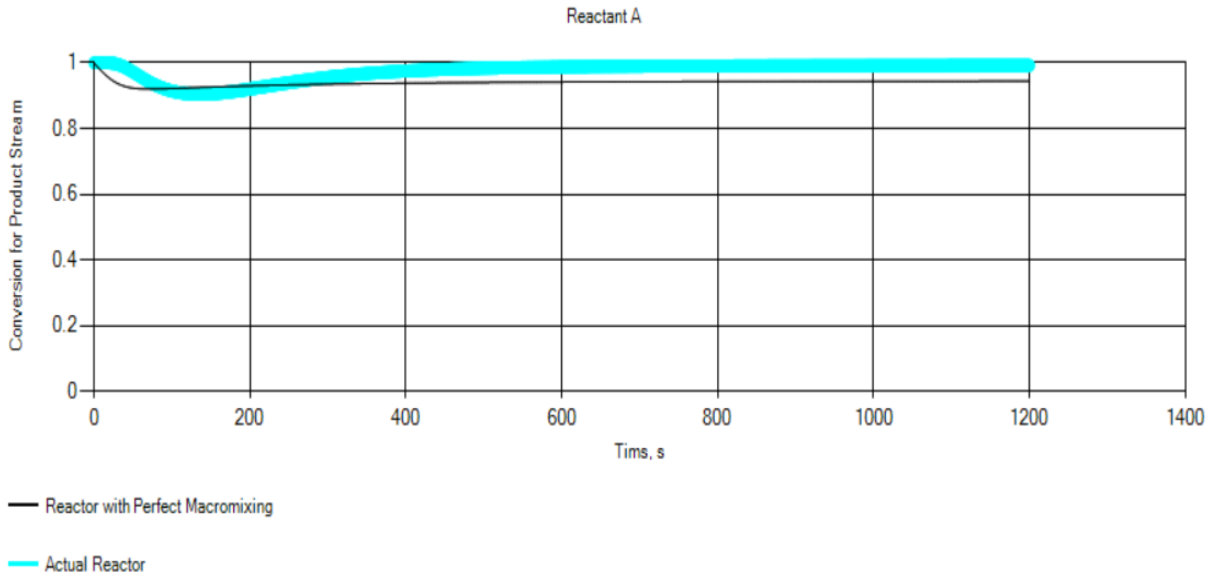


Figure 11. Conversion Vs time graph – Reactant A

The graph shows that initially, the conversion fluctuates slightly during the transient phase as the system stabilizes. Ultimately, Reactant A achieves a conversion of 0.99 in the actual reactor which is 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.

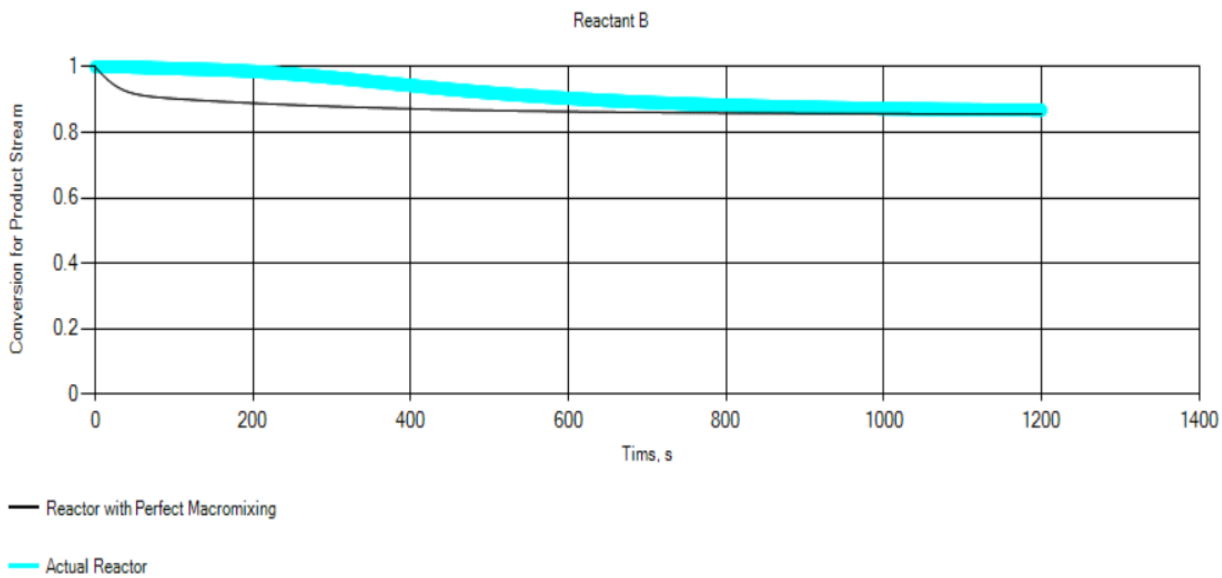


Figure 12. Conversion Vs time graph – Reactant B

This graph shows that Reactant B achieves a conversion of 0.86 in the actual reactor, which is slightly higher than the 0.85 observed in the ideal reactor.

Results Overview:

The investigation demonstrates the combined impact of feed inlet position and the incorporation of baffles on reactor performance. In the previous study, with the feed inlet positioned near the bottom of the reactor (radius of 500 mm and a height 120 mm from the base), without baffles, Reactant A achieved a conversion of **0.97** in the actual reactor, slightly exceeding the ideal reactor's conversion of **0.94**. Reactant B also performed well, achieving a conversion of **0.87** in the actual reactor compared to **0.86** in the ideal reactor.The by-product concentration was found to be **0.05 mol/L.**

With the addition of baffles, Reactant A's conversion increased further to **0.99** in the actual reactor, surpassing the ideal reactor's conversion of **0.94**. Reactant B exhibited a similar trend, with a conversion of **0.86** in the actual reactor compared to **0.85** in the ideal reactor. However, the by-product concentration in this configuration was found to be **0.06 mol/L**. These findings emphasize that optimizing feed position and incorporating baffles can significantly improve mixing, reduce non-idealities, and enhance overall reactor performance while influencing by-product formation.