NEWSLETTER

Continuous reaction optimization with VisiMix Chem: Role of feed position and Baffles in Multi step reactions

No.4 - Jun 2025

School of Scale-Up (SOS): A New Concept Offering

• Increasing productivity in research, scale-up and manufacturing are key goals for all chemical industries as the time to market shortens to meet fast-paced technology needs.

• With the resources at your disposal, how can you achieve the next level of productivity.

• Technologists need to think outside-of-the-box with novel methods and approaches to solve the practical challenges of Scale-up and Scale-down quickly.

Utilizing your lab and facility resources we will design simple test experiments to show your team how mixing influences your process challenges and how to overcome your existing limitations.

With VisiMix software we will show you how to quickly analyze and understand your process to achieve successful scale-up.

Our training is intuitive, insightful and practical. The hands-on demonstrations are accessible to technicians, chemists and engineers at all levels. We are two companies working together with a unique offering.

Register for SOS

Introduction

Continuous flow reactors are increasingly favored in the chemical and pharmaceutical industries for their enhanced control over reaction conditions, improved safety, and scalability. However, achieving optimal performance in multi-step reactions depends heavily on the reactor's internal configuration—particularly the location of feed entry and the presence or absence of baffles. Feed position influences local concentration gradients, mixing zones, and residence time distribution, all of which directly impact conversion and selectivity. Similarly, baffles affect flow patterns, turbulence, and energy dissipation, playing a crucial role in determining the overall mixing efficiency.

This edition of our newsletter focuses on optimizing continuous flow reactions using VisiMix Chem, with a special emphasis on the role of feed location and baffle configuration in multi-step reaction systems.

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 study focuses 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.

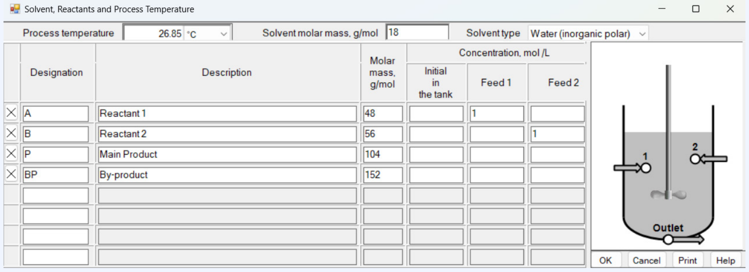
Case-I: Feed inlet positioned along the shaft near the **top** of the reactor, **without baffles**

Case-II: Feed inlet positioned near the **bottom** of the reactor, **without baffles**

Case-III: Feed inlet positioned near the **bottom** of the reactor, **with three baffles.**

VISIMIX SIMULATION

Case-I: Feed inlet positioned along the shaft near the **top** of the reactor, **without baffles**

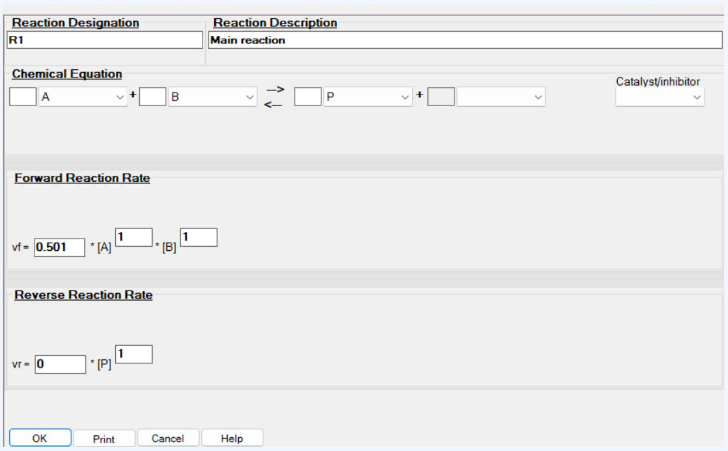


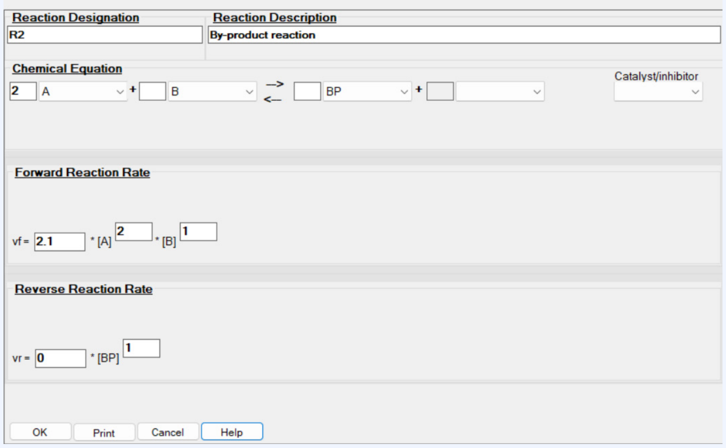
Solvent, Reactants and Process Temperature

Process temperature 26.85 °C | Solvent molar mass, g/mol 18 | Solvent type Water (inorganic polar)

Designation	Description	Molar mass, g/mol	Initial in the tank	Feed 1	Feed 2
A	Reactant 1	48		1	
B	Reactant 2	56			1
P	Main Product	104			
BP	By-product	152			

Next, enter the reaction details for both the main and side reactions, and update the corresponding kinetic data.





Next, enter the tank dimensions, baffle, impeller specifications, and the inlet and outlet locations of the reactant and product. Then, input the feed flow rate, density, and dynamic viscosity of the reaction mass in order to obtain simulation results.

Simulation Results - Case-I

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

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

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		

Reactant A achieved a high conversion of 0.95, slightly above the ideal 0.94, indicating efficient local micro-mixing. In contrast, Reactant B showed a lower conversion of 0.81 vs. the ideal 0.86, likely due to poor flow distribution or dead zones.

The by-product concentration was 0.07 mol/L, highlighting a trade-off between main reaction efficiency and by-product control.

This case emphasizes the impact of feed position on both reactant conversion and selectivity.

Case-II: Feed inlet positioned near the **bottom** of the reactor, **without baffles**

Now, we evaluate the continuous flow process by modifying the feed inlet position for Reactant B. In this setup, Inlet 2 is placed near the bottom of the reactor without baffles.

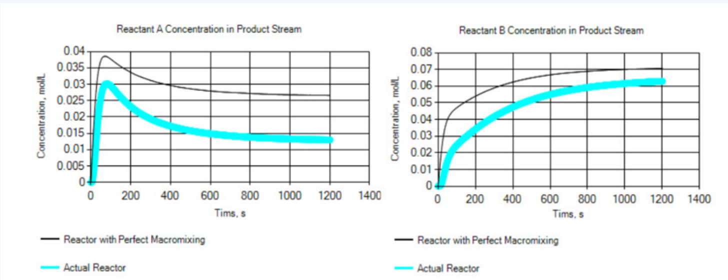
This change helps us understand how feed location affects mixing, conversion, and by-product formation.

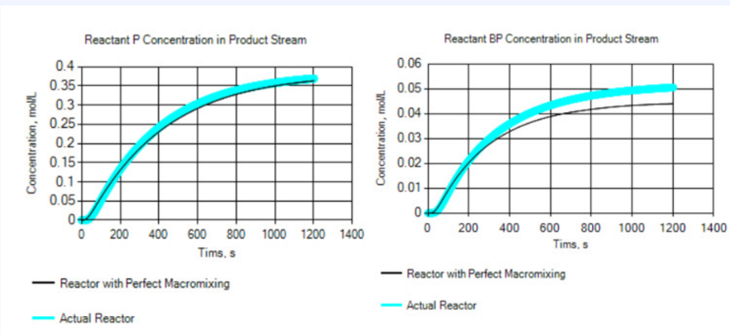
The results are compared with the previous configuration to assess the impact on reaction performance and process yield.

Simulation Results - Case II

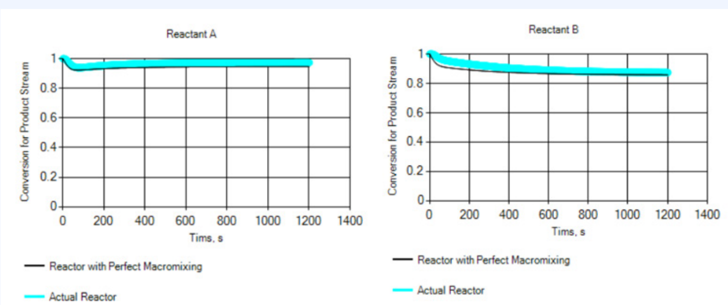
VisiMix generates results in both table and graph formats, making it easy to interpret process behavior and performance.

Concentration profiles





Conversion profiles



Reactant A showed improved conversion of 0.97, surpassing both the perfect maco mixing value (0.94) and the previous case (0.95).

Reactant B also improved, reaching 0.87 compared to 0.86 (perfect macro mixing) and 0.81 in the earlier setup.

By-product concentration decreased to 0.05 mol/L (from 0.07 mol/L), indicating enhanced selectivity.

These results highlight the positive impact of bottom feed positioning in improving both conversion efficiency and by-product control, emphasizing the value of feed location as a key design parameter in continuous flow systems.

Case-III: Feed inlet positioned near the **bottom** of the reactor, **with three baffles.**

In this, we evaluate the continuous flow process with the addition of three baffles, combined with the bottom feed inlet position. Baffles are known to improve mixing by disrupting vortex formation and promoting better radial flow and uniform reactant distribution. This setup is assessed for its impact on reactant conversion, by-product formation.

By comparing the results with the previous configuration without baffles, this study highlights the effectiveness of baffles in enhancing mixing efficiency, reducing flow irregularities, and improving reaction performance in continuous systems.

Simulation Results - Case III

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

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

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		

Reactant A achieved a higher conversion of 0.99, significantly exceeding the ideal value of 0.94, while Reactant B reached 0.86, closely aligning with the ideal 0.85. The by-product concentration was slightly higher at 0.06 mol/L, compared to 0.05 mol/L in the non-baffled setup. These findings highlight how combining optimal feed placement with baffle incorporation enhances mixing, reduces flow non-idealities, and improves conversion efficiency, though with a minor trade-off in by-product selectivity.

COMPARATIVE ANALYSIS

VisiMix Chem was used to simulate and analyzed three cconfigurations to understand the effect of feed position and baffle design on reactor performance.

Parameter	Case-I (Feed at the top, No baffles)	Case-II (Feed near the bottom, No baffles)	Case-III (Feed near the bottom, 3 baffles)
Feed Inlet position	Top	Bottom	Bottom
Baffles	No	No	Yes (3)
Initial concentration of A and B (mol/L)	1	1	1
Reactant A Conversion	0.95	0.97	0.99
Reactant B Conversion	0.81	0.87	0.87
By-product concentration (mol/L)	0.07	0.05	0.064

The results clearly demonstrate that:

- Bottom feed improves both conversions and selectivity compared to top feed.
- Incorporation of baffles further improves conversion (notably Reactant A: 0.99), though there is a minor trade-off in by-product selectivity.

These insights were quickly obtained through VisiMix Chem, eliminating the need for multiple physical trials and helping guide smarter, data-backed design decisions.

CONCLUSION

This study demonstrates how VisiMix Chem enables rapid, predictive evaluation of reactor configurations, helping engineers identify the optimal setup for reaction efficiency, selectivity, and scale-up reliability.

Key Conclusions:

- **Feed positioning** plays a critical role in maximizing conversion and minimizing by-products.
- **Incorporating baffles** enhances mixing, further improving conversion, though with slight increase in by-products.
- **Simulation insights** eliminate the need for extensive physical trials, accelerating scale-up and improving design reliability.

VisiMix empowers engineers with data-driven tools for smarter process development and scale-up.

Please refer: **Feed position near the top**
Feed position near the bottom
Baffle Influence