

Introduction

Complex enzymatic reactions in continuous reactors involve intricate interactions between reactants, enzyme activity, intermediate complex formation, and competitive side reactions. The performance of such systems depends on the dynamic evolution of concentration fields, reaction pathways, and hydrodynamic conditions throughout the reactor volume. Accurate prediction of these phenomena requires an integrated approach that captures both the chemistry and the physical environment in which the reaction occurs.

VisiMix Chem provides a comprehensive modeling platform that unifies detailed reaction kinetics, reactor geometry, impeller configuration, feed positioning, power input, and fluid properties into a single predictive framework. It simulates the actual behavior of multi-step reaction networks under real operating conditions, allowing engineers to evaluate concentration profiles, intermediate accumulation, conversion rates, and by-product formation as a function of time in continuous processes.

In this study, a complex five-step enzymatic reaction system is modeled in a continuous stirred tank reactor using VisiMix Chem. The analysis demonstrates how the software delivers deep insight into reaction progression, mixing-driven effects, and overall reactor performance, enabling confident design decisions and optimized process outcomes before plant implementation.

Consider the following enzymatic reaction, which includes a complex intermediate reaction, a main reaction and side reactions that result in by-product formation.

Intermediate reaction 1
$A + E \leftrightarrow C1$
Main Reaction
$C1 \leftrightarrow E + P$
Byproduct reaction 1
$B + E \leftrightarrow C2$
Byproduct 1 generation
$C2 \leftrightarrow E + BP1$
Byproduct 2 generation
$A + B \leftrightarrow BP2$

“Where A and B are the reactants, P is the main product, E is the enzyme, C1 and C2 are the intermediate complexes, and BP1 and BP2 are the by-products”.

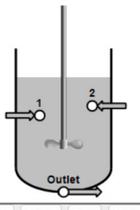
Objective

To determine the concentration of each reactant, enzyme species, intermediate, desired product, and by-product as a function of time under continuous operating conditions, analyze the corresponding conversion rates, and generate concentration versus time and conversion versus time profiles to illustrate the dynamic progression and kinetics of the complex enzymatic reaction within the continuous reactor system.

VisiMix Simulation

The simulation begins by defining the complete chemical system under the Chemistry input section of VisiMix Chem. In this module, the process temperature, solvent properties, and all participating chemical species are specified, including reactants, enzyme, desired product, intermediate complexes, and by-products, along with their molecular weights and concentration data in the reactor and feed streams. This ensures that the reaction system is fully defined before proceeding with kinetic and reactor modeling.

		Process temperature	26.85 °C	Solvent molar mass, g/mol	88.1	Solvent type	Organic polar (alcohol)
Designation	Description	Molar mass, g/mol	Concentration, mol/L				
			Initial in the tank	Feed 1	Feed 2		
A	Reactant 1	101		2			
B	Reactant 2	86			1		
P	Main product	101					
BP1	By-product 1	86					
E	Enzyme	1800	0.01		0.05		
C1	Intermediate 1	1900					
C2	Intermediate 2	1890					
BP2	By-product 2	187					



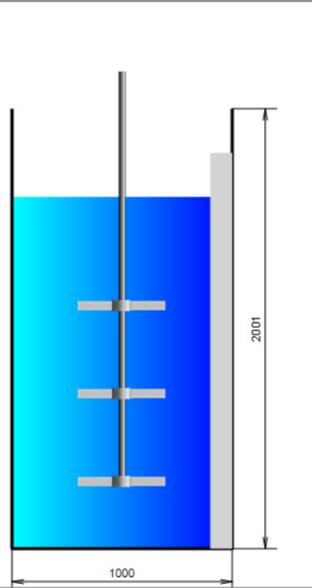
The complete reaction network is then defined under the Chemical Reactions section, including intermediate formation, the main reaction, and by-product pathways with their respective kinetics. This allows VisiMix Chem to simulate the full multi-step enzymatic mechanism under continuous operation.

Reaction List			
Designation	Description		
R1	Intermediate reaction 1 $A + E \leftrightarrow C1$	Edit	✓
R2	Main Reaction $C1 \leftrightarrow E + P$	Edit	✓
R3	Byproduct rereaction 1 $B + E \leftrightarrow C2$	Edit	✓
R4	Byproduct 1 generation $C2 \leftrightarrow E + BP1$	Edit	✓
R5	Byproduct 2 generation $A + B \leftrightarrow BP2$	Edit	✓

Next, the reactor was modeled as a 1000 mm internal diameter flat-bottom tank with a 1600 mm working fluid height, equipped with four flat baffles.

Paddle	
Tip diameter	400 mm
Number of blades	2
Blade width	50 mm
Distance from the bottom	305 mm

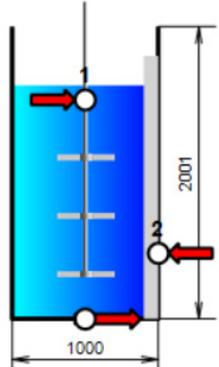
Number of impellers	3
Distance between the stages	400 mm
Rotational speed	60 rpm
Motor power	1.49 hp



The mixing system consisted of a three-stage paddle impeller with a 400 mm tip diameter operating at 60 rpm.

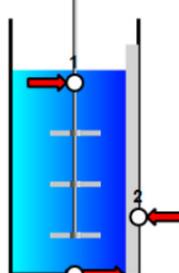
The inlet and outlet positions were strategically defined to reflect realistic continuous operation. Feed 1 was introduced along the shaft axis near the upper region of the reactor to promote uniform dispersion, while Feed 2 was introduced radially at a lower height to enhance localized mixing interaction. The outlet was positioned at the bottom center to maintain steady continuous discharge.

Inlet and Outlet Locations	
INLET 1	
Radius	0 mm
Height	1500 mm
INLET 2	
Radius	500 mm
Height	450 mm
OUTLET	
Radius	0 mm
Height	0 mm



The reactor was operated under continuous flow conditions with equal feed rates of 100 L/min for both inlet streams, resulting in a total product flow rate of 200 L/min. The transient simulation was performed for a duration of 2000 seconds to evaluate the evolution of concentration profiles and conversion behavior until steady-state conditions were achieved.

CP—Flow Rates and Transient Process Duration	
Feed 1 Flow Rate	100.0 L/min
Feed 2 Flow Rate	100.0 L/min
Note	
Product Stream Flow Rate = 200.0 L/min (Feed 1 + 2 Flow Rates)	
Transient Process Duration	2000.0 s



Results

Upon completion of the simulation, VisiMix Chem generated steady-state concentration profiles, reactant conversion behavior, and quantitative analysis of species distribution within the continuous reactor. The results provide clear insight into the influence of real mixing conditions on reaction progression, intermediate accumulation, and by-product formation, enabling accurate performance evaluation under practical operating conditions.

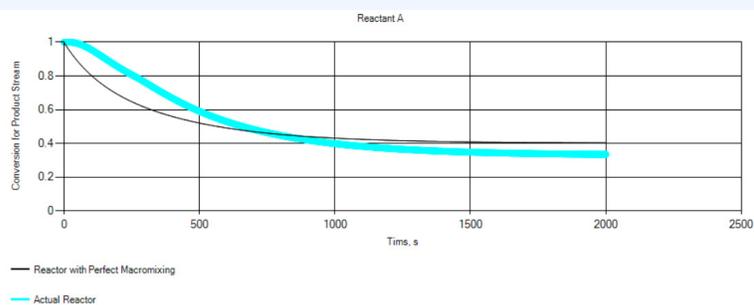
Continuous Flow Process—Average Concentrations, mol/L

At the end of the transient process of requested duration

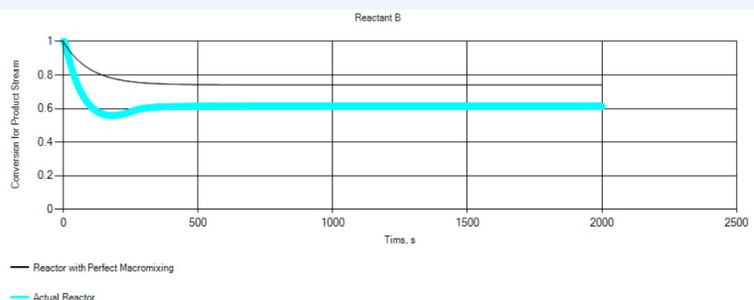
	Reactant Designation	Actual Reactor—Tank	Actual Reactor—Product Stream	Reactor with Perfect Macromixing
▶	A	0.9942	0.6648	0.5964
	B	0.1072	0.1929	0.1293
	P	0.01657	0.01731	0.02418
	BP1	0.001394	0.001632	0.002503
	E	0.01067	0.01547	0.01444
	C1	0.006823	0.008441	0.009587
	C2	0.00058	0.001059	0.000898
	BP2	0.2513	0.3027	0.3648

Average concentration profile in the reactor

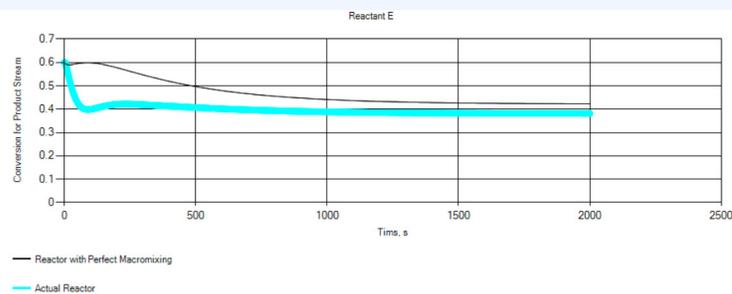
Conversion profiles



Reactant A



Reactant B



Enzyme E

Results Overview

- This study evaluates a five-step enzymatic reaction system involving Reactants A and B, enzyme (E), desired intermediate (C1), undesired intermediate (C2), and by-products (BP1 and BP2) under both Actual Reactor and Perfect Macromixing conditions. The comparison clearly demonstrates the influence of realistic mixing behavior on overall reaction performance.
- Under actual reactor conditions, Reactant A conversion reached approximately **33%** compared to 40% under perfect macromixing, while Reactant B stabilized at 61% versus ~74% under perfect macromixing. Enzyme conversion also showed lower stabilization (**~38% vs ~42%**), reflecting the impact of localized concentration gradients on reaction efficiency.
- In terms of intermediate behavior, the desired intermediate C1 accumulated at a slightly lower concentration in the actual reactor (**0.0084 mol/L vs 0.0096 mol/L**), whereas the undesired intermediate C2 showed higher accumulation (**0.0012 mol/L vs 0.0008 mol/L**). Despite this, overall by-product formation remained lower in the actual reactor, suggesting that localized kinetic limitations restricted the progression of secondary reactions.

These results highlight the critical role of mixing quality in controlling reaction pathways, conversion efficiency, and final product distribution in continuous enzymatic systems.

CONCLUSION

- This case study demonstrates the capability of VisiMix Chem to accurately simulate complex multi-step enzymatic reactions under realistic continuous reactor conditions. By integrating reaction kinetics with reactor geometry, impeller configuration, and hydrodynamic behavior, the software provides reliable prediction of concentration profiles, conversion efficiency, and by-product formation.
- The comparison between actual reactor performance and ideal macromixing conditions highlights the critical influence of mixing on reaction progression, intermediate distribution, and overall process efficiency.
- VisiMix Chem enables engineers to predict real reactor behavior prior to scale-up, optimize operating conditions, and make informed design decisions with confidence. This predictive capability helps improve process efficiency, reduce development risks, and support successful implementation of continuous reaction systems.
- Optimizing mixing, feed distribution, and concentration uniformity enables maximum reactant utilization, significantly improving conversion and overall reactor performance.

Start Your Free Trial of VisiMix Today

Want to model your own process and avoid costly mistakes?

[Click here to download your free trial of VisiMix](#)