VISIMIX CHEM
Batch Reaction (Esterification): Effect of Solvent type (Organic polar)

Previous Study Overview:

In the previous report titled **Batch Reaction (Esterification) Using Water as Solvent**, we explored the effects of water on the concentration and conversion rates of the esterification reaction. The findings indicated a maximum conversion of 68%, with reactant A's concentration decreasing from 1.2 mol/L to 0.38 mol/L over a duration of 10 seconds.

Current Study Overview:

This report aims to investigate the **esterification reaction using an Organic polar solvent(alcohol).** The choice of solvent plays a critical role in determining the reaction kinetics, solubility of reactants, and overall product yield. By substituting new solvent for water, we aim to evaluate how this change influences the efficiency of the reaction and the behavior of the reactants.

Through a comparative analysis of the results obtained with Organic polar solvent against those from the initial report, this study aims to enhance our understanding of solvent effects in esterification processes and identify optimal conditions for improved reactant conversion and yield.

Objective:

This report aims to investigate the esterification reaction using an organic polar solvent (alcohol).

The Solution:

Update the **Solvent type and molar mass** in the 'Solvent, Reactants, and Process Temperature' section of the edit menu; all other inputs will remain constant."

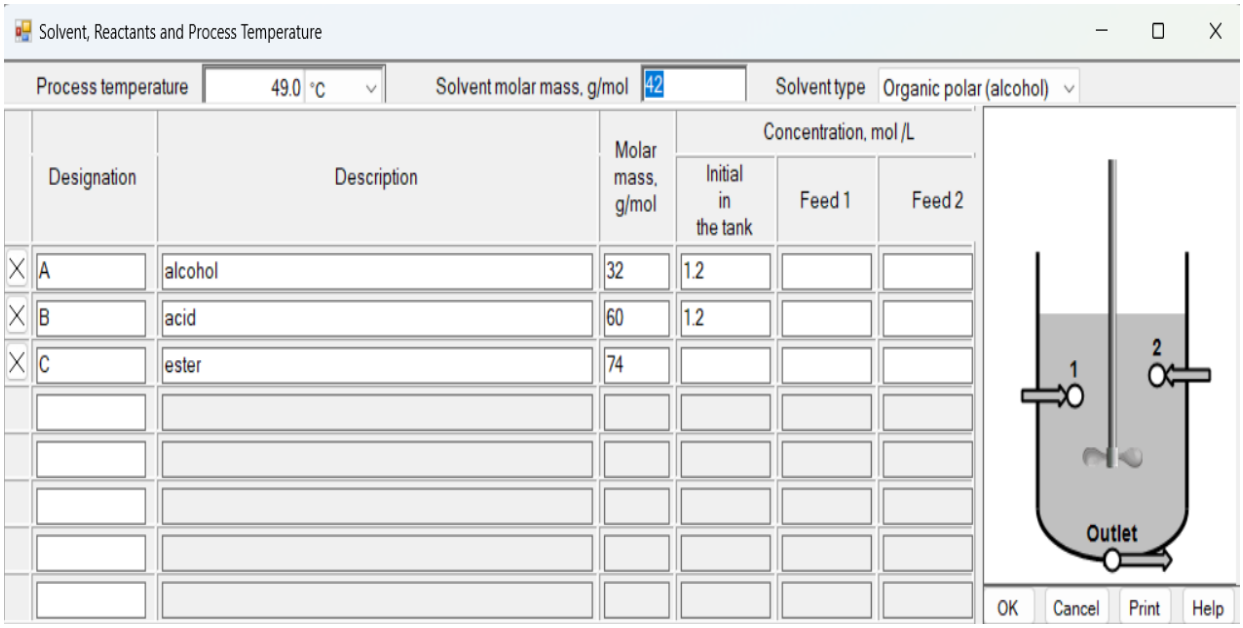
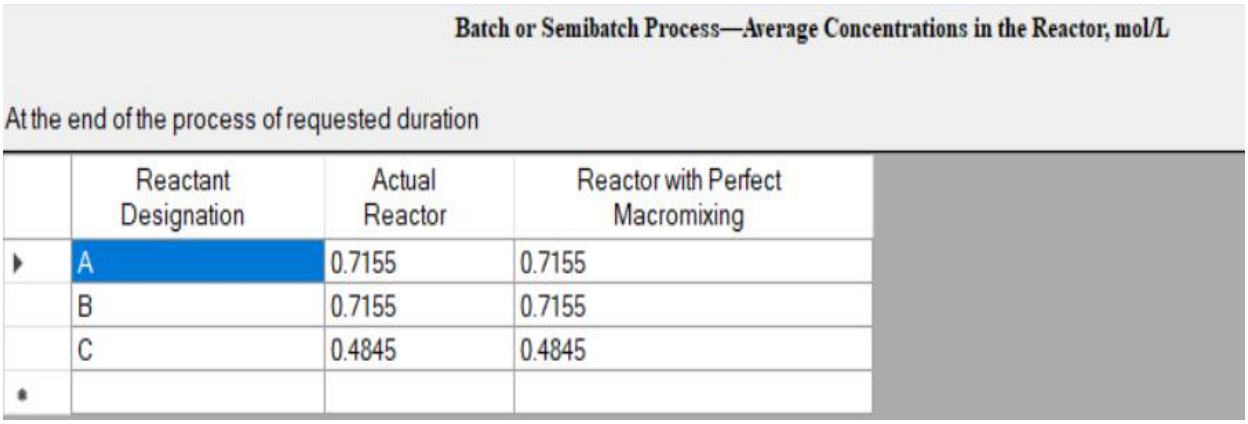


Figure 1. Update the solvent type and molar mass

RESULTS:

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



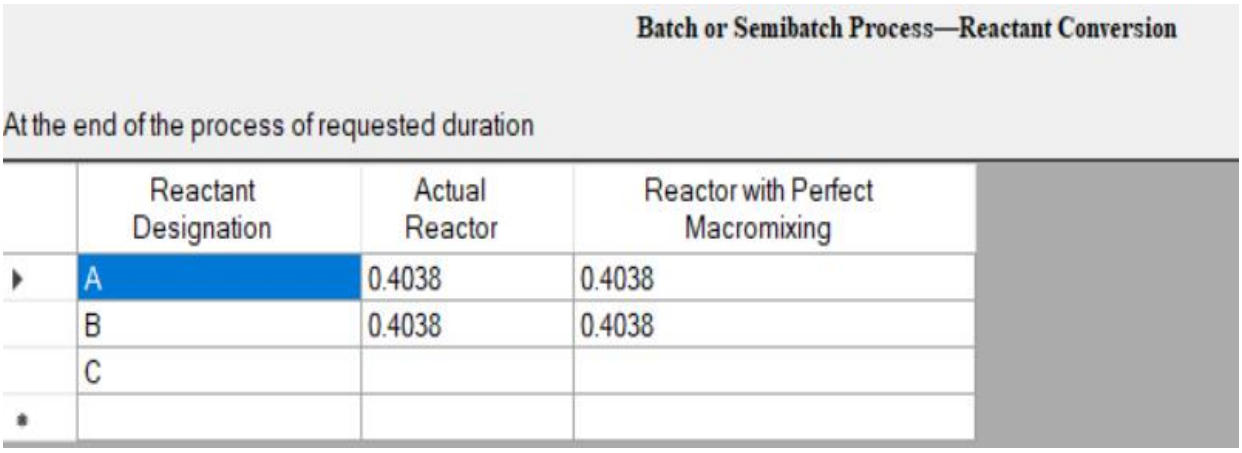
Batch or Semibatch Process—Average Concentrations in the Reactor, mol/L

At the end of the process of requested duration

	Reactant Designation	Actual Reactor	Reactor with Perfect Macromixing
▶	A	0.7155	0.7155
	B	0.7155	0.7155
	C	0.4845	0.4845
*			

Figure 2. 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	0.4038	0.4038
	B	0.4038	0.4038
	C		
*			

Figure 3. 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.

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

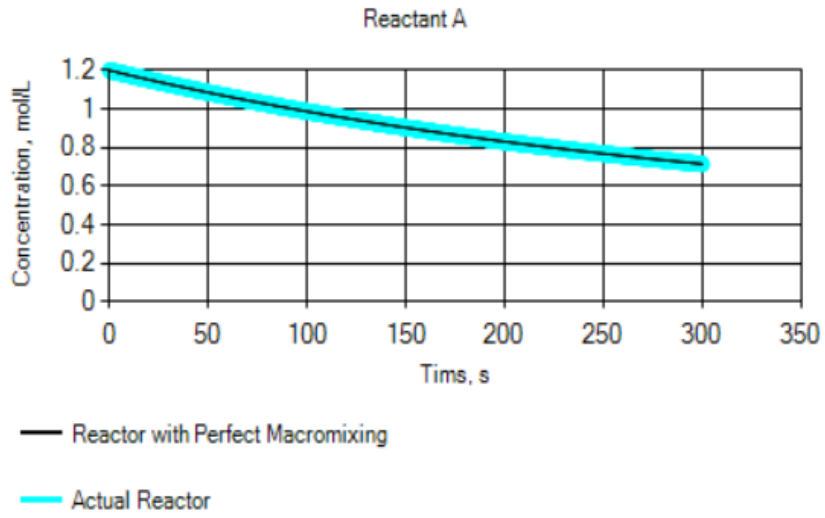


Figure 4. Concentration Vs time graph-Reactant A

Reactant B

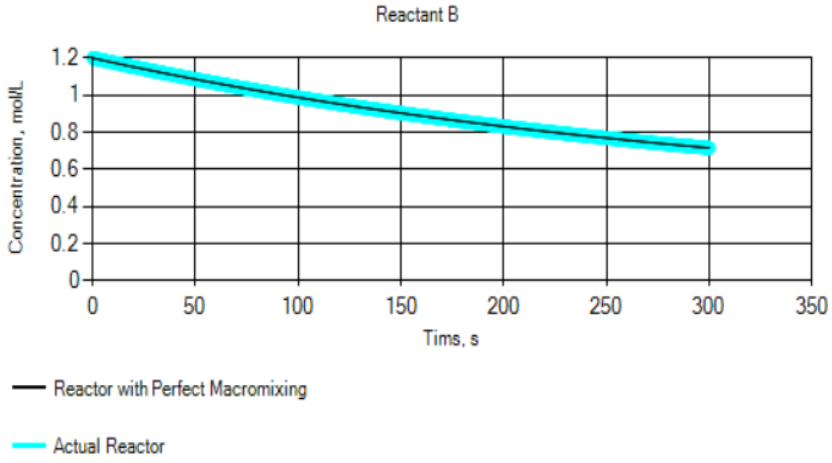


Figure 5. Concentration Vs time graph-Reactant B

The concentration versus time graph illustrates a decrease in concentration from 1.2 mol/L to 0.71 mol/L over a duration of 300 seconds.

Product C

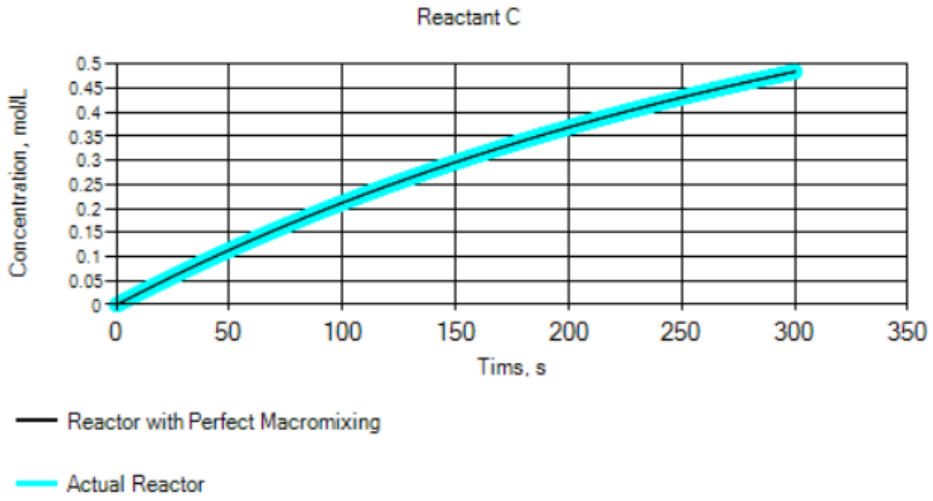


Figure 6. Concentration Vs time graph-Product C

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.

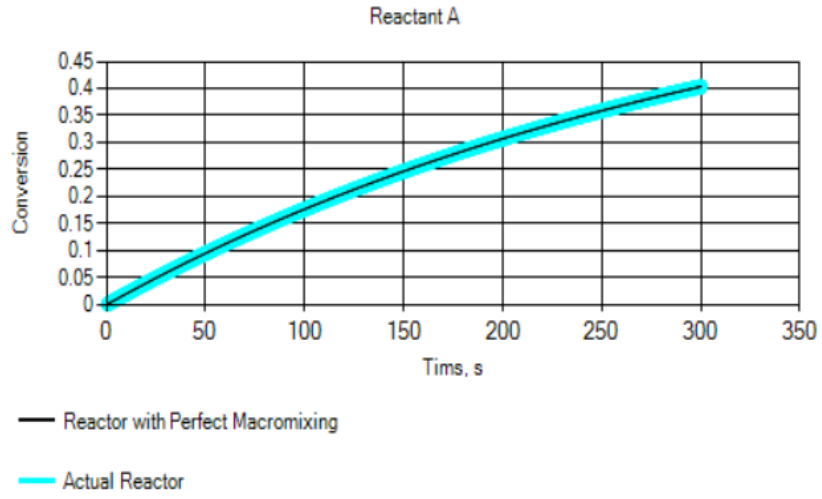


Figure 7. Conversion Vs time graph-Reactant A

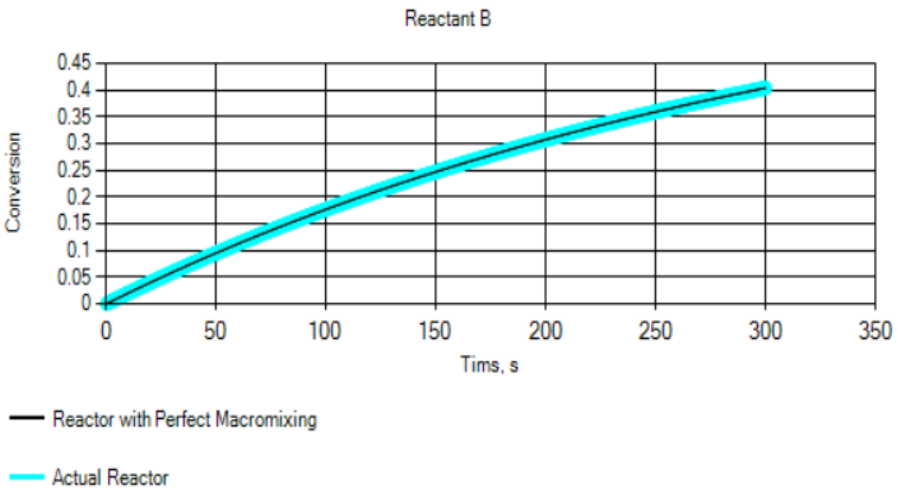


Figure 8. Conversion Vs time graph-Reactant B

Analysis of the graph indicates that the conversion rate is comparatively low, i.e., 40%, when utilizing an organic polar solvent (alcohol) over a duration of 300 seconds.

Results Overview

This report examined the batch esterification reaction utilizing an **Organic polar solvent**. The results demonstrated a conversion rate of 40%, with the concentration of reactant A decreasing from 1.2 mol/L to 0.71 mol/L over a duration of 300 seconds.

These findings indicate that the Organic polar solvent influences reaction kinetics, resulting in a lower conversion compared to the previous experiment using water as the solvent. By utilizing the VisiMix Chem simulation, we can minimize the need for some laboratory experiments, streamlining the analysis of different reaction conditions.

Understanding the impact of different solvents on esterification is crucial for optimizing reaction conditions and enhancing product yields in further studies. This research contributes valuable insights into solvent selection for esterification processes and lays the groundwork for further exploration of solvent effects.