VISIMIX CHEM
Batch Reaction (Esterification): Effect of Mixing Intensity

Previous Study Overview:

In the previous report titled **Batch Reaction (Esterification) Using Water as Solvent at 180 Rpm**, 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 water as solvent at low rpm of 30.** By conducting the reaction at this lower mixing intensity, we seek to evaluate how the reduction in agitation affects the conversion rates. The study will focus on assessing the impact of low RPM on the concentration of reactants throughout the reaction duration. We will monitor how the slower mixing influences the formation of the ester, particularly in terms of yield and efficiency.

Through a comparative analysis of the results obtained at different mixing intensities, we aim to elucidate the relationship between agitation speed and reaction efficiency, identifying how varying levels of mixing impact conversion rates and product yield. This analysis will provide insights into the optimal conditions for maximizing esterification processes and enhancing overall reaction performance.

Objective:

This report aims to investigate the esterification reaction using water as solvent at low rpm of 30.

The Solution:

Update the **Rotational speed** in the Impeller details section of the Mechanical design-edit menu; all other inputs will remain constant."

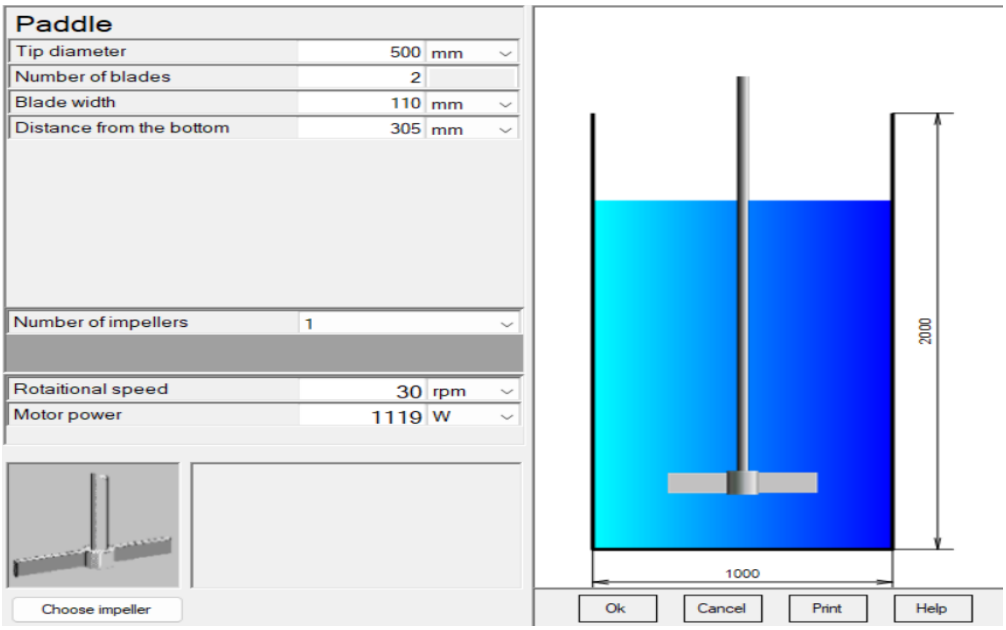

Figure 1. Update the Rpm

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	0.3822	0.3822
	B	0.3822	0.3822
	C	0.8178	0.8178
*			

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	0.6815	0.6815
	B	0.6815	0.6815
	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

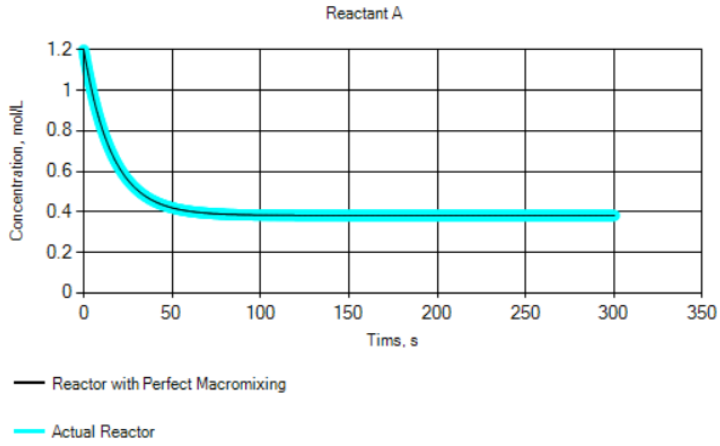

Figure 4. Concentration Vs time graph-Reactant A

Reactant B

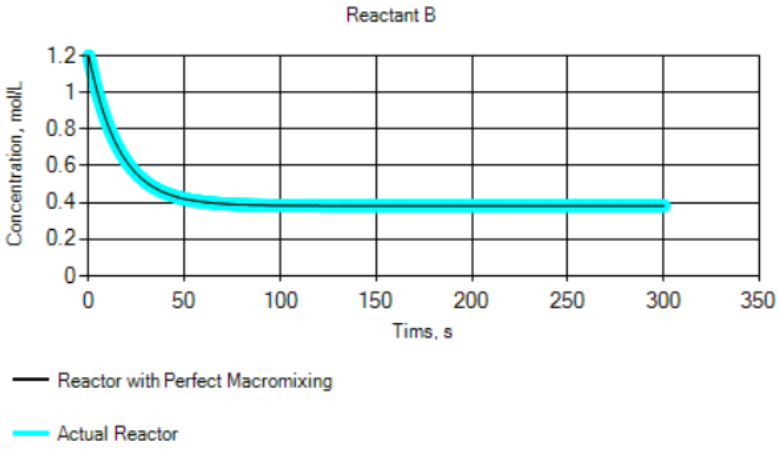

Figure 5. Concentration Vs time graph-Reactant B

The concentration versus time graph illustrates a decrease in concentration from 1.2 mol/L to 0.38 mol/L over a duration of 45 seconds.

Product C

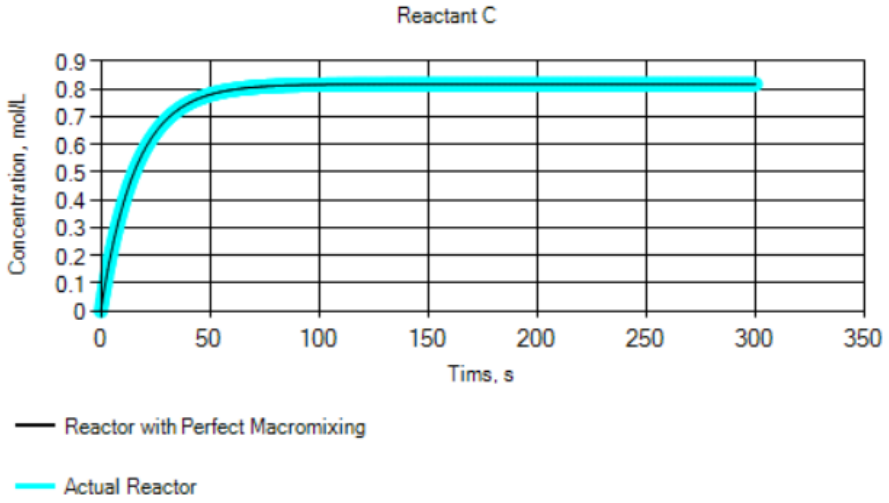

Figure 6. Concentration Vs time graph-Product C

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.

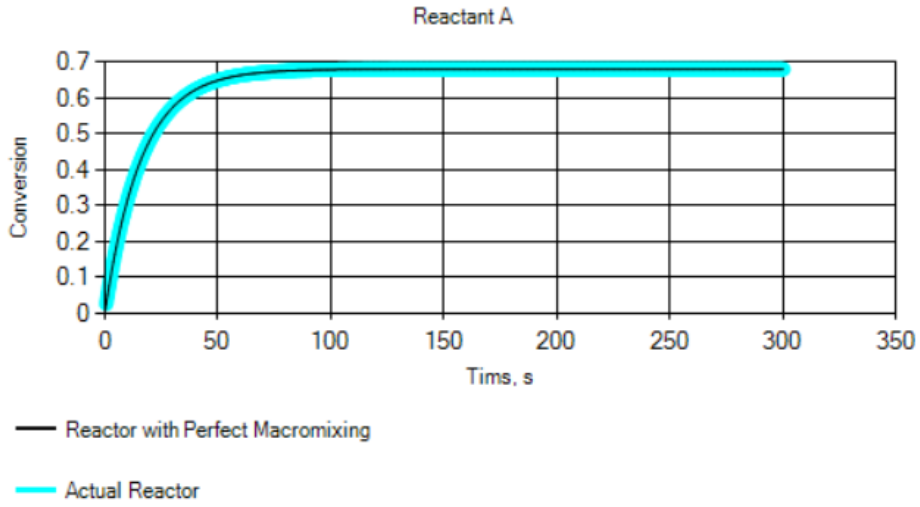

Figure 7. Conversion Vs time graph-Reactant A

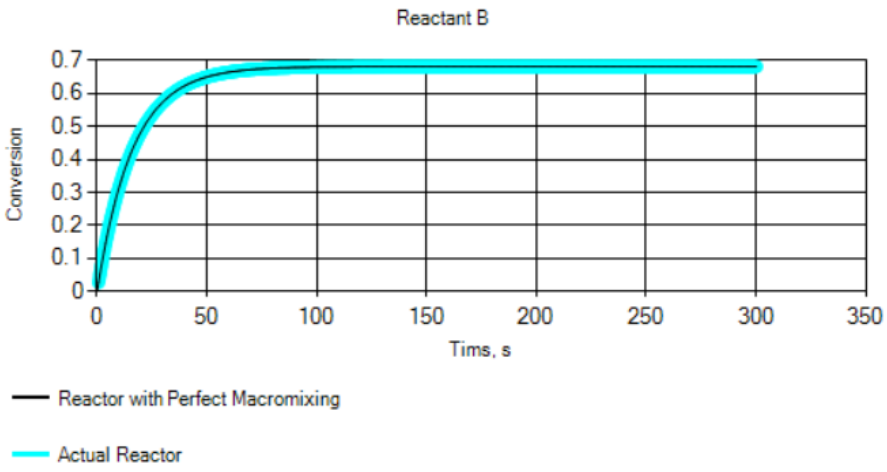

Figure 8. Conversion Vs time graph-Reactant B

Analysis of the graph indicates that 68% conversion is achieved in 45 seconds at 30 Rpm.

Results Overview

This report examined the batch esterification reaction utilizing **water as solvent at low rpm of 30**. The results demonstrated a conversion rate of 68% over 45 seconds, with the concentration of reactant A decreasing from 1.2 mol/L to 0.38 mol/L.

The findings indicate that the reaction rate at this lower mixing intensity may be constrained by molecular diffusion. While the conversion rate achieved was equivalent to that observed in the previous study at 180 RPM, it required significantly more time to reach this level of conversion**.**

These results enhance our understanding of how mixing intensity affects reaction kinetics in esterification processes, emphasizing the balance between agitation speed and reaction time.