NEWSLETTER

Heat Transfer Analysis for Semi-Batch Reactors Using VisiMix Turbulent

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Introduction

- Efficient heat transfer is a critical aspect of many chemical, pharmaceutical, and specialty chemical manufacturing processes. In semi-batch reactors, where reactants are added during operation and the reaction may consume or release heat, accurately predicting the heating profile is essential for maintaining product quality, reducing batch cycle time, and optimizing energy consumption.
- Traditional methods of estimating heating performance often rely on empirical calculations or plant trials, which can be both time-consuming and costly.

The Heat Transfer section of the VisiMix Turbulent module provides a simulation-based approach that enables engineers to evaluate heating performance under actual process conditions by considering reactor geometry, agitator design, jacket configuration, fluid properties, and reaction heat effects. By predicting heating behavior before plant implementation, VisiMix helps reduce development time, minimize costly plant trials, optimize steam utilization, and improve confidence in process scale-up decisions. This example demonstrates the application of VisiMix to simulate a steam-heated semi-batch reactor with a heat-consuming reaction and predict the time required for the reactor contents to reach the desired operating temperature.

The Process Challenge

Many industrial processes involve heating a reaction mixture while continuously adding reactants in a semi-batch reactor. In heat-consuming reactions, achieving the desired process temperature can be challenging due to the combined effects of reactor design, agitation, steam heating, and reaction heat demand.

Key challenges include:

- Maintaining the desired reactor temperature during continuous reactant addition.
- Compensating for the heat absorbed by the chemical reaction.
- Predicting the heating time required to reach the target temperature of **80°C.**
- Understanding the influence of reactor geometry, agitator design, and steam jacket configuration on heat transfer performance.
- Minimizing plant trials by evaluating heating performance through simulation before implementation.

Objective

The objective of this study was to evaluate the heating performance of a steam-heated semi-batch reactor using Heat Transfer section of **VisiMix Turbulent module.**

The study aimed to:

- Predict the temperature profile of the reaction mass during the heating process.
- Estimate the time required to heat the reactor contents from **60°C to 80°C.**
- Assess the impact of a heat-consuming reaction on the overall heating process.
- Evaluate the performance of the steam jacket and agitation system under the specified operating conditions.

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- Support process optimization and reduce development time by evaluating heating performance before plant implementation.

VisiMix Simulation Approach

To evaluate the heating performance of the semi-batch reactor, the process was simulated using the Heat transfer section of the **VisiMix Turbulent** module. The simulation integrates reactor geometry, agitation, heat transfer, and process conditions to predict the transient temperature profile throughout the heating cycle.

The following process parameters were incorporated into the simulation:

- **Reactor Configuration:** Unbaffled semi-batch reactor with an elliptical bottom.
- **Agitation System:** Anchor agitator operating at 30 RPM.
- **Heating System:** Conventional steam jacket using atmospheric steam as the heating medium.
- **Reactor and Jacket Characteristics:** Shell material, wall thickness, jacket dimensions, and heat transfer configuration were incorporated into the simulation model.
- **Process Fluid Properties:** Density, viscosity, specific heat, and thermal conductivity of the reaction medium were considered.
- **Operating Conditions:** Initial temperature of 60°C with a target temperature of 80°C.
- **Semi-batch Operation:** Continuous addition of the second reactant over 25 minutes, including inlet flow properties.
- **Process Characteristics:** Heat consumed by the chemical reaction was incorporated to accurately predict the transient heating profile.

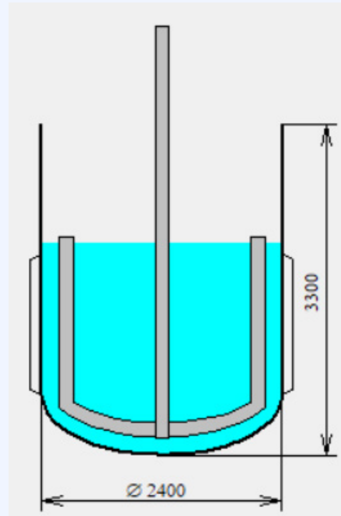
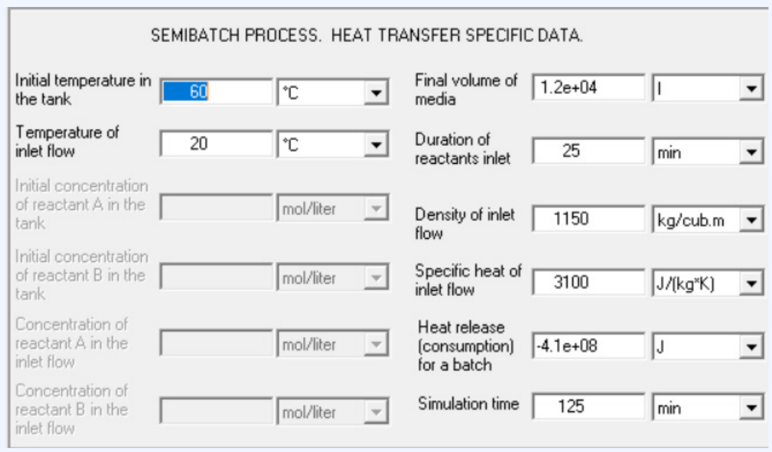


Figure: Semi-batch Reactor Model Used in the Heat Transfer section of VisiMix Turbulent



SEMIBATCH PROCESS. HEAT TRANSFER SPECIFIC DATA.

Initial temperature in the tank	60	°C	Final volume of media	1.2e+04	l
Temperature of inlet flow	20	°C	Duration of reactants inlet	25	min
Initial concentration of reactant A in the tank		mol/liter	Density of inlet flow	1150	kg/cub.m
Initial concentration of reactant B in the tank		mol/liter	Specific heat of inlet flow	3100	J/(kg*K)
Concentration of reactant A in the inlet flow		mol/liter	Heat release (consumption) for a batch	-4.1e+08	J
Concentration of reactant B in the inlet flow		mol/liter	Simulation time	125	min

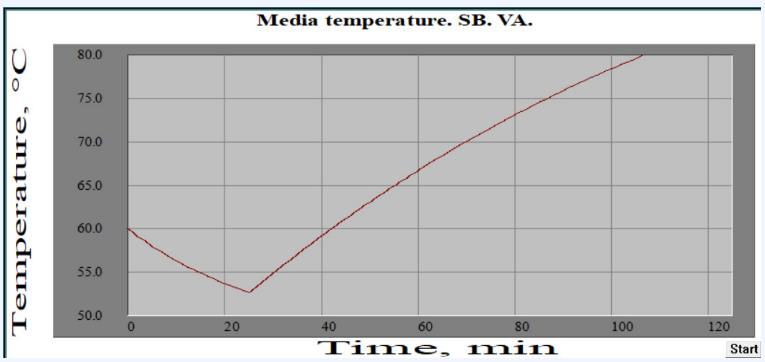
Figure: Key Simulation Input Parameters for Heat Transfer Analysis in a Semi-Batch Reactor

By integrating these process parameters, VisiMix predicts the temperature profile over time, enabling engineers to estimate heating time and evaluate reactor performance before plant implementation.

Simulation Results

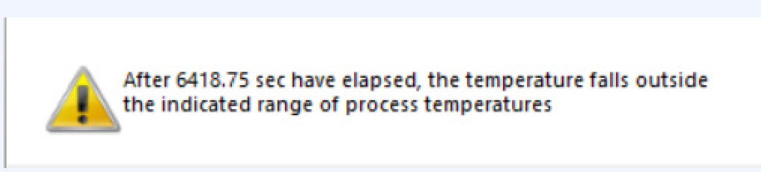
The VisiMix Turbulent (Heat Transfer) simulation successfully predicted the transient temperature profile of the reaction mass throughout the semi-batch heating process. By accurately estimating the heating time under the specified operating conditions, engineers can evaluate reactor performance before implementation, reducing engineering effort, minimizing plant trials, and accelerating process development.

Media Temperature Profile During the Semi-batch Heating Process



The graph illustrates the predicted temperature profile of the reaction mass during the semi-batch heating process. A gradual increase in media temperature was observed, with the reaction mass reaching the target temperature of 80°C in approximately **107 minutes.** The simulation captures the transient heating behavior under the specified operating conditions and demonstrates the effectiveness of VisiMix in predicting batch heating performance.

VisiMix Simulation Notification Indicating the Predicted Heating Time



The simulation notification confirms that the reaction mass reaches the specified upper process temperature after approximately **6418.75 seconds (≈107 minutes).**

Key Observations

- The simulation predicted that the reaction mass reached the target temperature of **80°C** in approximately **107 minutes** under the specified operating conditions, enabling engineers to estimate batch heating time before plant implementation.
- The simulated temperature profile exhibited a gradual and stable increase throughout the semi-batch heating process, demonstrating effective heat transfer from the steam jacket to the reaction mass.
- By incorporating reactor geometry, agitator configuration, jacket design, fluid properties, and reaction heat effects, the simulation provides a realistic representation of the heating process, allowing engineers to evaluate thermal performance with greater confidence.
- In addition to predicting the heating profile and heating time, the Heat transfer section of the VisiMix Turbulent module provides engineering parameters including the **overall heat transfer coefficient, inside and outside film heat transfer coefficients, heat transfer area, heat transfer rate, and overall reactor heat transfer performance** for comprehensive heat transfer analysis.
- These predictive insights help engineers optimize process performance, reduce dependence on costly experimental trials, improve scale-up confidence, and lower project risks.

Conclusion

- Efficient heat transfer is essential for achieving consistent product quality, minimizing batch cycle time, and improving overall process efficiency in semi-batch operations.
- The Heat Transfer section of VisiMix Turbulent enables engineers to accurately predict transient heating behavior before plant implementation, helping organizations reduce development costs, optimize steam utilization, shorten process development timelines, and make confident scale-up decisions.
- By minimizing trial-and-error experimentation and providing key engineering parameters such as **overall heat transfer coefficient, film heat transfer coefficients, heat transfer area, and heat transfer rate,** VisiMix supports faster process optimization while reducing technical and financial risks.

Please refer: **Heat Transfer Process in a Semi-Batch Reactor with Heat Consumption**

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