Hydrodynamics and Heat Transfer Characterization in an Automated Taylor Vortex Reactor for Imine Synthesis

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Highlights

- Axial dispersion model with energy balance developed for imine synthesis in a TVR.
- Heat transfer is governed by Reynolds number, with negligible Taylor number influence.
- Model predicts reactor outlet temperature and reactant conversion under varied conditions.

1. Introduction

Flow reactors are increasingly central to chemical manufacturing, with the Taylor Vortex Reactor (TVR) emerging as a promising platform due to its superior mixing characteristics [1]. Despite this advantage, the heat-transfer behaviour of TVRs remains poorly understood [2], which limits their predictive capability and broader application in continuous processing. Accurate modeling of coupled hydrodynamic and thermal transport is therefore essential for rational TVR design. In this work, we demonstrate the automated operation of a TVR for continuous imine synthesis and develop an axial dispersion model incorporating heat transfer and hydrodynamics. Real-time control of rotation speed, flow rate, and temperature enables precise control of the reactor environment.

2. Methods

All experiments were performed in an automated TVR system controlled using a LabVIEW-based data acquisition and control platform. The reactor consists of a longitudinally ribbed rotor inside a stationary concentric cylindrical shell, providing an annulus volume of 21 ml. Pumps, temperature sensors, rotor drive, and a Huber heating/cooling circulator were integrated into the automated control system. Temperature probes were installed at multiple axial locations within the reactor annulus and jacket to capture axial temperature profiles.

Heat transfer experiments were conducted to investigate the influence of flow rate, rotation speed, and jacket temperature. A one-factor-at-a-time approach was employed, with rotor speeds of 60, 180, and 300 rpm, residence times of 2.5, 5, 7.5, and 10 min, and jacket temperatures of 5 and 15 °C. Seven K-type thermocouples were positioned along the reactor length (TR1–TR4) and within the jacket (TJ1–TJ2) to obtain temperature profiles. Macro-mixing was studied using step-input experiments by monitoring the tracer's concentration (Rhodamine B) with inline UV–Vis spectroscopy. Reaction progress during imine synthesis was monitored inline using Raman spectroscopy, with spectra acquired every 10 s. Reactant conversion was calculated in real time and displayed on the LabVIEW interface, enabling continuous assessment of reactor performance. For reactor modeling, the system was divided into four distinct zones to realistically represent the experimental configuration. The first zone ($z < 9$ mm) involves natural convection without heat exchange or reaction. The second zone ($9 \leq z < 100$ mm) includes jacket cooling without reaction. The third zone ($100 \leq z < 291$ mm) corresponds to the onset of reaction with jacket cooling, while the fourth zone ($291 \leq z \leq 300$ mm) represents continued reaction under natural convection.

3. Results and discussion

Heat transfer experiments conducted over a range of Reynolds and Taylor numbers were used to investigate the influence of rotor speed and flow conditions on the thermal behavior of the TVR. Upon rotor activation, the temperatures along the reactor decreased, indicating an increase in heat transfer efficiency due to intensified mixing and enhanced convective transport. The rotor motion disrupts the thermal boundary layer promoting improved heat transfer performance. Flow in the annular gap between rotor and shell is characterized by the Taylor number, representing the ratio of centrifugal to viscous forces. The experimental results indicate that heat transfer is primarily governed by Reynolds number ($Re = u(r_o - r_i)/ \nu$), with no significant dependence on Taylor number ($Ta = \omega r_i(r_o - r_i)/ \nu$) within the investigated operating window. Here, ω denotes the rotor speed (rad/s), r_i the rotor radius excluding rib (m), r_o the internal radius of the shell (m), and v the kinematic viscosity (m^2/s) of fluid. The empirical Nusselt number correlation developed ($Nu = 0.045 \pm 0.18 * Re^{1.642 \pm 0.09} Ta^{0.032 \pm 0.07}$) within the parameter ranges $0.81 < Re < 3.5$ and $100 < Ta < 700$, exhibited R^2 value of 0.94. However, the data appears clustered into three distinct bands, suggesting that the deviations are systematic rather than random, and needs further investigation.

To account for spatial non-idealities inherent to Taylor vortex flow, the reactor was divided into axial sections, allowing local variations in hydrodynamic and thermal behavior to be captured within the axial dispersion model (ADM). Zone-wise overall heat transfer coefficients were estimated by fitting the experimental reaction temperature data for each zone. The discrete zone-wise model predicted temperatures at locations TR2 and TR3 with good agreement, whereas larger deviations were observed at TR1 and TR4 i.e. inlet and exit of the reactor, respectively. These discrepancies may be attributed to additional heat effects not included in the model, such as heat generation from the mechanical seal and heat exchange through the reactor end caps with the ambient environment. Despite these deviations, the model captured the temperature rise at the onset of the reaction arising from its exothermic nature. The model-predicted outlet temperature (TR4) and conversion exhibited Root Mean Square Error (RMSE) of 3.79 K and 16.42 %, respectively, relative to the experimental values. All reaction experiments were performed in triplicate to assess reproducibility. The low standard deviation (0.10-2.02) in conversion confirms satisfactory experimental reproducibility (Figure 1B).

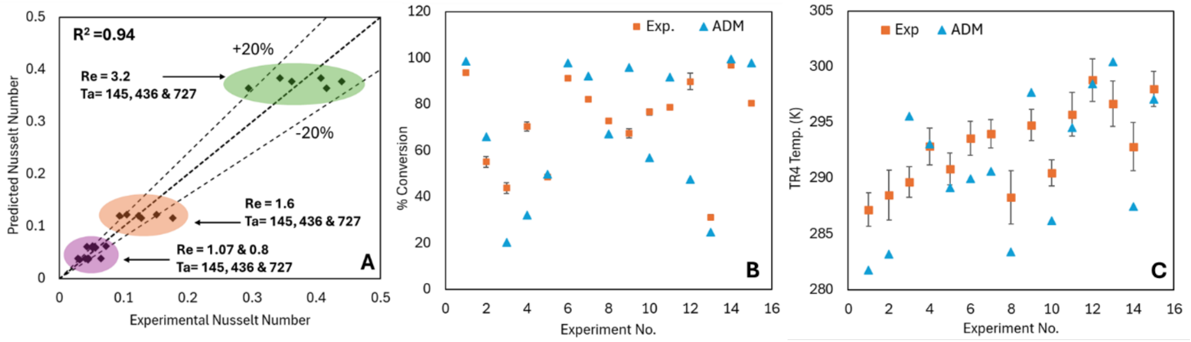

Figure 1. A) Parity plot showing the comparison between experimentally measured and predicted overall Nusselt numbers. Comparison of ADM predicted and experimental B) conversion and C) reactor outlet temperature. Experimental Conditions: Benzaldehyde Conc.: 0.5-1.5 M, Benzylamine Conc.: 0.5-1.5 M, Temperature: 5-25 °C, Rotor Speed: 100-300 rpm, Space time: 1-10 min.

4. Conclusions

The developed empirical Nusselt number correlations indicate that heat transfer in the TVR is primarily governed by Reynolds number, with negligible dependence on Taylor number within the investigated operating regime. A zone-wise ADM was developed to account for axial variations in thermal and hydrodynamic behavior. The model predicted reactor outlet temperature as well as the outlet temperature (TR4) and conversion, with RMSE of 3.8 K and 16.42%, respectively, relative to the experimental values. Overall, the developed framework enables reliable prediction of reactor performance and provides a basis for process analysis and scale-up.

References

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Keywords

Taylor Vortex Reactor, Axial Dispersion Model, Heat Transfer, Residence Time Distribution