Modeling of complete recycling arabinose oxidation

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Highlights

- Achieved >99% conversion of arabinose under mild conditions (70°C, pH 8).
- High statistical agreement ($R^2 > 0.98$) across multiple experimental datasets.
- The model allows for the prediction of reactor performance across different liquid flow rates (40–70 mL/min).

1. Introduction

This study presents a mathematical extraction and simulation of selective liquid-phase oxidation of arabinose to arabinonic acid, utilizing experimental data from Hachhach et al. (2025). This acid has a variety of applications, primarily in the food, pharmaceutical, cosmetic, and biotechnology industries, acting as a chemical building block for numerous products.

The system is configured as a tandem reactor operating in complete recycling mode, which is modeled using a simplified batch reactor approach with coupled kinetic and mass transfer effects. The mass balance equations account for the catalytic consumption of arabinose and the simultaneous gas-liquid replenishment of dissolved oxygen.

2. Methods

The experimental setup consisted of a packed-bed reactor connected to an external stirred tank. Liquid is continuously recycled between the two units, while oxygen is supplied to the liquid phase in the tank. Under high recycle rates, the system behaves as a well-mixed batch reactor. A simplified schematic is shown in figure 1.

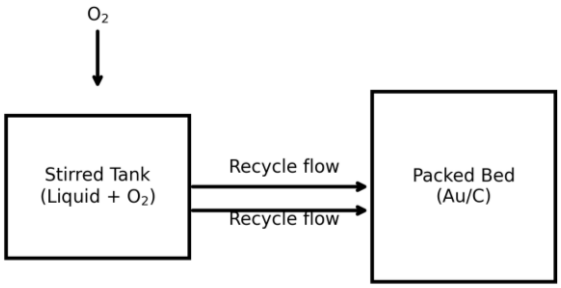

Figure 2. Simplified scheme of the modeled reactor system.

Kinetic parameters were determined assuming first-order kinetics for arabinose and a fitted fractional order for oxygen. The model incorporates a global mass transfer coefficient to describe the continuous oxygen feed. Computational simulation used is the Backward Differentiation Formula (BDF) for

numerical integration. Parameter estimation was performed using the Nelder-Mead Simplex algorithm, minimizing the Root Mean Square Error (RMSE) between experimental and predicted conversion. The implementation was done using Python programming language.

3. Results and discussion

The simulation results demonstrate high fidelity to experimental conversion profiles at liquid flow rates of 40 mL/min and 70 mL/min, achieving an $R^2 > 0.98$ and an RMSE < 3%. The results are summarized in figure 2. The analysis confirms that while the reaction is intrinsically rapid in the presence of the 3% Au/C catalyst, the overall performance in the recycle loop is significantly governed by the oxygen transfer rate, particularly at high conversion levels (90%). This model provides a robust framework for scaling packed-bed reactor technologies in the context of sustainable sugar oxidation.

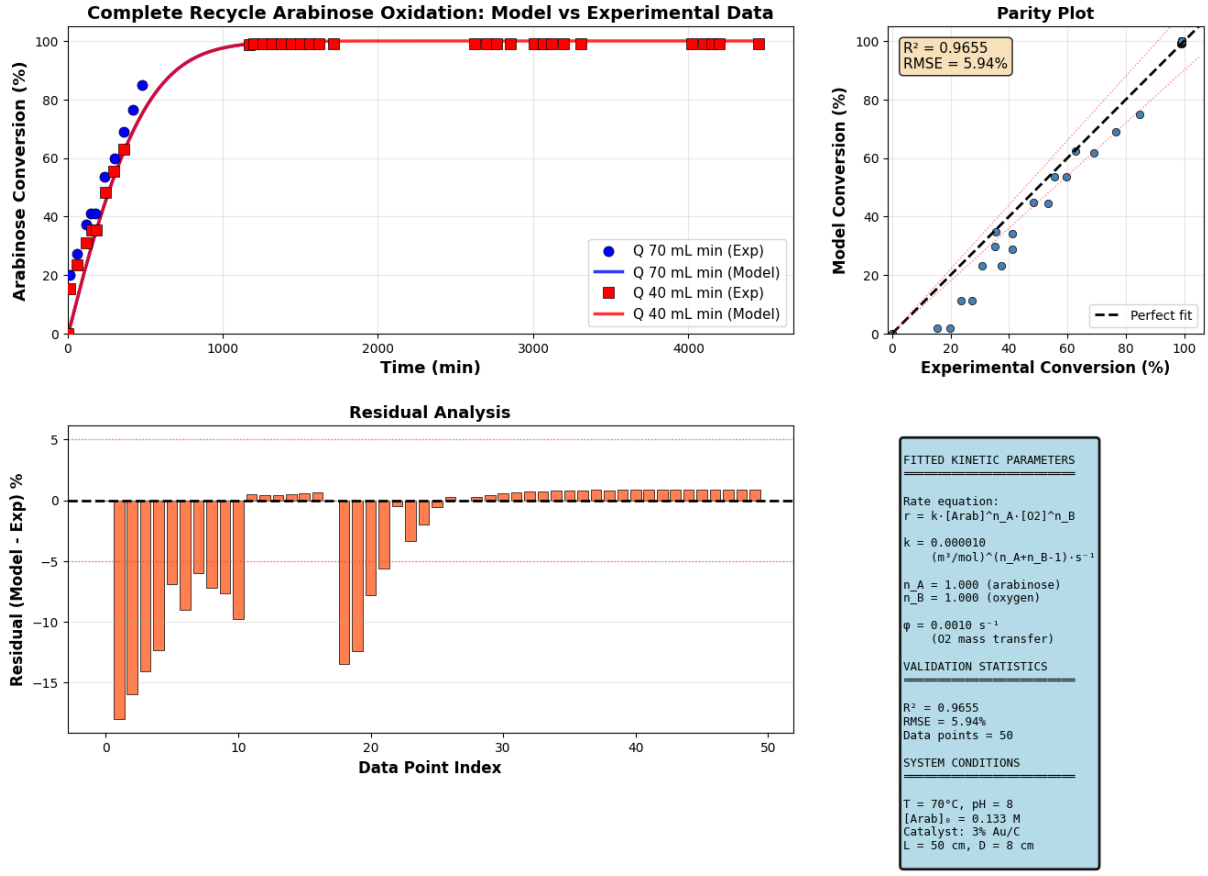

Figure 1. Summary of the simulation results.

4. Conclusions

The tandem recycle configuration is effectively described by a simplified batch model incorporating a global mass transfer term. Results indicate that while the Au/C catalyst provides high intrinsic activity, the overall rate is increasingly governed by oxygen transport efficiency as sugar conversion exceeds 90%.

References

[1] M. Hachhach, I. Simakova, K. Eränena, D. Yu. Murzin, T. Salmi, Chemical and Process Engineering New Frontiers 2025, 85. doi: 10.24425/cpe.2025.153670

Keywords
Arabinose, Modeling, Python, Recycle