Electrification of endothermic fixed-bed catalytic reactors: multiphysics computational modeling of a Joule-heated fixed-bed reactor, experimental validation and Joule-heating design optimization

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Highlights

- Development of a fully coupled 3D multiphysics computational model for Joule-heated fixed-bed reactors
- Explicit resolution of electrical current distribution and local Joule heat generation
- Experimental validation of thermal behavior in a fixed-bed catalytic reactor
- Optimization of heating-element design enabling uniform temperature and high conversion

1. Introduction

Electrification of catalytic reactors via Joule heating is increasingly recognized as a key pathway for the decarbonization of endothermic chemical processes and the improvement of energy efficiency [1]. Electrically heated fixed-bed reactors offer direct heat generation, fast dynamic response, and enhanced thermal integration. However, their development is challenged by several critical issues, including achieving thermal uniformity within the catalyst bed, controlling the temperature of heating elements, preventing local hotspots [1, 2, 3]. These challenges are particularly pronounced for endothermic reactions such as ethanol dehydration to ethylene, where hot spots may promote secondary reactions and catalyst deactivation. Advanced modeling approaches are therefore required to capture the strong coupling between electrical, thermal, and reaction phenomena in Joule-heated catalytic systems.

2. Methods

To address these challenges, a dedicated 3D multiphysics computational model was developed to support the design and optimization of an electrified fixed-bed catalytic reactor. The model couple fluid flow through a fixed catalyst bed, reactions kinetics of ethanol dehydration, heat transfer by conduction, convection, and axial and radial thermal dispersion. Joule heating is explicitly represented through the solution of the electrical field within the heating elements, allowing direct calculation of local heat generation as a function of material resistivity, geometry, and applied current.

This modeling framework enables the investigation of key design and operating aspects, including thermal uniformity, heating-element temperature, hotspot formation in low-conversion zones. The thermal component of the multiphysics model was experimentally validated using a dedicated warm-scale fixed-bed reactor prototype (Fig. 1a). The experimental setup consists of a vertical metallic tube with a length of 2 m, an inner diameter of 45 mm, filled with approximately 3 L of catalyst particles. A cold air stream flows through the packed bed, while heat is supplied indirectly via steam condensation in a double-jacket surrounding the reactor, providing a well-controlled and spatially uniform heat-flux boundary condition.

3. Results and discussion

Axial temperature profiles within the catalytic bed were measured under steady-state conditions and directly compared with numerical predictions obtained from the computational model (Fig. 1b). The simulations accurately reproduce the measured temperature gradients along the reactor length, demonstrating good agreement between experimental and calculated results. This validation confirms the model's ability to reliably capture heat-transfer mechanisms in wall-heated fixed-bed reactors, including conduction, convection, and thermal dispersion in porous media. As these heat-transfer processes are analogous to those governing Joule-heated electrified fixed-bed reactors, the validated model provides a robust foundation for the subsequent design, benchmarking, and optimization of electrically heated reactor concepts (Fig. 1c). Following validation, the model was employed to benchmark and optimize several Joule-heating concepts by varying heating-element materials, geometries, and spatial distributions, with the objective of maximizing temperature homogeneity and reactor selectivity.

The optimum design achieved a uniform temperature distribution across the catalyst bed and enhancing catalytic activity. The electrified reactor operated efficiently with a reaction conversion rate exceeding 98% for bioethanol dehydration conversion, facilitated by the elimination of axial temperature gradients and the reduction of preheating requirements. This approach also significantly reduced the need for carrier steam dilution, resulting in a process that is both energy-efficient and environmentally sustainable.

Economic evaluations indicate that for a green ethylene production unit via bioethanol dehydration with industrial production capacity, the electrified reactor concept enables a significant annual energy consumption reduction. Additionally, it achieves a significant reduction in CO_2 emissions per year compared to standard design. This highlights the potential of electrification to not only improve process efficiency but also substantially contribute to decarbonization efforts [4].

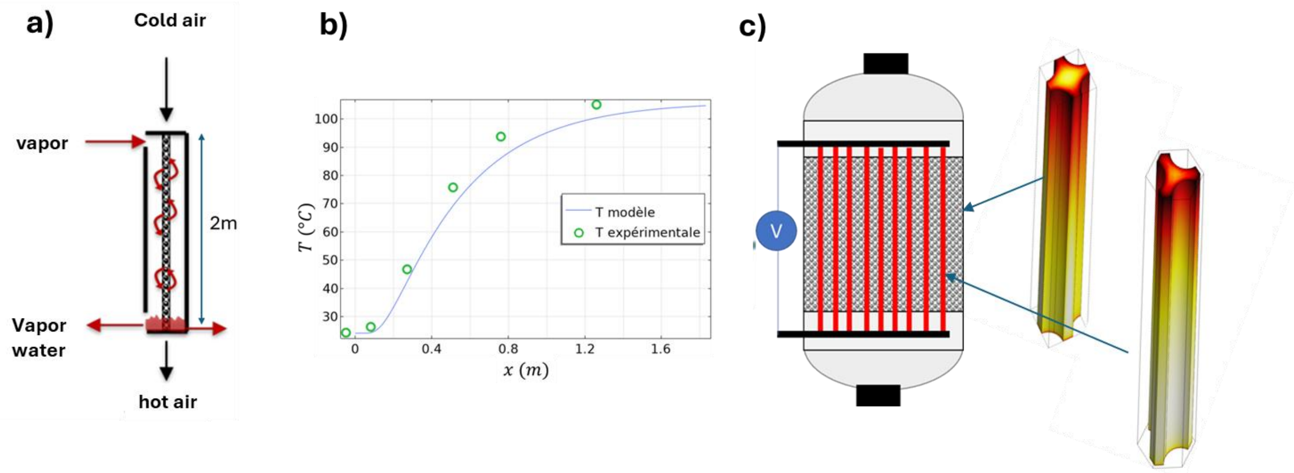

Figure 1. a) Schematic of the warm-scale experimental setup used to investigate heat transfer in a fixed-bed reactor. (b) Example of a comparison between temperature profiles predicted by the model and experimental measurements. (c) Illustration of the parametric study and optimization of the heating elements

4. Conclusions

This work demonstrates that the successful implementation of Joule-heated fixed-bed catalytic reactors for endothermic reactions requires integrated control of electrical, thermal, and reaction phenomena. The combination of multiphysics computational modeling and experimental validation provides a robust framework for reactor design and optimization, enabling the identification of heating-element configurations that ensure thermal uniformity, stable operation, and improved energy efficiency. The results confirm the strong potential of electrified catalytic reactors as scalable solutions for process intensification and decarbonization.

References

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Keywords
Electrification; Joule heating; endothermic catalytic reactor; multiphysics modeling; process intensification; decarbonization