Digital Twins of Steady-State and Dynamic Joule-heated Reactors

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Highlights

- Computational fluid dynamics simulations reveal Joule-heated reactors' flow patterns, transport effects, and heating rates at steady state and in transient operation.
- Flow recirculation and low energy loss to gases occur under many conditions.
- Heating elements with high electric conductivity and low volumetric heat capacity result in milliseconds response time.
- Rapid pulse Joule-heating enhances heat transfer and modulates the residence time.

1. Introduction

Process heating of chemical manufacturing accounts for 36% of the total energy consumption of the manufacturing sector. This underscores an urgent need to develop and deploy scalable and sustainable technologies that decouple economic growth from greenhouse gas emissions to decarbonize the industrial sector using renewable electricity. An effective decarbonization approach involves developing new processes for chemical production that replace fossil fuels with energy from wind and solar sources. Electrification methods, such as Joule heating, transform electrical energy directly into thermal energy.

Recent studies proposed that reactor internal Joule heating elements can eliminate heat transfer limitations and save 2x the energy compared to a furnace for high-temperature endothermic reactions.[1] Our previous work used a carbon fiber paper (CFP) heating element and achieved high heating rates (~14000 °C/s) and a near-isothermal catalyst surface.[1] Despite advances, the spatiotemporal flow and temperature fields in Joule-heated reactors are hard to obtain experimentally but are crucial for efficient reactor operation. Computational Fluid Dynamics (CFD) can be employed as digital twins of experiments to provide temperature and flow fields non-intrusively, insights into operation, and transients with unprecedented spatiotemporal resolution.

In our study, we first compare CFD simulations with experimental data and then examine flow and temperature patterns in Joule reactors under steady state and rapid pulse heating operation. We found that carbon heating elements can achieve high, uniform temperatures, crucial for efficient catalyst use, and localize hot zones near the element to mitigate unwanted gas-phase reactions. We observe reverse flows influenced by the element's steady-state temperature. Strategies are proposed to reduce reverse flows and enhance the reactor's temperature uniformity. Rapid pulse Joule heating enhances heat transfer. Finally, we elucidate all key parameters affecting catalytic performance in these reactors.

2. Methods

We model a carbon fiber paper in a quartz tube in continuous gas flow. A constant voltage V is applied across the carbon fiber paper. Heat loss due to natural convection is imposed outside the quartz tube. We also consider radiation loss from all surfaces. We solve the electric current, fluid dynamics, and heat-transfer equations using the COMSOL Multiphysics software. We include microkinetic models for typical endothermic reactions, e.g., methane reforming, to understand the impact on catalytic reactions. We compare nitrogen (N_2) and helium (He) as carrier gases to understand the relevant forces on flow patterns and transport. To provide insights into flow and heat transfer, we estimate the heating and cooling rates (upon turning the power off), the time to steady state, and the steady state temperature.

3. Results and discussion

CFD temperatures for continuous Joule-heated reactors at various voltages are in excellent agreement with experimental data (Figure 1a). Figure 1b presents the Nusselt number, Nu, calculated over the element versus position at steady state in continuous Joule-heated reactors. The Nu exhibits a U shape with enhanced heat transfer near the leading and trailing edges. Nu remains constant with increasing fluid velocity under typical experimental conditions, indicating the dominance of free convection. Continuous Joule heating reactors show recirculation and vortex formation (Figure 1c), impacting the reactor's temperature contours (Figure 1d). Minimizing recirculation by increasing the inlet velocity is essential to reduce dead zone formation and increase the reactor's temperature uniformity. We computed the critical conditions beyond which flow recirculation and dead zones are eliminated. Under dynamic pulse conditions, we found that rapid pulse heating enhances the heat transfer, manifesting process intensification from dynamic operation (not shown). Furthermore, we included and will present results on methane reforming to explore the steady and dynamic operation of Joule-heated reactors. Finally, the effect of heating element on reactor performance is discussed.

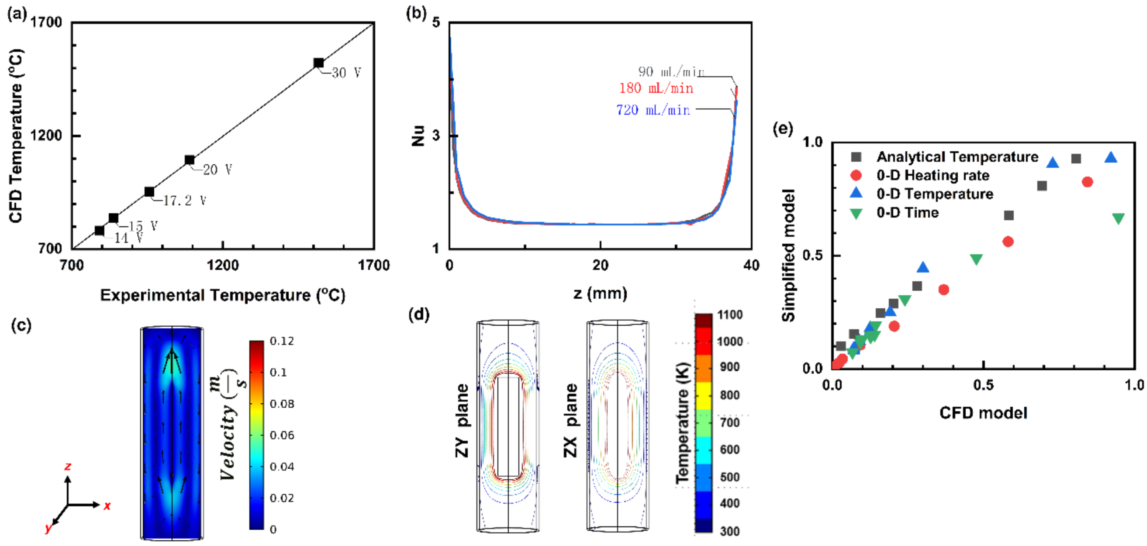

Figure 1. (a) Comparison of CFD and experimental data of average steady-state element's surface temperature for continuous Joule-heated reactors at various voltages. (b) Nu over the element vs position at various flow rates of He. (c) Velocity profile and (d) temperature contours for He. (e) Parity plot of simplified and CFD models for heating rate, temperature at steady state, and time to steady state scaled to 0 to 1 range. Nominal flow He at 90 mL/min.

To provide insights into the transient operation, we developed a simplified (0D) dynamic model for rapidly predicting the temperature of the Joule heating element, the time to reach a steady state, and the heating and cooling rates. This model achieves prediction with 15% accuracy compared to CFD data (Figure 2). We derived analytical expressions for the quantities of interest that can assist with reactor optimization, fast reactor response, and temperature control (Figure 2).

4. Conclusions

We developed a CFD model as a digital twin to capture the spatiotemporal behavior of Joule-heated reactors. We found significant flow recirculation at typical laboratory conditions due to buoyancy and Nu values consistent with free convection. The recirculation impacts temperature isotherms, necessitating higher flow rates for a uniform reactor temperature. We demonstrate that one can reach ~2000 °C in milliseconds with suitable materials, enabling rapid response, unattainable even with conventional microreactors. Rapid pulse Joule heating enhances heat transfer and offers superior control and responsiveness to transient operation. Finally, we demonstrate how catalyst structure affects endothermic reactions, guiding improved reactor designs.

References

[1] K. Yu, C. Wang, W. Zhang and D. G. Vlachos, ACS Energy Lett., 2023, 8, 1050-1057.

Keywords

Joule heating, flow patterns, heat transfer, dynamics, timescales.