Electrification Of Chemical Reactions

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Abstract

Many industrial processes involving chemical reactions rely on heat addition, which accounts for approximately 50% of all energy consumed in the United States' industrial sector. Examples include metallurgical processes, chemical processing, and heating process fluids. Traditionally, this heat is generated through combustion, which transfers heat to a reactor via its external walls. This method, although mature, is often inefficient in terms of energy use and can have negative environmental impacts. Electromagnetic heating enables enhanced energy efficiency, reduced emissions, and improved process intensification compared to traditional combustion-based methods. This approach to process heating creates a complex multiphysics environment where electromagnetic interactions, fluid dynamics, heat transfer, and chemical reactions must be carefully balanced.

In this study, we simulate three variants of a steam-methane reformer that utilize electromagnetic heating (Figure 1). These include the resistive (Joule) heating of the reactor tube, induction heating of a soft iron susceptor to heat a non-magnetic porous catalyst bed, and hysteresis heating of ferromagnetic catalyst particles. To simulate each of these reactors, we couple the Magnetic Fields, Heat Transfer, Free and Porous Media Flow, Transport of Concentrated Species, and Chemistry interfaces in COMSOL Multiphysics®. The kinetics of steam methane reforming are modeled using the mechanism reported by Xu and Froment [1]. The magnetic hysteresis behavior of the ferromagnetic particles is taken from the experimental work in [2].

We plot the temperature and methane conversion distributions for each reactor in Figure 2. The resistively heated reactor shows strong radial and axial temperature gradients as the heat of reaction in the catalyst coating is balanced by the Joule heating in the reformer tube. We additionally observe a slow, non-uniform conversion of methane along the length of the reactor. The inductively heated susceptor generates heat at the centerline of the reactor, which promotes a more even distribution of the temperature field and more rapid conversion of methane. Finally, the ferromagnetic particle reactor demonstrates the most uniform temperature distribution among the reactors studied, as heat is generated in a distributed manner throughout the catalyst bed. This yields a very rapid conversion of methane, which enables future work to design for process intensification. The improved thermal distribution is beneficial for process efficiency and the mechanical integrity of the reactor.

Multiphysics simulations of electromagnetically heated chemical reactors allow for the design and optimization of reactors with complex flow systems. By capturing the interactions between multiple coupled physical phenomena, these simulations make it possible to evaluate design trade-offs efficiently. Our findings offer valuable insights into enhanced reactor heating strategies and can be further leveraged to improve process yield and operational efficiency.

Reference

[1] J. Xu and G. F. Froment, "Methane steam reforming, methanation and water-gas shift: I. Intrinsic kinetics", AIChE Journal, vol. 35, pp. 88-96, 1989
[2] M. G. Vinum, M. R. Almind, J. S. Engbæk, S. B. Vendelbo, M. F. Hansen, C. Frandsen, J. Bendix, P. M. Mortensen, "Dual-function cobalt–nickel nanoparticles tailored for high-temperature induction-heated steam methane reforming", Angewandte Chemie, vol. 130, pp. 10729-10733, 2018.

Figures used in the abstract

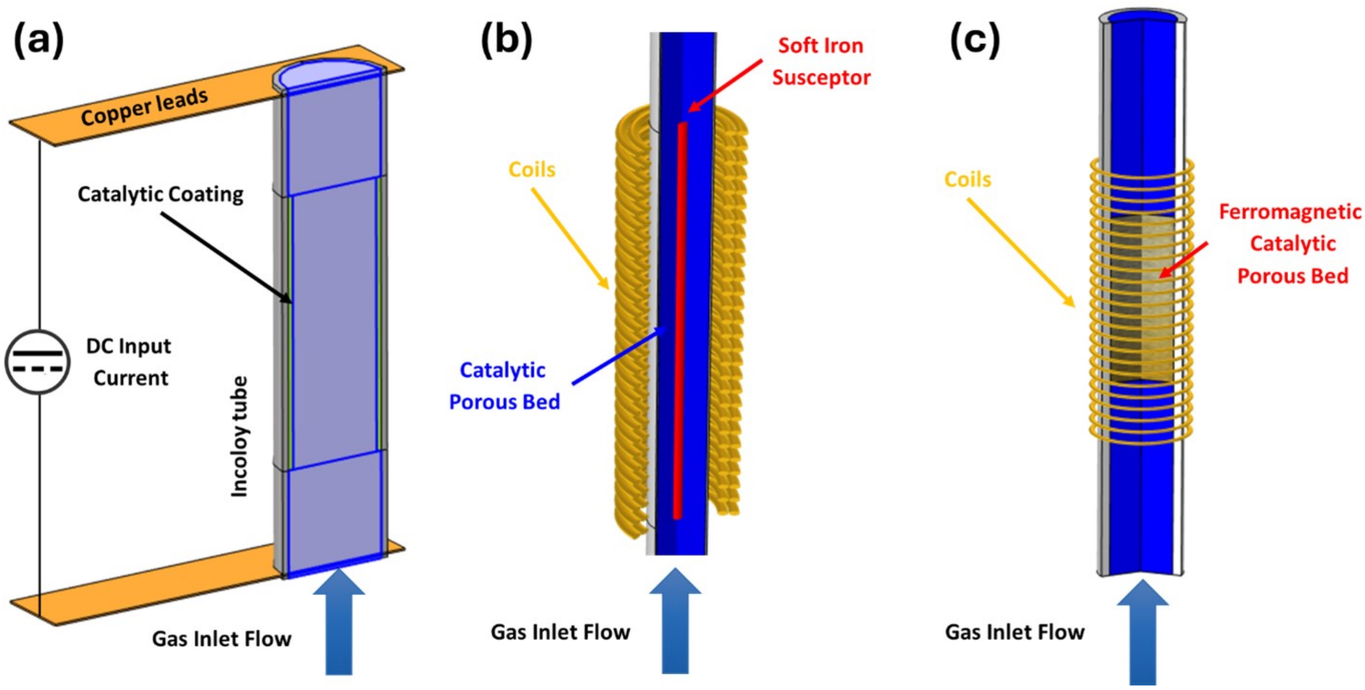

Figure 1 : Reactor configurations considered in this study: (a) resistive heating of the reformer tube, (b) induction heating of an internal susceptor, and (c) hysteresis heating of ferromagnetic catalyst particles.

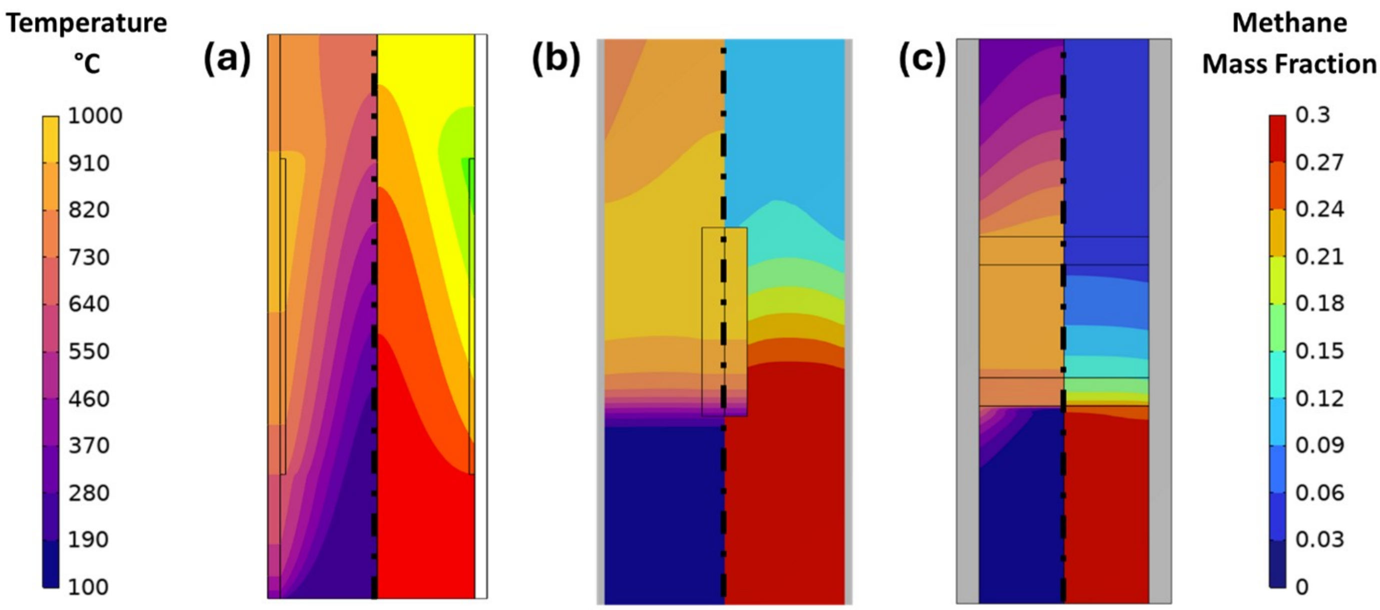

Figure 2 : Temperatures (left half) and methane mass fractions (right half) for the three reactor configurations. Reactor dimensions scaled down 20X in axial direction.