Mathematical Modelling of an Electrified Steam Reformer

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Introduction

Electrification is proposed as a viable option for decarbonizing high temperature endothermic catalytic processes. Among the different options for power-to-heat, Joule heating can deliver high temperature heat power with unitary theoretical efficiency and it is the most mature technology towards scale-up and retrofitting[1].In particular, Electrified Methane Steam Reforming (e-MSR) is a promising concept for low-carbon H_2 production. Among the alternatives proposed in the literature, an interesting solution consists in a reactor with an electrically heated structured ceramic Ni-based catalyst where heating wires are inserted in the channels of a washcoated monolith[2]. This solution provides very high volumetric mass transfer coefficients, low pressure drops and unprecedented heat transfer performances thanks to the combination of radiative and convective heat transfer mechanisms. To unlock the potential of this solution, an engineering model that accounts for relevant thermal and chemical phenomena is required to allow the rationale scale-up of the concept.

Materials and Methods

A 1D steady-state heterogeneous mathematical model was developed in Matlab, which consists of energy and momentum and species mass balance. The reactor, consisting of parallel channels with identical geometry, is simplified to a single channel under the assumption of uniform variables at the inlet section and negligible heat dispersion. Ideal gas behavior, fully developed laminar flow, T-dependent properties and radiation from the wire to the catalyst were considered. For the kinetics, the Xu and Froment's model was implemented[3]; the effect of the wire eccentricity is accounted by considering transport coefficients available in the literature[4].

Results and Discussion

Two simulations have been performed using the following input data: T^{IN} = 573.15K, P^{IN} = 8 barg, S/C = 2, $\mathrm{GHSV}_{\mathrm{CH_4}}$ = 3600 1/h, PD = 12.3 MW/m^3. For the concentric reactor configuration, a small gas-solid temperature gradient is present leading to an equilibrium approach of 69K. With this configuration, 86% methane is converted, and external mass transfer resistances are negligible. Conversely, introducing 30% wire eccentricity, deviations are present due to the negative impact of eccentricity on mass and heat transport coefficients. In particular, the methane conversion decreases to 82%, due to the onset of external mass transfer resistances. This, under constant input power, raises the outlet gas temperature, impacting the equilibrium approach negatively. The gas-solid temperature differences become more pronounced due to the reduction of the convective heat transfer mechanism. Here, in fact, radiation plays a major role: at the inlet, the catalyst is hotter than the gas due to the radiative exchange between the wire and the catalyst surfaces. In summary, the model shows the high sensitivity on the wire eccentricity, that has significant impacts on both conversion and temperature profiles. Further experimental studies are required to determine the effective eccentricity of the system.

Acknowledgments

This project has received funding from the European Research Council (ERC) under the European Union's Horizon 2021 research and innovation programme (GA No. 101058608 - 'EReTech').

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