Parametric investigation of an electrified steam methane reforming process using CFD modelling

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Significance and Relevance

The present work introduces a Computational Fluid Dynamics (CFD) tool for modelling an electrified steam methane reforming (e-SMR) process. The intended use of the developed model is the evaluation and optimisation of e-SMR reactors. In this framework, the developed CFD models predict the performance of an electrically heated reactor unit within a broad spectrum of operating conditions. The resulting simulation data are presented in a comparative manner and provide a clear overview of the key operating parameters and their effect on the output of the e-SMR process.

- *Preferred and 2nd choice for the topic:* "Multiscale modeling and advanced simulation aspects" / "Catalysis to electrify the chemical production"
- *Preferred presentation*: Oral only

Introduction and Motivations

In 2022, more than 90% of the hydrogen produced in Europe was a product of a reforming process,[1] while globally, hydrogen production by methane-containing natural gas reforming is estimated to be around 48%.[2] Steam methane reforming (SMR) is an energy-intensive catalytic process, thus the efficient electrification of this process is of great importance for the decarbonisation of hydrogen production.[3] For that reason, a lot of research is conducted both on the development of more efficient e-SMR systems,[4,5] but also on the techno-economic viability of such solutions.[6] For enhancing the ability to assess and optimise such systems, the introduction of specialized numerical tools is crucial. The present work introduces a CFD-based model designed to numerically simulate, evaluate, and optimize e-SMR reactors.

Materials and Methods

A Computational Fluid Dynamics (CFD) model is developed to simulate the e-SMR process that takes place inside an experimental, electrically heated, FeCrAl reactor tube, partially coated with a Nickel-based catalytic washcoat.[7] The model is built in the ANSYS Fluent® environment and accounts for the conservation of mass, energy and momentum within the system. An in-house code is developed to describe the chemical kinetics and mass diffusivity within the catalytic washcoat. The developed functions describing the chemical kinetics are based on the work of Xu & Froment,[8] while the diffusivity model is based on the publication of Rostrup-Nielsen and Christiansen.[9] The model is validated against experimental data for a wide range of operating conditions in terms of mass flow rates and power load.[7] The validated model is used to predict the performance of a given system in the case of various operating conditions and catalytic properties. Eventually, the developed model can be effortlessly modified and used as an optimisation tool for reforming reactors.

Results and Discussion

The operating pressure of the unit, the mass flow rate of the methane mixture, the provided steam-to-fuel ratio, and the power supplied for heating the reactor are the key operating parameters examined in the CFD simulations. From the catalyst side, two main properties are investigated, namely the porosity and the average pore diameter of the catalytic washcoat. In total, twenty sets of operating conditions are simulated. For each set of conditions and properties, the resulting data are presented in terms of methane conversion, net power usage, temperature variation within the reactor domain

and species mole fraction distribution along the tube length, whereas the flow field and the pressure drop within the channel are also reported for each case. Indicative results from the numerical campaign can be found in **Figure 1**. The resulting data are presented in a comparative manner and provide a clear overview of the correlation between the operating parameters and the products of an e-SMR process. Since the model can be easily adapted and used with various reactor arrangements, it can function as an effective optimisation tool for compact e-SMR reactor for hydrogen production.

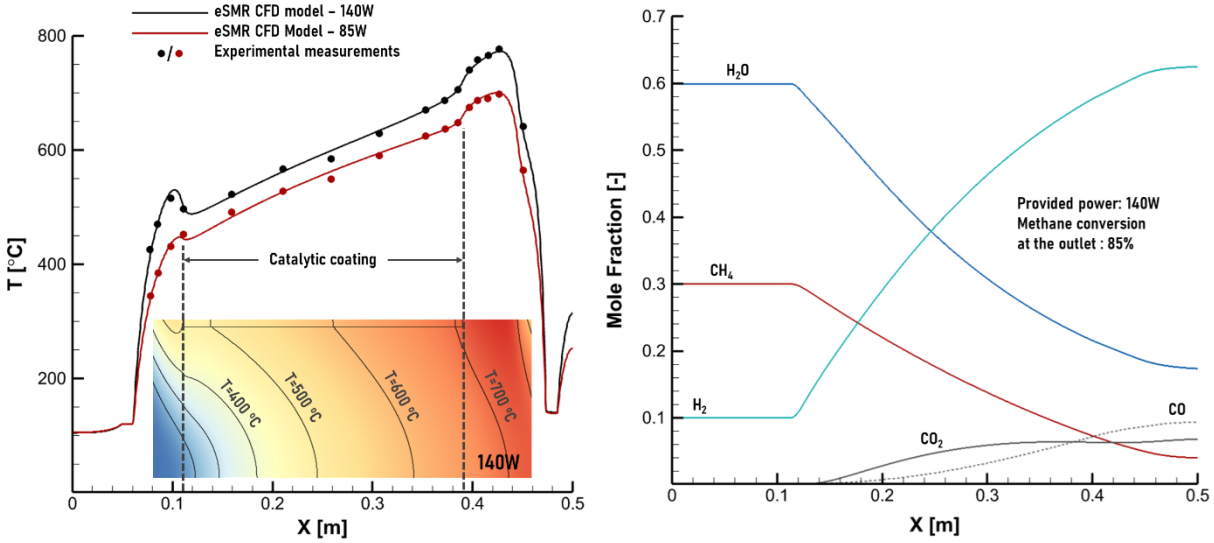

Figure 1. *Experimental measurements[7] and corresponding numerical predictions of the e-SMR CFD model for power load of 140 and 85W. A contour plot of the temperature of the reactor domain is presented on the bottom of the diagram (left). Line diagram of the evolution of the mole fractions of the reacting species along the reactor length, as measured at the axis of symmetry (right).*

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