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3D Modeling of a CPOX-Reformer including Detailed Chemistry and Radiation Effects with DUO

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Highlights

- 1. 3D modeling of a honeycomb CPOX reformer for the conversion of methane on rhodium
- 2. Calculation domain comprises the flow region and two monoliths (one of them coated)
- 3. Modeling includes detailed surface chemistry and solid body radiation
- 4. Comparison of concentrations and fluid/solid temperatures with measured data
- 5. Radiation influences heat distribution but the effect on the chemical conversion is weak

ABSTRACT

The impact of radiation heat transfer and radial heat losses in small-scale monoliths, as often used for testing catalysts or qualifying process conditions, are an important consideration to design and predict performance of commercial size reactors. The paper presents the 3D modeling of a honeycomb CPOX (Catalytic Partial Oxidation) reformer, including detailed surface chemistry for the conversion of methane on rhodium. The calculation domain comprises the flow region and two monoliths (one of them coated) which are positioned in a glass tube. For the simulations the software tool DUO (coupling between OpenFOAM and DETCHEM^{TM}) was used. The objective was to model the system without any boundary conditions for the temperature (aside from the inlet). As the temperature level is above 900 K solid body radiation has to be included. The comparison of the results with detailed experimental data shows that it is possible to reproduce the species concentrations and the temperature fields of the flow and solid structures well. The effect of radiation, leading to a heat transfer between the two monoliths, can clearly be indicated. However, this effect plays only a minor role with respect to the chemical conversion. The simulations capture the measured effect of radial heat loss on the conversion process in different channels inside the catalyst.

Keywords: CFD; 3D; DUO; OpenFOAM; DETCHEM; CPOX; Simulation; Modeling; Monolith Catalyst; Honeycomb Catalyst; Reformer; Detailed Chemistry; Solid Body Radiation