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Subject Area	Energy and Environment

CFD Analysis of Ammonia Reforming in a Micro-Channel Reactor

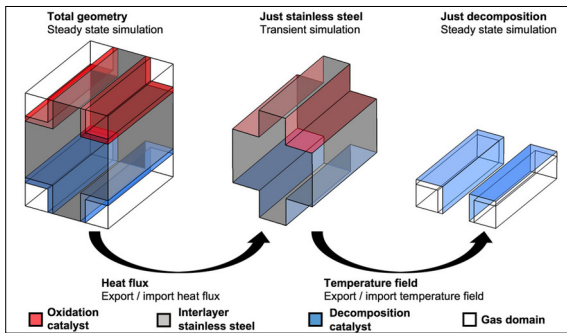


Figure 1: Division of the entire model for the transient solution procedure (geometry scaled in length 1:100).

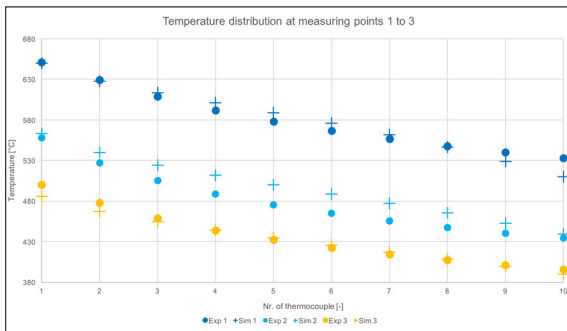


Figure 2: Steady-state comparison of temperature distribution in micro-channel reactor for three operating conditions.

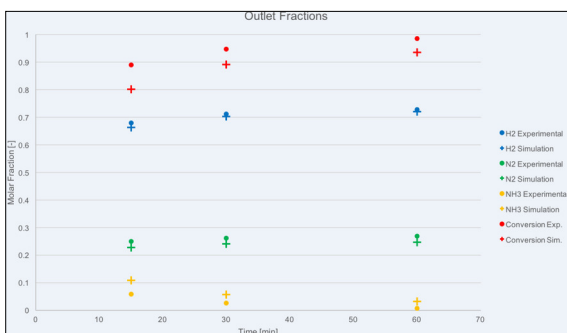


Figure 3: Outlet NH3 decomposition product fractions after one hour since initiating transient operation.

Introduction: In this work, a computational fluid dynamic (CFD) model is developed to describe the unsteady (transient) behaviour of ammonia reforming in an auto-thermal micro-channel reactor. An experimental reactor is modelled to determine heat and mass transfer effects within the micro-channels. Characterising reactor start-up enables an accurate interpretation of temperature dependence and hydrogen production in dynamic operation. Appropriate governing equations were used to account for mass, momentum, energy and species transport. Specifically, Knudsen diffusivity is defined to describe diffusion in the porous catalyst domains. Ultimately, future reactor designs can be improved to minimise time loss during start-up by identifying increased heat and mass transfer through CFD simulation. For the chemical reaction, the time step size is in the order of 10^{-5} seconds in the CFD simulation.

Procedure / Result: This simulation problem is solved in a stepwise procedure (Fig. 1). First, a steady state simulation of the entire model is created. From this result, the calculated heat flux of the interface areas between catalysts and interlayer is exported. These heat flux values are applied on a geometry reduced to the interlayer. Because the geometry now contains only one fluid-free solid, a transient simulation can be performed with large time steps. As in the experimental investigation, a temperature of 300°C is used to initiate the transient phase of six hours during simulation. The temperature distribution in the interlayer can be reconstructed using result files with a defined time interval. The resulting wall temperature, on the same inter-facial areas as was used for heat flux, can be exported to a geometry reduced to the decomposition side. This wall temperature is used as a boundary condition in a steady-state fluid simulation, incorporating the chemical reaction for decomposition. With this solution procedure, the product gas composition from the decomposition reaction and the temperature distribution in the reactor can be calculated.

Result: Both the transient and steady-state simulations show a good correlation to the experimentally determined values. The reactor was evaluated by varying NH_3 decomposition flow rate (2-6 NL/min) and NH_3 oxidation flow rate (2-4 NL/min) at an oxidation fuel-to-oxygen ratio of 1.4. Figure 2 illustrates the temperature distribution over the entire length of the reactor for three different operating points, under stationary operating conditions. During the experiments, the temperature is measured at ten different points with thermocouples. The simulated temperature is recorded at the same locations and used for this comparison. In Figure 2 and 3, the experimental values are represented with a dot and the simulated values represented with a cross. Figure 3 compares the product gas composition (NH_3 , H_2 and N_2) for the decomposition outlet after one hour of transient operating time for one operating point between experimental values and simulation results. By solving the simulation problem in a stepwise procedure, the experimental results can be accurately simulated and provide unique insight into the transient behaviour of the chemical reactions and the heat propagation throughout the reactor. These CFD results can therefore be used to successfully design and further develop reactors with quick transient response times for H_2 production technology.