Virtual Functional Product Development of a µ-Methane Steam Reformer

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Abstract

1. INTRODUCTION:

One of the pillars of the "Energiewende" of the Federal Republic of Germany is energy efficiency [1]. The need for reduced energy consumption leads to the question of energy saving potentials. Decentralized cogeneration, production of heat and energy, according to the actual demand with a high efficiency energy converter like a fuel cell is capable of delivering highest energy savings in regards to primary energy consumption [2, 3]. In Figure 1 a process flow chart of a Methane Steam Reformer Fuel Cell system is shown. The target of this work is the study and a design proposition of a Methane reformer - catalytic burner compound. This abstract covers the catalytic burner.

2. USE OF COMSOL MULTIPHYSICS®:

For the description of a chemical reactor it is necessary to solve multiple conservation equations. In order to study the kinetics of a system you have to account for convective and diffusional transport of species to and within the catalyst and heat transport over the whole geometry. COMSOL Multiphysics is known for its capabilities in combining different physical effects and offering appropriate and optimized solvers. The programming environment already proved advantageous in the simulation of a high temperature proton exchange membrane fuel cell [4].
Solving for the temperature and the concentration field gives the opportunity to examine the reaction mechanisms. With the reaction engineering module first results for 0D problems can be obtained, which are beneficial for the estimation of contact time and turnover. Only the full space dependent model is able to predict accurate results. Figure 2 depicts the 2D axisymmetric model geometry and the calculation domains for the catalytic burner. It consists of a single reactor channel with a catalyst coated wall. The gap size is with 500 µm in the sub millimetre region.

3. RESULTS:

Besides the obviously interesting results like the temperature profile shown in Figure 3a the simulation can be used to calculate:
• total turnover
• local maximum temperature

• local combustion power
• heat losses
Impacts of changing the geometry like the gap size or different material pairings are easy to probe. Another source of information is the time dependant simulation. Figure 3b represents the ignition process of a Hydrogen air mixture at 25°C and with reaching the catalysed ignition temperature of Methane the onset of Methane oxidation (/footnote Only heterogeneous reactions were considered.).

4. CONCLUSION:

The simulation is able to describe the catalysed oxidation of Methane and Hydrogen. In order to validate these results, especially in regards to the kinetic approach, it is necessary to compare the simulation with experimental data. For setups modelled after experiments extracted from the literature [5] the results were in good agreement. Still the kinetic data represents a loose edge. Therefore an experimental setup was developed (Figure 4), which is based on the boundary conditions of the simulation. This setup combined with the information about the applied catalyst should deliver a validated kinetic data. This data set can be applied to an enhanced simulation consisting of the burner and the reformer channels.

Reference

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[2] F. Barbir, PEM fuel cells: Theory and practice, second edition, 2nd ed., Academic Press, Waltham, Mass. 2013.
[3] G. Kolb, Fuel Processing, Wiley-VCH, Hoboken 2008.
[4] T. J. Kazdal, S. Lang et. al., Modelling of the vapour–liquid equilibrium of water and the in situ concentration of H3PO4 in a high temperature proton exchange membrane fuel cell, Journal of Power Sources 2014, 249, 446.
[5] N. S. Kaisare, D. G. Vlachos, A review on microcombustion: Fundamentals, devices and applications, Progress in Energy and Combustion Science 2012, 38 (3), 321.

Figures used in the abstract

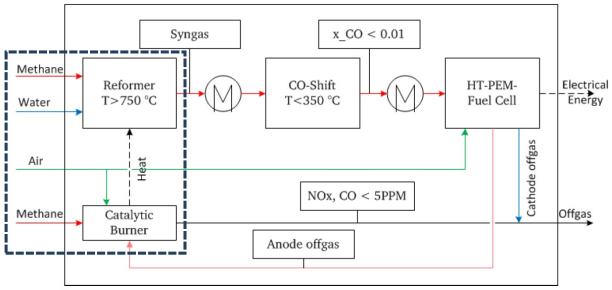

Figure 1: Figure 1: Process flow chart for the Methane Steam Reformer Fuel Cell System

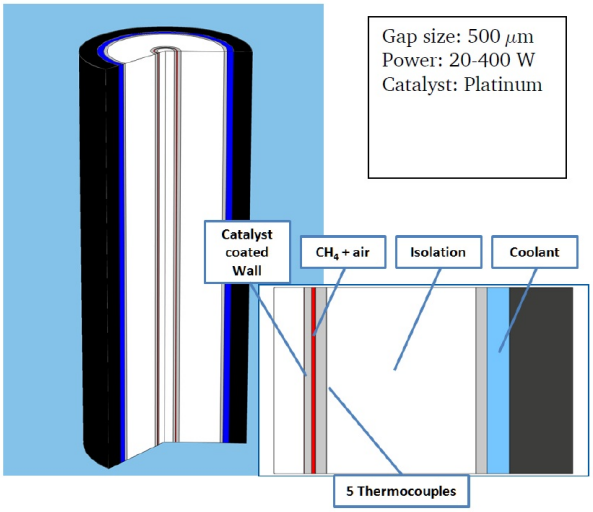

Figure 2: Figure 2: 2D axisym. calculation domains

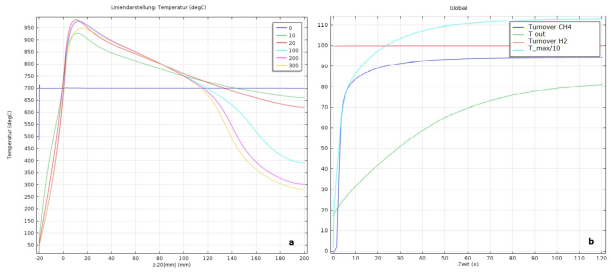

Figure 3: Figure 3: a) Temperature along the z-axis for different time stamps. Starting from uniform 700°C. b) Hydrogen assisted ignition starting at 25°C and onset of Methane oxidation.

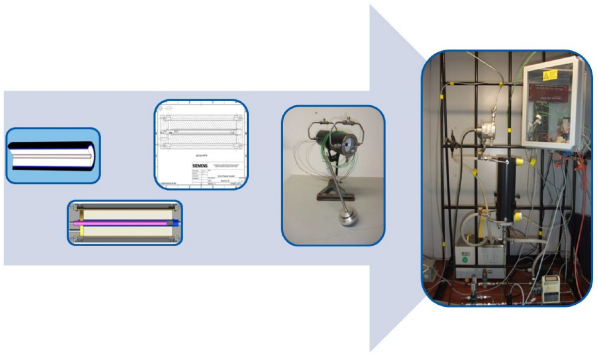

Figure 4: Figure 4: Experimental setup adapted from boundary conditions of the model. COMSOL model – CAD model – CAD drawing – fabricated reactor – experimental setup