Experimental and numerical investigation of the catalytic partial oxidation of methane on rhodium coated honeycomb catalysts

Summary

The catalytic partial oxidation (CPO) of light alkanes on the noble metals Pt and Rh at very short contact times has been shown to offer a promising route to convert natural gas into more useful chemicals such as synthesis gas, higher hydrocarbons, and oxygenates.[1,2]

The catalytic reactor used for these processes, such as foam or extruded monoliths, wire glasses, or sintered spheres, show a complex interaction of transport and chemical reactions occurring on the catalytic surface and in the gas phase. Therefore, the description of the reactor requires detailed models of the flow field, chemistry and their coupling.

We studied the chemical reactions at the Rh and Pt surfaces for the partial oxidation of methane, and the coupling with the surrounding reactive fluid flow. Selectivity, conversion, and reactor temperature as function of temperature, velocity, and methane/oxygen ratio derived from a detailed numerical simulation are compared with experimental data.

The simulation applies elementary step reduction mechanisms for gas phase as well as surface chemistry, which are coupled with three- and two-dimensional flow field simulations including detailed models for mass and heat transport. The computations are based on the CFD-code FLUENT® which is coupled with the chemistry modeling package DETCHEM.[3]

The study reveals that partial oxidation of methane is a purely heterogeneous process at atmospheric pressure, while homogeneous (gas phase) reactions become significant at elevated pressure.[4]

Acknowledgments:

The authors would like to thank S. Tummala and L. D. Schmidt (University of Minnesota) for fruitful collaboration on interaction of transport and chemical reactions short contact times.

Literature: