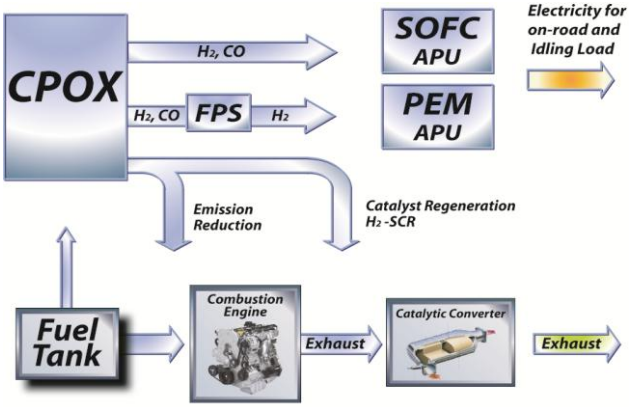
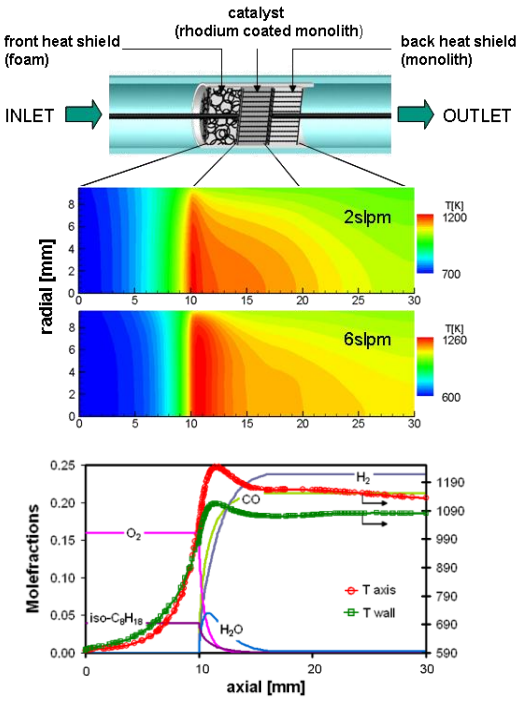
Conversion of gasoline and diesel to hydrogen

Background: A considerable long term interest in hydrogen as a fuel in relation to the scarcity of fossil fuels and the associated pollution problems excites the development of systems using catalytic partial oxidation for the production of hydrogen-rich synthesis gas from conventional fuels such as gasoline, diesel and jet propulsion. Two examples of such systems being currently of great technological interest are the Solid-Oxide Fuel Cell (SOFC) when operated with non-pure hydrogen fuels, e.g. partially reformed logistic fuels, and short-contact time reactors for reforming gasoline and diesel, as first stage of an on-board auxiliary power unit (APU). The non-linear coupling of complex homogeneous and heterogeneous chemical reaction kinetics with heat and mass transfer in such systems matters for reactor behavior, often even superimposed by transient modifications of the active catalytic phase, e.g. by oxidation and coking





Project: The main task of this project is the study on catalytic partial oxidation of gasoline and diesel for hydrogen production in the monolithic short-contact time reactors both experimentally and numerically. Our experimental setup allows well-defined accurate mixing of fuels with boiling points up to 280°C with synthetic air to feed the catalyst with a homogeneous, pulse free reactant flow and a uniform temperature profile. The product stream is analyzed by a variety of simultaneously applied methods such as FT-IR, MS and GC/MS allowing both a time resolved monitoring of the reaction and a fast screening of a diversity of fuel surrogates and gas mixtures. The mixture of a large number of intermediates and radicals (over 200 chemical species) formed in the complex heterogeneous and homogeneous reaction network presents a challenge for the numerical simulation. The implementation of detailed chemical kinetics in a two-dimensional parabolic flow model for individual monolith channels and the coupling with heat balances of the catalytic monolith as well as heat shields, insulation, and reactor wall provides a simulation tool that is able to analyze the behaviour of structured CPOX reactors in great detail. The simulation can provide guidance to reactor design and optimization of the operating conditions such as flow rate and fuel/oxygen ratio.

Co-workers: Lubow Maier, Torsten Kaltschmitt

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Selected publications: M. Hartmann, L. Maier, H. D. Minh, O. Deutschmann. Combustion and Flame, 157 (2010) 1771-1782; M. Hartmann, L. Maier, O. Deutschmann. Appl. Catalysis A: General 391 (2011) 144-152; L. Maier, M. Hartmann, S. Tischer, O. Deutschmann. Combustion and Flame 158 (2011) 796-808; T. Kaltschmitt, L. Maier, C. Hauck, O. Deutschmann Proceedings of the Combustion Institute 33 (2011) 3177-3183; T. Kaltschmitt, C. Diehm, O. Deutschmann. Industrial & Engineering Chemistry Research, accepted (12.01.2012)