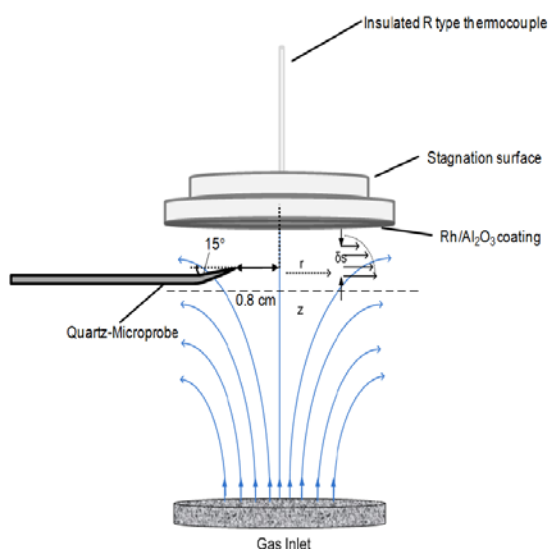# Catalytic conversion of H_2, CO, CH_4, C_3H_8 over rhodium

Background: Today, catalytic applications play an important role for academic and industrial research; especially for the development of environmentally friendly technologies to generate alternative ways of energy and material production for future sustainable economies.Among the catalysts belonging to group VIII transition metals (Rh, Pt, Ru, Ni), Rh is an effective catalyst with its high product efficiency over a wide range of temperatures and its stability against impurities in the fuel such as sulphur.

Many industrial applications involve Rh catalysts in their processes such as synthesis gas (H_2+CO) production technology via reforming of hydrocarbons, i.e., catalytic partial oxidation (CPOx), auto-thermal reforming, steam reforming and gasification of coal or biomass, preferential oxidation of CO and water-gas shift (WGS) reaction technologies, where CO concentration in the fuel stream should be less than 10 ppm for H_2-operated low temperature fuel cell power generation systems, and reduction of emissions (NO_x, CO, HC) in exhaust gas after-treatment systems.

Current focus in the catalytic technology is on the search for alternative catalytic materials to increase the product selectivity and on understanding the interaction of the catalyst and surrounding reactive . This leads to the optimization of catalytic processes and reactor geometries.

Project: Our primary objective is an understanding of the reactive flows and their interaction with surrounding media to develop a reliable unified surface reaction mechanism for C_1-C_3 light hydrocarbons over Rh catalysts. For this purpose, a stagnation-flow reactor (SFR) is used to facilitate computational modeling of heterogeneous surface chemistry coupled with 1D convective and diffusive transport properties within the gas-phase boundary layer.

A stagnation-flow reactor enables exact computational solutions of chemical and physical properties of the reactive flow with its well-defined concentration and temperature profiles in the catalytic region wherein heat and mass transport effects are minimized.

Microprobe sampling technique is used to measure the gas-phase composition in the boundary layer adjacent to the catalyst surface. Data is used to build up a thermodynamically consistent elementary-step surface reaction mechanism based on the mean field approximation. Detchem[STAG] and Chemkin-SPIN programs are used for computational simulations.

Stagnation flow field and micro probe sampling technique in SFR

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Selected publications: Baer J., Karakaya C., Deutschmann O., Proceedings of the Combustion Institute, Accepted (2012); O. Deutschmann, Modeling and simulation of heterogeneous catalytic reactions : from the molecular process to the technical system, in, Wiley-VCH, Weinheim, 2012, pp. 354; N.E. McGuire, N.P. Sullivan, O. Deutschmann, H. Zhu, R.J. Kee, Applied Catalysis A: General, 394 (2011) 257-265; M. Hartmann, L. Maier, O. Deutschmann, Applied Catalysis A: General, 391 (2011) 144-152.