Simulation of stagnation flow reactors with DETCHEM^{STAG}

Background: Stagnation flow reactors have gained significant attention within the last two decades. Stagnation flow on a catalytic plate offer a simple configuration which enables coupling the catalytically active surface with the surrounding flow. This coupling gives insight into heterogeneous chemical processes on the surface and fluid-mechanical properties inside the gas-phase boundary adjacent to the surface. All in all, this simple configuration enables developing reaction mechanisms for different chemical processes (steam reforming, dry reforming etc.).

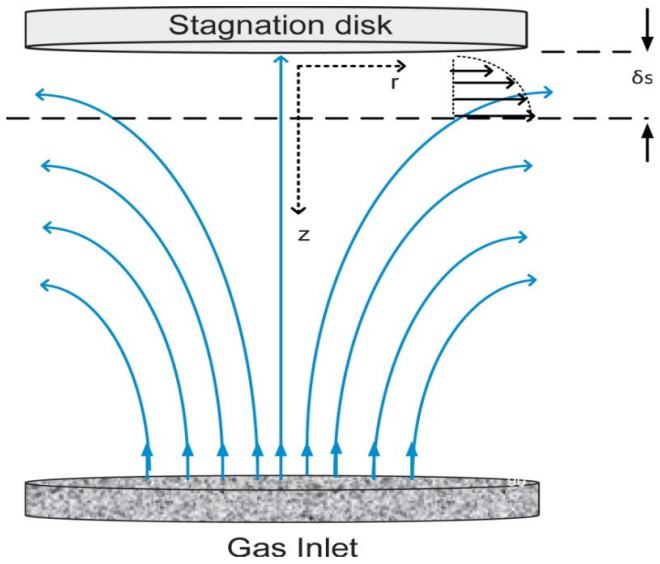

Figure: Schematic illustration of the stagnation flow configuration (C.Karakaya, O.Deutschmann, Chemical Engineering Science Volume 89 2013 171 – 184)

Project: We use a transient one-dimensional model to simulate the behavior of a catalytically active stagnation flow reactor. With this model, it is possible to predict the state of the catalytic surface (its coverages and temperature) and properties of the surrounding gas flow (species mass fractions, temperature and velocity). The model neglects edge effects and gives the attention to the center of catalytic surface. In more detail, the governing equations consist of three parts: gas-phase equations, surface equations, and boundary conditions. Gas-phase equations include the energy, species, mass conservation, momentum conservation and eigenvalue (radial pressure gradient) equations. Surface equations include the coverage of each adsorbed species on the surface. In order to completely describe the system, boundary conditions are also included. One boundary condition is introduced for the inlet stream and the other is introduced for the gas-surface interface. Since the model is one-dimensional, the variables (temperature, species etc.) do not change with respect to the radial coordinate. Therefore, independent variables are just the time and the axial coordinate. Detailed models for the chemical reactions and molecular transport are also included in the governing equations. Spatial discretization of the partial differential governing equations is applied by using finite difference approximations. The mesh points are obtained by using an adaptive-refinement procedure. This discretization results in a system of ordinary differential and algebraic equations which is finally solved by the software package LIMEX that uses an implicit extrapolation method.

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Selected publications: O. Deutschmann et al., Proc. Combust. Inst. 26 (1996) 1747-1754; www.detchem.com