# Modeling and numerical simulation of multiphase chemical reactions in exhaust after-treatment

Motivation: SCR-systems for NOx conversion have been used in the automotive industry for several years. In contrast to processes in the gas phase, the interaction between physical and chemical processes near the significantly colder wall in the exhaust pipe as well as on the walls, where liquid films and sometimes even solid deposits are present, are not completely understood. Besides the experimental investigation of these processes, the development of mathematical models to describe these phenomena and their integration in computer programs for numerical simulation of reactive turbulent flows in exhaust lines are also required.
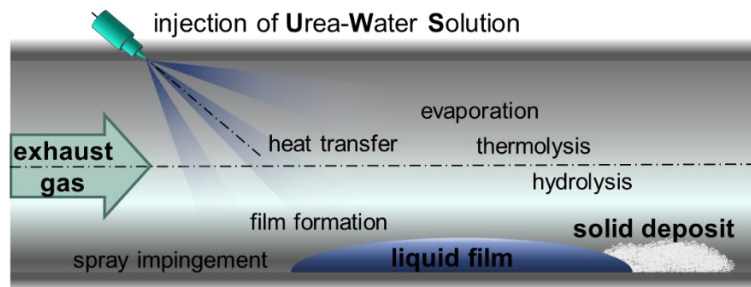
Chemical reactions in the exhaust line

Currently there exists neither a micro-kinetic description of the system nor a numerical algorithm to couple the chemical reactions at the respective phases and interfaces with the turbulent flow field.

Objectives: Our project has two primary objectives. The first is the development of mathematical models, capable of describing chemical reactions in multiphase flows in presence of solid walls based on molecular processes, which can be coupled with the simulation of reactive turbulent flow near the wall. The second is the application of the aforementioned models to study the decomposition of a urea-water solution taking into account undesirable side reactions. It should be noted, that the thermolysis and hydrolysis of the urea-water solution can proceed both in liquid and in gas phase. Moreover, solids can simultaneously deposit on the exhaust pipe, and crystallize wall films.
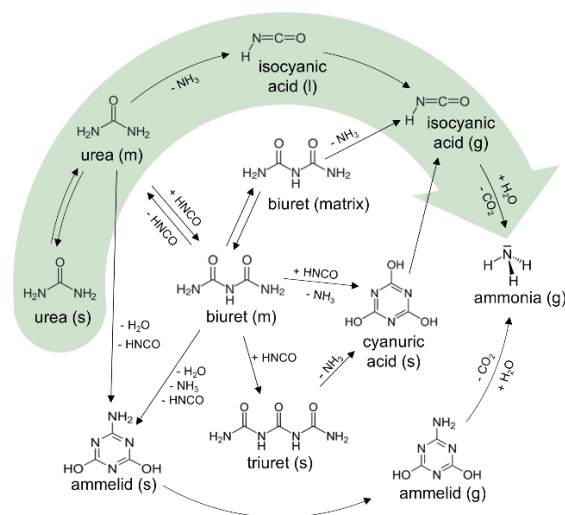

Reaction mechanisms for the forming and decomposition of the solid deposit, based on (Brack, Heine et al. 2014)

Approach: Chemical reaction mechanisms are developed to represent the elemental processes occurring at both single phases (gas, liquid, solid) and their interfaces (gas/liquid, gas/solid, liquid/solid) using consistent micro-kinetic

approaches. The mechanisms are particularly sophisticated for the liquid and solid phases and at the gas/liquid and liquid/solid interfaces. The mean-field theory based methods, which have been successfully applied to describe heterogeneously catalyzed gas-phase reactions in recent years, will be expanded for liquid and solid phases with their interfaces.

The software package DETCHEMTM offers a starting point for the planned investigations, which enables the numerical simulation of reactions in gas phase flows and on solid walls. During the course of the project, this software will be developed to compute the chemical source terms for species conservation equations in single phases and their corresponding interfaces.
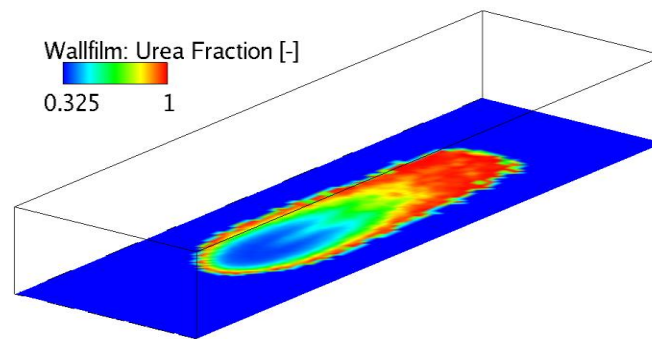
Simulation showing wall film formation (Birkhold, Ulrich Meingast et al. 2006)

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Collaboration: SFB TRR 150

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Selected publications:

Birkhold, F., Ulrich Meingast, P. Wassermann and O. Deutschmann (2006). "Analysis of the Injection of Urea-water-solution for automotive SCR DeNOx-Systems: Modeling of Two-phase Flow and Spray/Wall-Interaction." SAE International.

Brack, W., B. Heine, F. Birkhold, M. Kruse, G. Schoch, S. Tischer and O. Deutschmann (2014). "Kinetic modeling of urea decomposition based on systematic thermogravimetric analyses of urea and its most important by-products." Chemical Engineering Science **106**(0): 1-8.