Experimental studies of multiphase chemical reactions in exhaust aftertreatment systems

Background: The complex interaction between turbulence / turbulent flow and chemical reactions under real conditions inhibits the optimization of technical systems presenting these properties. This applies especially to multiphase reactive flows in the vehicle exhaust gas system, such as the selective catalytic reduction (SCR) of nitrogen oxides by means of urea-water-solution.

Project: The goals of the project are the development of space- and time-resolved examination methods, experimental characterization of selective catalyst processes and the establishment of a data basis for validation of numerical simulations. The measurements will be performed in a new chemical reactor with improved optical access that will enable the application of laser diagnostic techniques. The modeling and numerical simulation of these phenomena require well-defined initial and boundary conditions which reproduce the essential aspects of the technical application. These features are considered in the design of the reactor.

Objectives:

In this project an experiment will be conducted to study multiphase reactive flows in a model exhaust system. The following information can be obtained from the experiments:

- Appearance and physical properties of fluid films, solid deposits and their dependence on the operating parameters
- Chemical composition of deposits
- Correlations between films, deposits, local temperatures and gas concentrations of the single phases.

Sub- and complete numerical models can be validated using the results of the measurements.

Approach:

A model chemical reactor, equipped with a commercial injector featuring two different outlet configurations, will be used to study selective catalytic reduction of nitrogen oxides in the exhaust gas of a lean burn diesel engine. Within this project the use of urea-water-solution is planned. Therefore, all the processes illustrated in Figure 1 will be examined. The lean exhaust gas contains all the relevant components i.e. nitrogen, water, oxygen, nitric oxides (NO, NO2). Carbon dioxide won't be added due to analytic reasons. It will be treated as an inert gas in the exhaust stream, which justifies this approach. Controlled heating and cooling of this model reactor will be provided. The temperature differences between gas, spray and wall influence the formation of the liquid film and solid deposits on the exhaust pipe wall. These differences are related to the ambient temperature and are caused by heat conduction as well as by convection. The measurements will be performed in the CATHLEN lab (CATalysis at High Temperatures Laser ENvironment) located at the Campus Nord of KIT (Großforschungsbereich).

In-situ laser spectroscopic methods will be applied to record spatially and temporally relevant data, i.e. temperature and gas concentration profiles. Methods to be applied are laser-induced fluorescence, Raman spectroscopy and the infrared laser absorption spectroscopy. Laser diagnostics will unravel the film and deposits formation processes in the SCR. Thus, correlations will be derived from data that have been recorded experimentally. The methods will face some considerable challenges when attempting to characterize and define process parameters due to simultaneously presence of gas/liquid//solid phases.

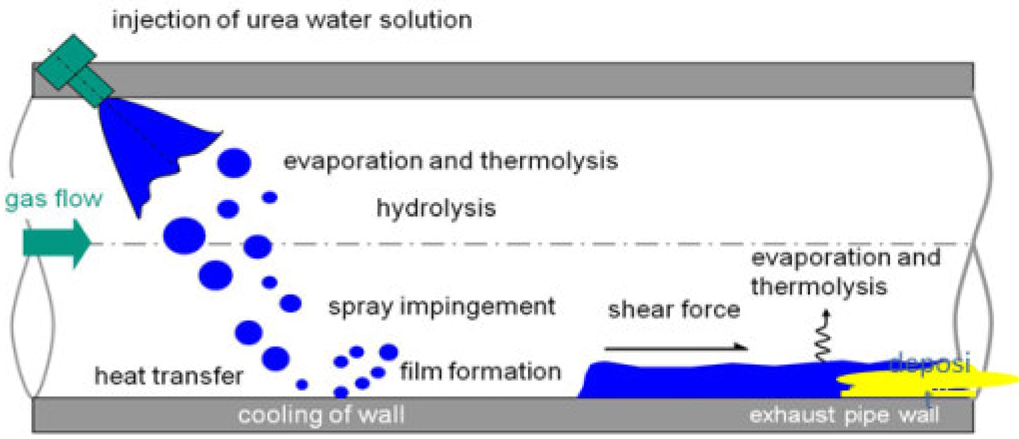
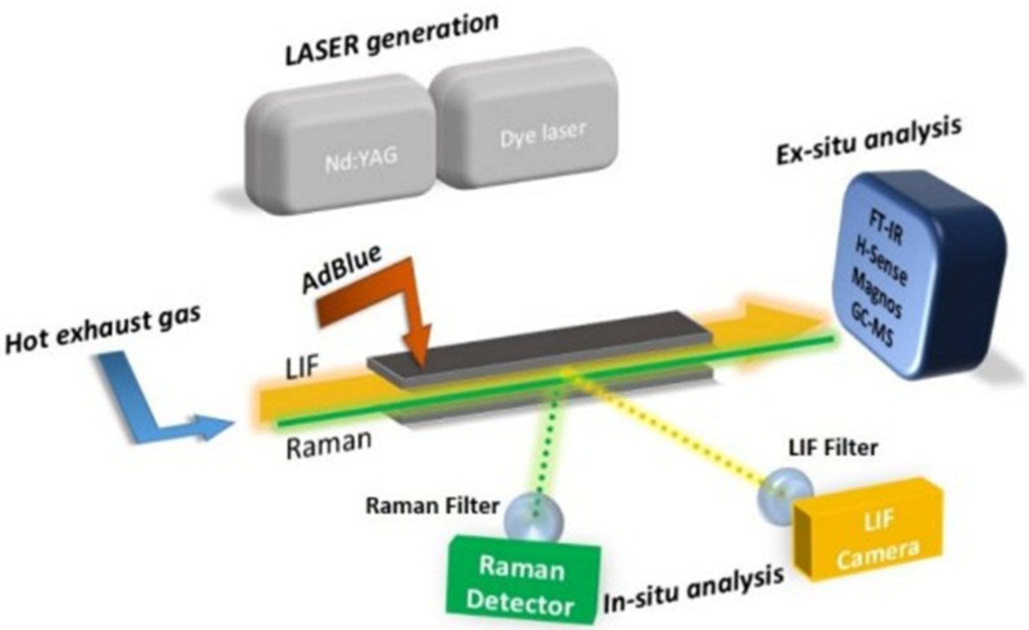


Fig. 1 Chemical and physical processes associated with the injection of urea-water-solution in a SCR catalytic converter

Further, ex-situ diagnostics will be applied at the CATHLEN-Lab to monitor the exhaust gas and characterize the solid deposits. Gas chromatography, mass spectrometry and FTIR- spectroscopy are already proved and tested in characterizing outflowing gas mixtures from other reactors. These techniques will provide information regarding of the minority species which cannot be directly measured by in-situ measurements. These methods can also be used for calibration and verification of the in-situ measured signals. Deposits and their decomposition products will be investigated by ex-situ thermogravimetric analysis (TGA) and differential thermal analysis (DTA). These experimental data sets are required to understand the multiphase reactive flows in the near-wall regions and serve for the validation and completion of the existing theoretical models for numerical SCR simulations.



Fig, 2 In-situ measuring equipment at the CATHLEN laboratory

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Funding: SFB/TRR150, Deutsche Forschungsgemeinschaft