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Gas phase reactions in diesel exhaust tract

Background: To meet the increasingly stringent emission standards, diesel vehicles currently mainly use a urea SCR (selective catalytic reduction) system for reduction of nitric oxides (NO_x). The precursor of the reducing agent is dosed into the exhaust pipe before the catalytic converter in the form of urea-water solution (commercial name AdBlue). The urea decomposes to the reducing agent ammonia (NH_3) and to isocyanic acid (HNCO) in the hot exhaust gas.

For optimal NO_x conversion at the so-called fast SCR conditions in the catalytic converter, the 1:1 ratio for NO/NO_2 and NH_3/NO_x is required. In diesel exhaust gas aftertreatment systems, the NO_2 amount is adjusted in the diesel oxidation catalyst, and according to the NO_x concentration in the exhaust gas, the urea-water solution is dosed in front of the SCR catalyst.

The increase of engine efficiency has led to a decrease of exhaust gas temperature, consequently the catalytic converters have been positioned closer to the engine to ensure the required temperature for catalytic converters. In addition, pre-turbine SCR is frequently used, in which the catalytic converter is positioned in front of the turbo charger. The increased temperature and pressure under pre-turbine conditions and the presence of NO_2 in the gas mixture bear the potential for non-negligible amounts of NO_x conversion or other reactions in the gas-phase. A possible change of the NO/NO_2 and NH_3/NO_x ratios, as well as HNCO-reactions in the exhaust pipe before the catalytic converter can lead to lower efficiency in the catalytic converter causing ammonia slip or NO_x emission. HNCO reactions are also important because of the significant role of HNCO in formation of urea deposits.

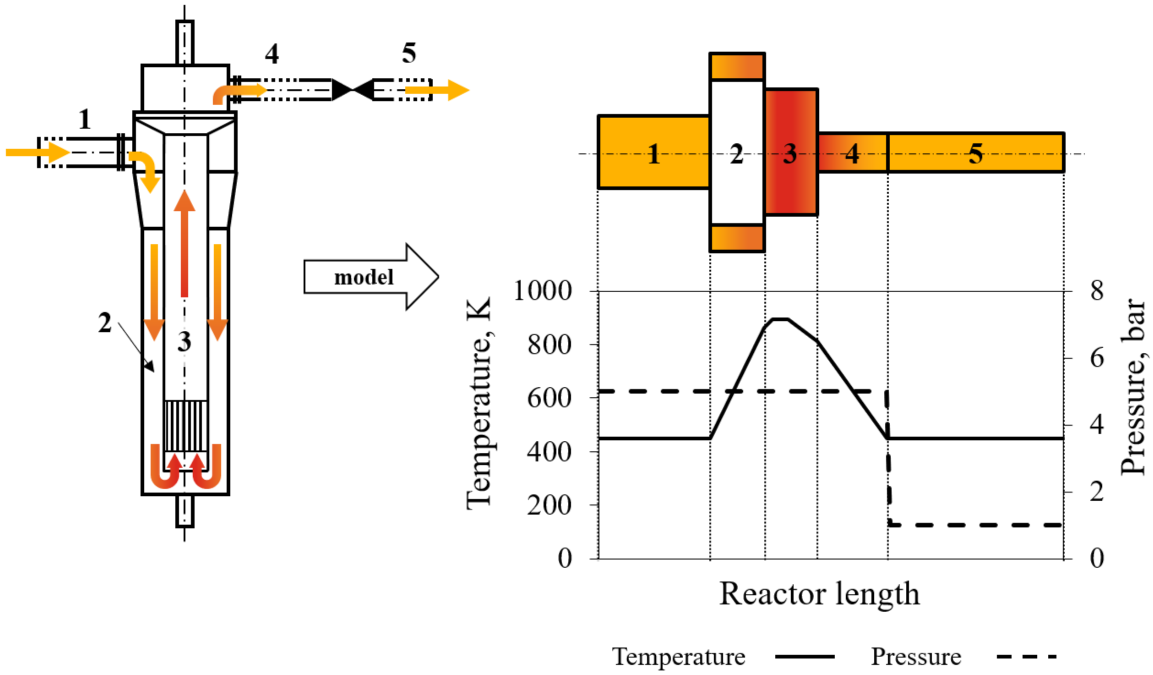

Figure 1 Schematic drawing of the experimental setup (left), plug flow model with the zone numbers used in the model and temperature-, pressure profile diagram of the measurement system (right). [1]

Project: In the current research, reactions of NH_3 with NO_x and HNCO with NO_x are investigated, focused on the effect of pressure (pre-turbine conditions) and on the effect of NO_2 in the gas mixture (Figure 2). For a better understanding of the chemical processes occurring, experiments are carried out and simulated with already published detailed reaction mechanisms (Figure 1). The development of a gas phase mechanism for HNCO reactions in the gas phase, relevant to diesel exhaust mixing is also part of the work. By analyzing the reaction paths, correlations in the reaction system of the gas mixture from the exhaust tract are also identified and explained.

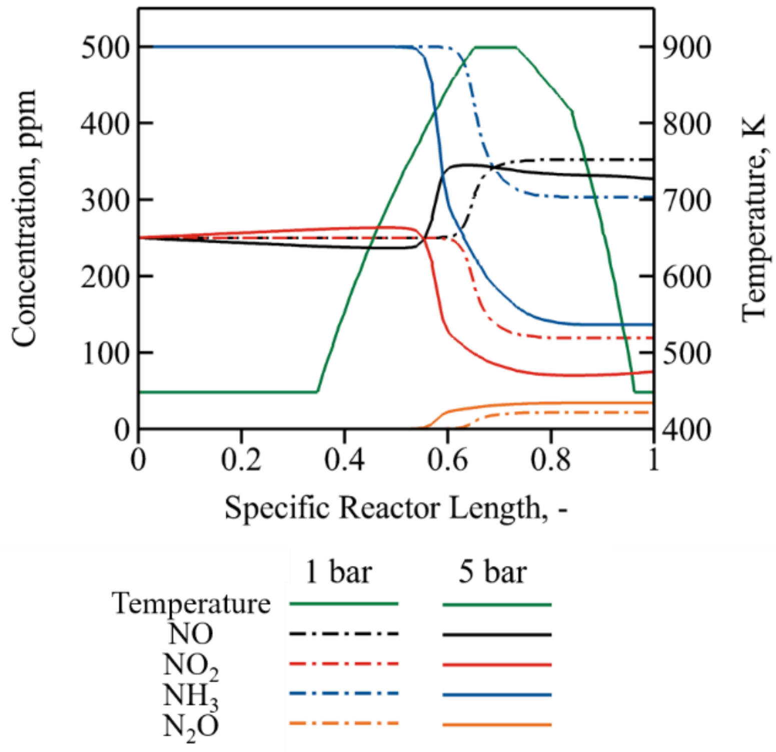

Figure 2 Simulated concentration profile along the reactor tube at 1 and 5 bar, 923 K reactor temperature, volume flow 12.6 L/min. Gas feed: 500 ppm NH_3, 250 ppm NO, 250 ppm NO_2, 10% O_2, 5% H_2O in nitrogen. [1]

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Publications:

1. Bertótiné Abai, A., Zengel, D., Janzer, C., Maier, L. et al., "Effect of NO2 on Gas-Phase Reactions in lean NOx/NH3/O2/H2O Mixtures at Conditions Relevant for Exhaust Gas Aftertreatment," *SAE Technical Papers* 2021, doi:10.4271/2021-01-5005.

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