Institute for Chemical Technology and Polymer Chemistry
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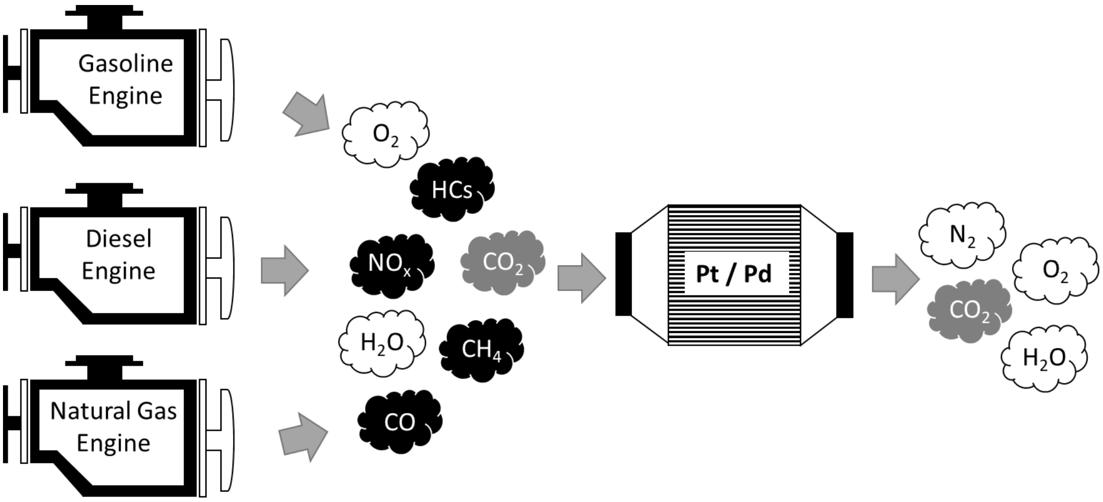
Master Thesis

Microkinetic Modeling for Exhaust Gas After-Treatment of Combustion Engines

Motivation/Background

The automotive sector has been related to the emission of various pollutants. The operating conditions of the gasoline and diesel combustion engines (air ratio, compression pressure, combustion temperature) and the fuel composition directly influence the composition of the raw exhaust gas. In addition to the products of complete combustion, namely water vapor and CO_2, the exhaust gas contains the CO, unburned and partially burned hydrocarbons (HC), nitrogen oxides (NO_x) and particles (particulate matter, PM). While the reduction of the CO_2 emissions is addressed by the improvement of the engine efficiency, the conversion of CO, NO_x and HCs to less harmful and more environmentally friendly gases is handled by the catalytic converter.

Even though a lot of efforts have been done in this area, the application of stricter regulations leads to the demand of a breakthrough in the design of the catalytic converter. Furthermore, the complexity of the catalytic system and its dynamic character in terms of structural modifications under various conditions necessitates the in-depth understanding of the catalytic system from the atomic level.



Description of Work

Scope of this thesis is the development of a reference microkinetic model for the emission control relevant applications. The reference mechanism will include sub-mechanisms for the oxidation of unreacted hydrocarbons and CO as well as the reduction of NO_x by CO under various conditions (e.g. lean conditions for Diesel Oxidation Catalysts). The catalysts in focus are Pt- and Pd-based catalysts. The initial detailed kinetic models of the sub-systems will be based on existing models in literature. The comprehensive analysis of the mechanisms will be conducted via reaction flow analysis and sensitivity analysis as well as numerical simulations under various reaction conditions by employing simulation tools. The comparison of the simulations with experimental results obtained in the exhaust gas center will enable the validation of the sub-mechanisms and the further development of the reference microkinetic model. Important aspect of the present thesis constitutes also the creation of a digital database of experimental and simulation results by using appropriate research data management tools.

Contact/Supervision

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