Modeling and Simulation of NO_x Abatement with Storage/Reduction Catalysts for Lean Burn and Diesel Engines

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Introduction

The unsolved problem of exhaust gas aftertreatment for diesel and lean burn engines still lead to enormous emissions of nitrogen oxides (NO_x). One of the most promising approaches is the NO_x Storage and Reduction Catalyst (NSR) which utilizes the NO_x storage on barium sites to form nitrates during the lean phase and their reduction to nitrogen in a rich atmosphere [1]. Detailed models, which are based on physical and chemical processes on the molecular level, are indispensable to exploit the full potential of this technique.

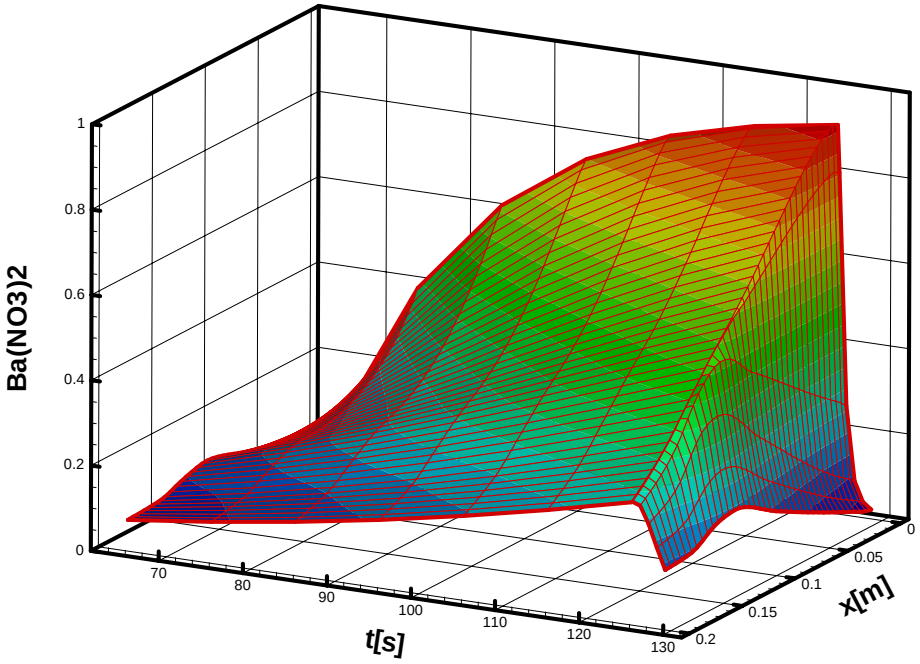
Numerical Model

The numerical simulations are carried out using the software package DETCHEM [2, 3], which uses detailed reaction mechanisms for the conversion on the noble metals and the storage and reduction processes on the barium particles. DETCHEM is a FORTRAN based package that is designed to couple chemistry models with Computational Fluid Dynamics (CFD) programs. It applies hierarchically arranged detailed models from an atomic scale up to reactor scale. The core is a library for the description of species properties based on atomistic models and for reactions among gas-phase and surface species based on elementary step reaction mechanisms. Upon this, the two-dimensional flow field in a single channel is modeled using the boundary-layer assumption. Radial transport models include composition dependent diffusion coefficients in the gas phase and an effectiveness factor approach for the washcoat. Inlet conditions and NO_x storage capacities of the single channel simulations vary in time.

Results

The present study aims at detailed insight into the processes on the catalyst surface and their interaction with the transport in the fluid flow at transient conditions by coupling the extensive description of the flow-field with elementary-step mechanisms on the noble metal catalyst [3] and the storage/reduction chemistry on barium. Based upon the reactions on the

noble metal and a shrinking core model for the NO_x storage [4], transient numerical simulations have been accomplished in order to predict the performance of the NSR in a temperature range from 250 to 450°C. The model predicts the experimentally measured concentration profiles in the lean as well as in the rich phase quite well. Simulated distribution of barium nitrate along the catalyst length as a function of time is obtained.



Axial and temporal profile of the simulated coverage with $Ba(NO_3)_2$ for a $Pt/Ba/Al_2O_3$ catalyst at 350°C

Literature

[1] Boegner, W., M. Kraemer, et al. (1995) Applied Catalysis, B: Environmental **7**(1-2): 153-71

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