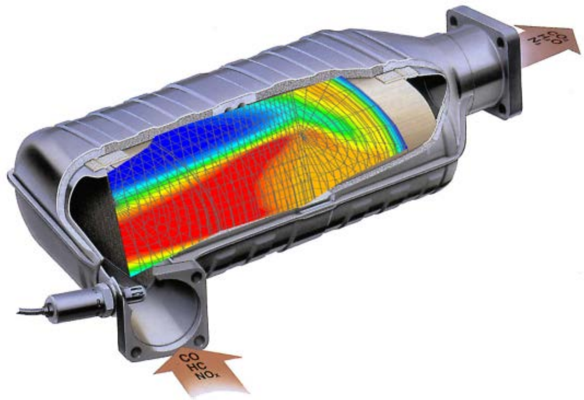
Three-way catalytic converters

Background: Three-way catalytic converters (TWCs) are the main technology for the reduction of tail-gas emissions in gasoline driven vehicles. Ever since their commercial market launch in the 1970s TWCs have become the most abundant technical catalytic reactors. Yet, increasingly stringent emission regulations induce ongoing research interest. A TWC consists of a ceramic support material; on its surface the catalytic active noble metals – namely platinum, rhodium and palladium – are embedded in a washcoat with high porosity. The catalyst enforces the oxidation of CO and unburnt hydrocarbons (HC) as well as the conversion of nitric oxides (NOx) to nitrogen. The efficiency of the pollutant reduction mainly depends on the operating temperature and feed composition. Both parameters are very volatile under real world traffic conditions, which is a challenge for a general optimization of the system.



TWC with simulated temperature profile, courtesy of J. Eberspächer GmbH & Co. KG

Project: Today's TWCs are a result of an evolution by test-bench experiments and numerical simulations. The latter have already helped to gain a fundamental understanding of the interactions between chemical reactions and transport processes. In general we have to consider four levels of modeling: the chemical reactions on the catalytically active particles, the transport of species in the porous washcoat structure, the flow of gases through channels of the monolithic structure, and temporal variations in the whole reactor system. Each of these processes can be covered by a large bandwidth of modeling detail depending on a judging between computational time and transferability of the results. However, for further simulation-based optimization of the system with respect to precious metal loadings and emissions we depend on both, speed and predictability. Our current research focuses on so-called zone-coated catalytic converters, where the washcoat consists of several layers of varying functionality and catalytic activity. The aim is to predict the influence of the spatial distribution of the catalytic components on the transient response of the TWC. In the long run this numerical model is a key step to design more resource-efficient converters.

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Funding: BMBF Project "Ressourceneffiziente Abgaskatalysatoren"

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