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Comparative simulation of reactive flow in catalytic filter using 3D pore-scale model on CT image and 1D effective model

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In order to improve the performance of the exhaust after treatment system and keep reasonable complexity, the number of the used devices is reduced by enhancing wall flow particulate filters with a catalytic functionality, like selective catalytic reduction in diesel or three way catalysis in gasoline vehicles. In this case the solid matrix of the filtering media consists from inert grains and active grains. For the simulation of such devices, effective 1D models are regularly used, because they are relatively simple and fast in comparison to higher dimensional models, while reproducing most of the experimentally observed phenomena with sufficient accuracy. The reduction of the complexity in the modeling, however, is achieved by introducing many simplifying assumptions.

As it will be seen in this presentation, 1D models do not always reproduce detailed 3D simulations. Here we compare a standard 1D homogenous wall model with a 3D pore-scale model. The latter describes convection and diffusion in the pores and in washcoat grains, and absorption in the washcoat grains. In fact, washcoat particles are nanoporous and surface reaction (adsorption) occurs at this scale. Softare tool called PoreChem [1] has been used for simulating the reactive flow at pore scale. A wall segment of a real particulate filter was used in the simulation. The three dimensional structure of the wall segment was obtained by X-ray microtomography, in which we resolved the different materials: Pores, (inert) Substrate and (active) Washcoat. A first order reaction was studied to examine if 1D simulations based on effective (Darcy scale) model can describe the behavior of a catalytic filter wall sufficiently well. In simulations the adsorption rate constant varied while the other properties, like temperature and flow speed remained constant. The conversion (adsorbed amount) was computed for different reaction rate. The discrepancy between the results obtained with the 3D and 1D models increase with higher reaction rates. They are caused by the inhomogeneous flow and washcoat distribution in the 3D system that cannot be described well with a homogenized 1D model. 3D models are therefore useful to optimize the microstructure of catalytic particulate filters.

References

[1] Iliev, O., Lakdawala, Z., Neßler, K. H., Prill, T., Vutov, Y., Yang, Y., & Yao, J. (2017). On the Pore-Scale Modeling and Simulation of Reactive Transport in 3D Geometries. Mathematical Modelling and Analysis, 22(5), 671-694.

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Primary authors: Mr GREINER, Robert (Technische Universität Darmstadt and Umicore AG & Co. KG); Dr PRILL, Torben (Fraunhofer ITWM); Prof. ILLIEV, Oleg (Fraunhofer ITWM, Kaiserslautern, Germany); Dr VAN SETTEN, B. (Umicore AG & Co. KG); Prof. VOTSMEIER, Martin (Umicore AG & Co. KG)

Presenter: Prof. ILLIEV, Oleg (Fraunhofer ITWM, Kaiserslautern, Germany)

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