Influence of the macropore structure on heat and mass transfer inside catalytic washcoats

Martin Kutscherauer[1], Gregor D. Wehinger [1]

[1]Institute of Chemical Process Engineering, Karlsruhe Institute of Technology, Karlsruhe, Germany

E-Mail presenting author: martin.kutscherauer@kit.edu

Technical reduction of pollutants and greenhouse gases is mainly preformed in catalytic coated monolith reactors. The catalytic performance of such reactors is strongly influenced by heat and mass transport limitations within the washcoated catalyst layer. Spatial resolved modelling of these systems can contribute to improve process understanding and to optimize reactor and catalyst design. However, it is challenging due to the multiscale nature of the reactor [1]. In this contribution, the impact of the macroscopic pore structure of a catalytic coated layer on heat and mass transfer is numerically studied. Realistic pore structures with different properties are generated synthetically and analyzed with the Python package PoreSpy [2]. Figure 1 shows results of CFD simulations (left) for two different macropore systems with equal porosity but different pore radius distributions (center) and the effect on the fluid-solid heat transfer coefficient α (right). In the future, catalytic reactions will be included to study heat and mass effects on reactor performance.

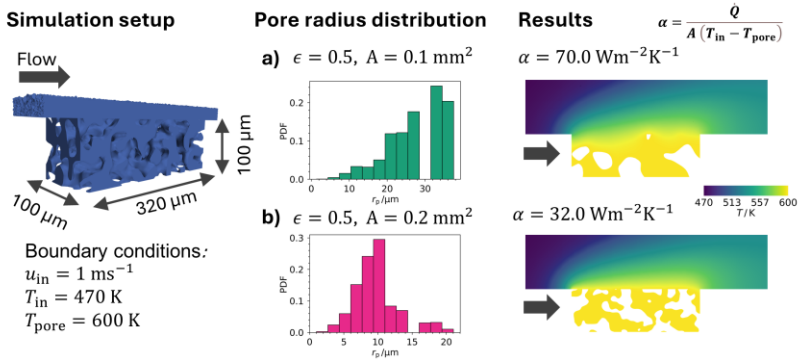

Figure 1: CFD simulation set up (left), pore radius distribution (center), temperature field at a plane through the pore system and calculated heat transfer coefficient α (right) for two different macropore systems. Left to right arrow indicates direction of flow.

[1] G. D. Wehinger et al., *Chem. Eng. Res. Des.* 2022, **184**, 39-58. DOI: 10.1016/j.cherd.2022.05.030.

[2] J. Gostick et al., *J. Open Source Softw*. 2019, **4 (37)**, 1296. DOI: 10.21105/joss.01296.