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On pore scale simulation of reactive flows in the case of complex catalytic reactions

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Pore scale simulation of reactive flows is a challenging and computationally intensive problem, especially in the case of complex reactions. In many applications, the complicated chemical reactions are handled via coupling a transport solver to a proper software tool for chemistry, e.g., such as ChemKin, Phreeqc. Reactoro. The practice, however, shows that such simulations can be very time consuming, and often are subject to severe time step restrictions.

Furthermore, it is an open question when the upscaling of reactive flow through thin porous media (e.g., filter membrane) is possible. While there are a lot of discussions when this can be done for single phase flow depending on the size and number of pores, there is a lack of understanding in the case of passive and reactive transport through thin porous media. In a recent paper [1] a simulation of reactive transport in a 3D CT image of a piece of a wall of a catalytic filter was performed for the case of simple first order reaction. It was shown that the particular problem can not be upscaled and only pore scale simulations can help to understand the performance of the filter. Our goal is to investigate reactive flow in catalytic filters on synthetic geometries, as well as on 3D CT images of real geometries, in the case of complex reactions. The first step toward achieving this goal is to develop efficient algorithms for pore scale simulation in the case of complex reactions. Our current results on this task are the subject of this presentation. Results from the numerical simulation will be presented and discussed.

Time Block Preference

Time Block C (18:00-21:00 CET)

References

[1] R. Greiner, T. Prill, O. Iliev, B.A.A.L. van Setten, M. Votsmeier. Tomography based simulation of reactive flow at the microscale: Particulate filters with wall integrated catalyst. Chemical Engineering Journal, 378, 2019, 121919

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