Contribution ID: **406** Type: **Oral Presentation**

FEATURES OF THE PORE SCALE REACTIVE FLOW WITH COMPLEX CATALYTIC REACTIONS

Monday, 30 May 2022 16:35 (15 minutes)

Most of the papers discussing pore scale simulation of reactive flow consider synthetic 2D geometry and/or simple reactions. On macroscale the engineers mostly use heuristically derived equations, for which the area of applicability is not clearly defined. Studies on the size of the Representative Elementary Volume, REV, are rarely presented for reactive flow, with effective coefficients computed as a function of the solution of microscale cell problems. A reason for this is the fact that pore scale simulation is a computationally intensive problem, especially in the case of complex reactions, and there is a lack of efficient algorithms for such problems.

A related question is when the upscaling of reactive flow through thin porous media (e.g., membranes) is possible. While there are a lot of discussions when this can be done for single phase flow depending on the pore size distribution, there is a lack of understanding in the case of passive and reactive transport through thin heterogeneous porous media. In [1] it was shown that a particular problem –reactive flow through real catalytic filter (converter), can not be upscaled, and only pore scale simulations can help to understand the performance of the filter in this particular case. Obviously, for other micro geometry or other process parameters upscaling might be possible.

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, Cantera end etc. The practice, however, shows that such simulations are very time consuming, and often are subject of severe time step restrictions

In the case of complex catalytic reactions the question about REV is much more difficult due to the presence of different reaction time scales. Our goal is to investigate reactive flow in catalytic filters on real and realistic geometry and 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.

We are developing an integrated solver for transport and reactions. Different coupled and splitting approaches are investigated, together with adopting proper methods for stiff ODEs when needed. Results from numerical simulation of reactive flow in catalytic porous converter on real and realistic geometries for different flow and reaction regimes are presented and discussed.

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References

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

Time Block Preference

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

Participation

Online

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