Pore scale simulation of reactive flow for industrial and environmental problems

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Reactive flows in porous media are important processes in many industrial and environmental applications. The reactive transport in porous media is influenced by the pore scale interplay between convection, diffusion and reaction, coupled with the heterogeneity of the pore space (e.g., pore size distribution and connectivity) and chemical heterogeneity.

A 3D pore-scale mathematical model describes convection and diffusion in the pores together with heterogeneous (surface) or homogeneous (volumetric) reactions. Some media can be considered as two scale (micro scale and macro scale) ones, where the size of the resolved pores defines the micro scale, and the size of the porous domain as effective (averaged, homogenized) media defines the macro scale. Example are functionalized materials (e.g., those used in water purification). Other media can be considers as three scale ones. In addition to the two scales defined above, one considers also nano scale. Examples are, e.g., catalytic filters, air and water filters exploiting granulated active carbon particles, etc. In this case the catalyst (washcoat) particles and the active carbon particles are nano porous. Resolving simultaneously all three scales is not feasible on the existing computers, therefore a common approach is to build computational domains with resolved microscale pores, and to consider the nanoporous materials as effective (averaged) porous media.
To perform the pore-scale simulations for the above described problems, Fraunhofer ITWM has developed PoreChem, [1, 2], a software package dedicated to the simulation of reactive flow in the case of heterogeneous or homogeneous reactions. It enables the simulation of reactive flows in resolved porous media in a reasonable time. The software can compute the flow of a fluid in the pore space, as well as the diffusive and advective transport of solute species. The flow is computed by solving the Navier-Stokes-Brinkman system of equations with a finite volume discretization on a regular voxel grid. The geometries are usually coming from CT imaging technique, virtually generated images are also considered. The reactive transport is simulated by solving the reaction-diffusion-advection equation using the same space discretization. Different reaction kinetics, parametrized by reaction isotherms can be taken into account. The fast voxel based solver enables calculations directly on CT-Images. Transient phenomena can be simulated, as well as steady state ones.

Pore scale simulations for two industrial problems will be presentated in this talk. Most attention will be paid on simulation for catalytic filters (in particular, diesel pariculate filter, DPF) [3]. The computational domain comes from a CT image of a piece of a manufactured filter. The role of the pore connectivity (manifested in channeling effects) and of the chemical heterogeneity (caused by the non-uniform distribution of the washcoat particles) will be discussed in details. Simulations with a generated, more homogeneous image, will also be presented. Further on, simulations for surface activated nonwoven filtering material will be also demonstrated.

Finally, some conclusions will be drawn, open questions will be formulated, and the forthcoming developments will be shortly announced.

References

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