

ON NUMERICAL SIMULATION OF REACTIVE FLOW IN POROUS MEDIA

Torben Prill¹, Oleg Iliev¹, Martin Votsmeier², Robert Greiner²

¹Fraunhofer Institut für Techno- und Wirtschaftsmathematik
(ITWM), Kaiserslautern,

torben.prill@itwm.fraunhofer.de

²Umicore

We discuss numerical simulation of reactive flow in porous media in case of surface (heterogeneous) and volumetric (homogeneous) reactions for geometries arising from 3D micro-CT images. A software tool, PoreChem, capable of direct numerical simulation at pore scale, as well as for solving cell problems defined in homogenization algorithms, is presented. Solutions of 3D pore-scale problems and respective macroscale models are compared to demonstrate the potential of the software in upscaling algorithms, as well as to identify the area of applicability of the homogenization approach. As an application we consider catalytic filters for automotive industry.