Pore scale modeling and simulation of flow and reactive transport on 3D CT images

O. Iliev [1], T. Prill[1], K.Nessler [2], Z. Lakdawala [3], G. Printsypar [4] , Ya.Vutov [5]

[1] Fraunhofer ITWM
[2] TU-Kaiserslautern
[3] DHI-WASY
[4] KAUST
[5] IICT-BAS

Abstract

Fibrous and sponge filtering media, as well as numerous other natural and technical porous media, usually have complex microstructures. In all applications, and in particular in filtration, the morphology of the filtering media influences its performance in one way or another. This is especially true for surface activated filtering media. Understanding the flow, transport and reaction/adsorption processes at the pore scale is important for explaining and interpreting the overall performance of such filtering media. In certain cases an effective media approach, which accounts for the membrane morphology in an average way (e.g., via porosity) can provide useful information. However, increasing the filtration efficiency needs a more detailed knowledge of the impact of the microstructure. Mathematical modelling and computer simulations are useful approaches, supporting researchers and manufacturers in their work on designing better filtering media and on selecting appropriate ones for a particular application.
Here we present simulation results for sponge functionalized membranes and for surface activated fibrous web. The microstructures can come either from 3D computer tomography (CT), or can be generated with specialized software tools (e.g., GeoDict). Navier-Stokes equations are used to describe the flow, the solute/contaminant transport is described by a convection-diffusion equation with reactive boundary conditions. The surface adsorption/reaction is modeled with Henry or Langmuir isotherms. Results from computer simulations are presented and discussed.

The developed algorithms and software are applicable to a broad class of scientific and industrial applications, where the morphology of the porous media has a significant impact on the studied flow and reactive transport.