## 3D simulations of gas transport in porous media with adsorption and comparison to 1D models

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**Abstract:** Fluid flow and mass transport in porous media involving mass transfer between the fluid phase and the solid matrix occurs in a great variety of applications. One such application is capturing a contaminant from a carrier fluid forced through a porous adsorbing bed. Describing this process in realistic 3D porous geometries is complex. A standard approach involves reducing the governing equations describing the process to one spatial dimension via averaging procedures [1, 2]. These models can be solved analytically in some limiting cases. The obtained solutions can be implemented in optimisation routines to find unknown parameters of the process such as the adsorption rate [3]. However, the details of the 3D microstructure are difficult (or impossible) to capture in 1D models and they are often lost in the averaging procedure. This makes it difficult to analyse the possible effects of the microstructure in the adsorption process. In this talk, we will formulate and solve a 3D mathematical model of contaminant capture by adsorption in 3D idealised porous media. The results of the simulations will be compared with the solutions of averaged 1D models. We will show how structure-related features such as porosity and structure homogeneity affect the adsorption process

## **References:**

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