

CONTINUUM AND DISCRETE MODELS OF ADSORPTION AT PORESACLE AND CORESCALE

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Porescale modeling has reached a stage where computational models are able to simulate very complex physics occurring in fluid and solid phases. It is now possible to study effects beyond first order which may have a significant impact on the pore-scale itself and on the up-scaled models of first order phenomena. Examples include reactive transport upscaling from core to pore and modeling of flow and transport with a large range of flow rates. The scientific significance of the findings depends however not only on the size of representative volumes but also on the required level of detail in representative geometries which is inversely proportional to the computational complexity of porescale models. In this talk we focus on flow and transport with adsorption. When accounting for adsorption in continuum models at corescale and beyond, we typically use adsorption equilibrium or kinetic models associated with one of IUPAC canonical types and known isotherms. At porescale however the physics of adsorption is obviously quite different, and various continuum and discrete statistical mechanics models have been proposed. A successful computational model needs to be general enough to allow for multiple components, threshold phenomena and hysteresis, microporous diffusion, evolution of pore-space and so on. In addition, it should remain stable with respect to the coarseness of the porescale geometry and provide information useful for upscaled models. We discuss several computational models and provide perspectives on these issues.