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# Transient and stationary transport of adsorbing pollutants in model porous media

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Departments of adsorption thermodynamics and kinetics and their influence on the different transport regimes

Understanding the transport of pollutants inside different porous structures remains a complex task as pollutants can adsorb to the solid surface following specific underlying adsorption kinetics. Transport is dominated by the pollutant specific adsorption behaviour coupled to the porous structure. We investigated the coupling between transport and adsorption in a two-dimensional regular porous medium by means of an extended Lattice Boltzmann approach [1-4]. We focused on the behaviour of molecules following: (1) the Henry model in which the adsorbed quantity is proportional to the adsorbate concentration and (2) the Langmuir model that describes monolayer adsorption and accounts for surface saturation.

The effect of the adsorption/desorption parameters on the transport behaviour in model porous media was investigated. For all adsorption conditions, we observed the three well-known transport regimes: diffusion-dominated regime (small times), transient regime (intermediate time range) and Gaussian or nearly Gaussian dispersion regime (large time range). However, there were important differences induced by the adsorption models. Particularly transient regimes, characterized by an asymmetric concentration profile, strongly depend on system parameters [5]. Concentration profiles become Gaussian (or nearly Gaussian) in the asymptotic long-time regime when the dynamical adsorption equilibrium is reached. We observed that the characteristic time to reach this equilibrium depends on the system's parameters and can be very long. In practice, such results may explain experimental observations where transport is found to be non-Gaussian even at a very large time scale. Consequently, for a better evaluation of pollutant transport in the subsoil or in water remediation processes it is crucial to consider the long-lasting transient regimes.

#### **Biography**

Daniela Bauer has her expertise in modelling flow and transport problems in porous media. She is particularly interested in the transport behaviour of adsorbing molecules. She focuses on the different adsorption thermodynamics and kinetics and their influence on the different transport regimes. Her flow and transport simulations are performed by means of an extended Lattice-Boltzmann code accounting for adsorption.

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