Spatial homogeneity analysis of packed bed chromatography

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Packed bed chromatography is usually modeled in one or two spatial dimensions, for example by the general rate model. Such models assume that fluid flow and solute molecule concentrations are homogeneously distributed over column cross sections. Moreover, concentration gradients within the beads are at most considered along the radial coordinate.

These homogeneity assumptions are studied with a three-dimensional model of the involved convection, diffusion and adsorption processes. Due to the complex geometry only bed sections with up to several hundred spheres can be computed without using supercomputers. Hence, a sphere packing algorithm was modified for cuboids with periodic boundaries perpendicular to the fluid flow.

The resulting concentration profiles indicate that the studied homogeneity assumptions are valid in many cases, even though complex flow profiles are observed in the interstitial volume. However, dominant wall effects justify the computational effort of spatially resolved simulations for small columns with volumes on the micro-liter scale.