Simulation of Chemical Separation Processes Using the Lattice-Boltzmann Method

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The separation of chemical species through adsorption, membrane separation, extraction, distillation, etc. is enhanced at the microscale due to the reduced length scales for diffusion transport. The ability to accurately simulate the performance of microscale separation devices, and the high level of detail provided by simulations, results in efficient design and optimization.

The lattice-Boltzmann simulation method provides accurate flow and thermal predictions for microscale systems with complex geometries. In addition, surface force terms can be included to model discreet liquid-vapor and liquid-liquid phase interfaces and surface adsorption. Although these effects are usually negligible in macroscale flows, they can dominate the behavior of flow in microscale devices. In addition to modeling multiphase systems, the lattice-Boltzmann method is expanded to include multiple chemical species with convection and diffusion transport. Each species is represented by a separate field and the diffusion coefficients can be independently specified. The ability to model multiple species is essential to simulating fluid reactor and separation systems. The chemical species model is verified by comparing simulation results with known analytical solutions. Results from simulations of actual microfluid systems will also be presented and compared with available data on system performance.