**Lattice Boltzmann method for pore scale flow and multi-physicochemical processes: Structure reconstruction and multiscale modeling**

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**Abstract:**

Mutli-physicochemical transport phenomena in porous and composite materials are everywhere found, particularly in various energy, earth and environment systems. Because of complexity and versatility of these materials the transport phenomena as well as the microstructures or the phase distribution can turn out to be a major challenge. Reconstruction algorithms, based on internal microstructure and geometry morphology, are developed for various (like granular, fibrous, open foam) heterogeneous multiphase complex structured porous materials. Lattice Boltzmann Method (LBM) is a kind of mesoscopic method based on statistical physics framework it is very beneficial for solving such type of problems involving multiple inter-particle interactions and complex geometry boundary conditions. The Lattice Boltzmann method and combined LBM and FVM (finite volume method) is adapted to solve various multi-scale diffusion, convection as well as diffusion-convection-reaction problems.

Initially lattice Boltzmann method is established to simulate fluid flow, mass transport and heat transfer through various building materials at pore scale level. The effect of Knudsen as well as surface diffusion is highlighted and obtained results of effective mass as well as heat diffusion coefficient are compared with experimental data

Then hybrid LBM- FVM is developed to study three different processes (i) VOC diffusion (ii) natural convection (iii) diffusion-convection-reaction problems. Flux balance approach and reconstruction operators for density–velocity distribution function and for concentration distribution function are used to transfer macroscopic variables (FVM) to distribution functions (LBM). Finally transport phenomena in complex porous GDL (gas diffusion layer), catalyst layer (CL) and GC (gass channel) will be discussed briefly.