Commun. Comput. Phys.
doi: 10.4208/cicp.361011.260112s

Vol. **13**, No. 3, pp. 801-822
March 2013

Validation of Pore-Scale Simulations of Hydrodynamic Dispersion in Random Sphere Packings

Siarhei Khirevich, Alexandra Höltzel and Ulrich Tallarek*

Department of Chemistry, Philipps-Universität Marburg, Hans-Meerwein-Strasse, 35032 Marburg, Germany.

Received 31 October 2011; Accepted (in revised version) 26 January 2012

Available online 29 August 2012

Abstract. We employ the lattice Boltzmann method and random walk particle tracking to simulate the time evolution of hydrodynamic dispersion in bulk, random, monodisperse, hard-sphere packings with bed porosities (interparticle void volume fractions) between the random-close and the random-loose packing limit. Using Jodrey-Tory and Monte Carlo-based algorithms and a systematic variation of the packing protocols we generate a portfolio of packings, whose microstructures differ in their degree of heterogeneity (DoH). Because the DoH quantifies the heterogeneity of the void space distribution in a packing, the asymptotic longitudinal dispersion coefficient calculated for the packings increases with the packings' DoH. We investigate the influence of packing length (up to 150 d_p, where d_p is the sphere diameter) and grid resolution (up to 90 nodes per d_p) on the simulated hydrodynamic dispersion coefficient, and demonstrate that the chosen packing dimensions of $10\,d_p \times 10\,d_p \times 70\,d_p$ and the employed grid resolution of 60 nodes per d_p are sufficient to observe asymptotic behavior of the dispersion coefficient and to minimize finite size effects. Asymptotic values of the dispersion coefficients calculated for the generated packings are compared with simulated as well as experimental data from the literature and yield good to excellent agreement.

PACS: 47.56.+r, 81.05.Rm, 05.40.-a, 61.43.Bn, 02.60.Cb

Key words: Packing microstructure, degree of heterogeneity, packing algorithm, hydrodynamic dispersion, random sphere packings.

1 Introduction

Mass transport in porous media is a central research theme in science and engineering, affecting such diverse fields as, e.g., separation of chemicals by chromatography, catalytic

*Corresponding author. *Email addresses:* khirevic@staff.uni-marburg.de (S. Khirevich), hoeltzel@staff.uni-marburg.de (A. Höltzel), tallarek@staff.uni-marburg.de (U. Tallarek)

reactions using fixed-bed adsorbents, migration of soil pollutants, and water recovery. Deriving morphology-transport relations to predict the transport properties of a porous medium from its pore space structure is therefore of fundamental as well as applied interest [1, 2]. The central structure-transport relationships can be established based on experimental data from high-resolution techniques that enable the physical reconstruction of a porous medium, such as X-ray tomography [3–5], nuclear magnetic resonance imaging [6], and confocal laser scanning microscopy [7, 8]. A real porous medium is the result of its formation process and has definite properties that cannot be altered at will by the researcher. Contrariwise, computer-generated models of porous media, such as random sphere packings (particulate fixed beds, in general), allow the systematic variation of packing properties (e.g., the final bed density, the particle porosity, as well as particle shape and size distribution functions) independent of other parameters. Random sphere packings, for example, can be computer-generated with high reproducibility over a range of bed porosities (interparticle void volume fractions), which is a pre-requisite to study the porosity-scaling of the transport coefficients for hydraulic permeability, effective diffusion, and hydrodynamic dispersion [9–11]. Another consideration is the observation of asymptotic behavior of the mass transport coefficients in the simulations, which requires packing models of sufficient size. As of now, samples that fit this requirement are difficult to obtain by physical reconstruction, whereas large computer-generated packings are readily available. The benefit of performing hydrodynamic dispersion simulations up to the asymptotic limit lies in the unequivocal meaning of the time-independent values of the transport coefficients. Only asymptotic values can be compared with certainty, which is of particular importance when packings with systematically varied DoH are studied, and asymptotic values for the mass transport coefficients are also needed to fit equations that link specific structural features of a porous medium to its (effective) mass transport properties [12].

The complex solid-liquid boundaries characterizing the pore space of a porous medium (whether a reconstructed sample or a computer-generated model) and the large model size required to observe asymptotic behavior of the mass transport coefficients needs supercomputing resources to perform pore-scale simulations of advective-diffusive transport. In this work, we perform pore-scale simulations of hydrodynamic dispersion in bulk (unconfined) random packings of uniform, hard spheres. These packings mimic infinitely wide, randomly packed beds without walls, and our simulations therefore selectively address bulk transport properties. A set of packings with targeted bed properties (final packing density, systematically varied DoH) are generated with two principally different algorithms, and fluid flow and advective-diffusive mass transport inside the packings' void space is simulated by the lattice Boltzmann (LBM) and random-walk particle-tracking (RWPT) methods, respectively. LBM and RWPT are attractive for use on supercomputers, because their local update rule minimizes the information transfer (communication time) between the processing units during execution of a parallel program, leaving the maximum amount of computation time for the calculations.

In this work we are interested in quantifying hydrodynamic dispersion resulting from