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A combined path-percolation – Lattice-Boltzmann model applied to multiphase mass transfer in porous media

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ABSTRACT

In this work, single-component single-phase, and single-component multi-phase Lattice-Boltzmann models were developed to investigate the effects of liquid formation on mass transfer in porous channels via path-percolation theory. A two-dimensional lattice with nine velocity components was used in both Lattice-Boltzmann models. A confidence level of 99% was utilized to obtain statistical results of porosity, effective porosity, and tortuosity of the system with 0%, 10%, and 20% liquid formation. Velocity distributions in randomly generated inhomogeneous porous channels with different solid–liquid–vapor combinations were analyzed. The statistical results show that the porosity range of the initially generated porous media lies between the specified error limit of 0.001 determined by the confidence level study for all three cases with 70%, 80%, and 90% target porosity. When target porosity decreases, the difference between porosity and effective porosity increases, and the effective porosity range gets wider than the range of porosity. Effective diffusion coefficient decreases with increase in liquid formation, since the effective porosity decreases. An application programming interface called OpenMP was implemented on the developed serial in-house program and the effects of 1–4 threads on program performance and efficiency were investigated. The maximum speedup and performance gained are 3.3553 and 1.275 GFlops for 4 threads of a personal computer with a 38.4 GFlops peak performance.

1. Introduction

The Lattice-Boltzmann equation was derived by Ludwig Boltzmann in 1872, and is counted as the cornerstone of the kinetic theory of gases [1]. The Lattice-Boltzmann Method (LBM) is an explicit technique based on Ludwig Boltzmann's kinetic theory of gases [2] used to simulate transport equations. In kinetic theory, a statistical treatment is performed for fluid particles, and the actions of these particles are described by streaming and collision mechanisms. Detailed information about the kinetic theory of gases can be found in references [1–4]. The LBM treats a group of particles as a lattice unit and investigates the behavior of the units in the system. In terms of computational fluid dynamics, LBM can be used to simulate single and multiphase flows, and in this study it was applied to simulate two-phase momentum transfer in porous media. Many studies with multi-phase LBM in porous media can be found in literature [5–13]. Among these, the authors decided to develop a single-component multiphase (SCMP) LBM model similar to that in the study of Chau et al. [14]. They used a two-dimensional, SCMP LBM code to investigate the effects of gravity on liquid formation, hence the gaseous diffusion in partially saturated porous media. They found that the relative (effective) diffusion coefficient shows about a 25% difference between different liquid configurations under zero gravity. The target of the current study is observing the effects of liquid formation on diffusivity by determining the effective porosity and tortuosity in randomly generated inhomogeneous porous channels with 0%, 10%, and 20% liquid formation based on a statistical point of view.

A statistical based "path-percolation theory" was developed by Jung et al. [15] to investigate the electrical property variations in inhomogeneous porous media. A process called "cluster labeling" was applied for a path determination scheme. Cekmer et al. [16] applied this theory with a combination of a single-phase Lattice-Boltzmann model to investigate the mass transfer in randomly generated inhomogeneous porous media. A new effective diffusion model was developed in terms of effective porosity obtained by eliminating the orphan pores, which were not connected to the

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Nomenclature

a	a parameter to include intermolecular attractive force into the van der Waals equation of state (m^6 Pa/mol^2)
b	a parameter to include the effects of non-negligible molecule volume into the van der Waals equation of state (m^3/mol)
CL	confidence level
c	unit lattice velocity (m/s)
c_s	unit lattice sound velocity (m/s)
D_{bulk}	bulk diffusion coefficient (m^2/s)
D_{eff}	effective diffusion coefficient (m^2/s)
F	intermolecular force (N)
f	the probability distribution function
f^{eq}	equivalent distribution function
G	intermolecular interaction strength
k	lattice index
N	number of floating point operations in the code
N_{RAE}	number of the representative area elements in a statistical representative area element set
n	total history number
n_c	number of threads used in parallel code
n_m	number of moles of the fluid
P	pressure of the fluid (Pa)
P_{peak}	peak performance of the computer (FLOP/s)
Pr	probability of any event to occur
p	the probability of a pore to occur in a node
q	the probability of a solid to occur in a node
R	gas constant of the fluid (J/mol K)
S	speedup
T	temperature of the fluid (K)
T_1	runtime of the code with a single thread (s)
T_{n_c}	runtime of the code with n_c threads (s)
t	time (s)
u	velocity, $u = \sqrt{u_x^2 + u_y^2}$ (m/s)
u_x	velocity in horizontal direction (m/s)
u_y	velocity in vertical direction (m/s)
V	volume of the fluid (m^3)
w	weighting factor of the lattice components
$\hat{X}$	arithmetic average of any property
x	horizontal distance (m)
y	vertical distance (m)
z	any parameter inside the error function

Greek letters

ε	error between the true and estimated probabilities of an event
$\varepsilon_{parallel}$	efficiency of the parallel code
ρ	density of the fluid (kg/m^3)
ρ_0	an arbitrary parameter (kg/m^3)
τ	tortuosity
τ_{eff}	effective tortuosity
ϕ	porosity
ϕ_{eff}	effective porosity
ψ	intermolecular interaction potential
ψ_0	an arbitrary parameter

Double-struck letters

$\mathbb{G}$	Gaussian function

pathways between the inlet and outlet of a channel. This model was also tested and compared with two well-known diffusion models [17,18]. In this study, the path-percolation theory was utilized to generate random inhomogeneous porous channels and determine the effective porosity after liquid particles plugged some of the paths for the particles in vapor-phase.

In addition, an application programming interface called open multi-processing (OpenMP) was implemented to the code to gain higher performance and speedup, which is defined as the runtime ratio of the codes with single- and multi- threads. OpenMP was applied to solve SCMP LBM for many representative area elements of random porous channels by multi threads simultaneously instead of sharing a single LBM simulation to avoid the time lost by message passing between the nodes. However, the main novelty of this article is its statistical results of multi-phase effective diffusion process for a number of different solid–vapor–liquid configurations determined by the confidence level studies.

The motivation of this work is to develop a statistical based diffusion behavior estimation of two-phase systems in inhomogeneous porous media, following on previously developed work valid for single-phase flow only [16]. This work will provide a better understanding of the effects of internal structure of the porous channels on multi-phase mass flow than macroscopic approaches. The novel methods introduced and the outcome of the work can be utilized in any application area of heterogeneous porous media involving single- and multi-phase mass and momentum transport. Furthermore, the increased performance of the computational model with OpenMP implementation is another significant improvement, since it has a potential to provide a more accurate statistical results with a higher confidence level using high performance computing systems.

2. Methodology

Three different models were used in this study to investigate the effects of liquid formation on mass transfer in randomly generated porous media. The first one is called the path-percolation model, and used for random porous media generation and cluster labeling process, which are explained in the following section. Then, a single-component single-phase (SCSP) LBM was utilized to solve the momentum balance equation and obtain the velocity distribution in representative area elements of the randomly generated channels. As the third model, a SCMP LBM was applied to observe the effects of liquid formation on mass transfer. Furthermore, parallel processing by OpenMP was implemented to the code and a performance analysis was performed.

2.1. Inhomogeneous porous media construction

The statistical based path-percolation theory was used to generate random inhomogeneous porous media as the first step of the current study. To start with, a confidence level study was performed to determine the necessary trial and node numbers of the simulations. A detailed analysis of confidence level studies can be found in [15,16,19]. In the current work, 99% confidence level was considered, and procedure of the history number determination is as follows:

The confidence level [19] defines the reliability of any estimate:

$$CL = Pr\left\{\left|\frac{k}{n} - p\right| \leqslant \varepsilon\right\} \tag{1}$$

In Eq. (1), p is the probability of a pore to occur in a node, which is called the porosity in this study. Total history number is represented by n, whereas k stands for the number of void generation in n histories. Error is defined as the difference between the true