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Three dimensional thermal diffusion in anisotropic heterogeneous structures simulated by a non-dimensional lattice Boltzmann method with a controllable structure generation scheme based on discrete Gaussian quadrature space and velocity

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ABSTRACT

A new Controllable Structure Generation Scheme (CSGS) based on discrete Gaussian quadrature space and velocity is presented and used to generate multiple-phase random isotropic homogenous and shape-constrained anisotropic heterogeneous structures. The primary advantage of the new CSGS over the existing random structure generation growth method is the ability to model a wide variety of structures by controlling the shape through relatively simple constraint indexes. The growth speed probability function is introduced to control the mesoscopic porosities and mixture/separation of material phases. The model is applied to generate four packed structure types (shapeless random, separated solid shapes, separated random-filled shapes, and random-mixture-filled shapes). Three-dimensional steady and transient thermal diffusion are simulated by Non-Dimensional Lattice Boltzmann Method (NDLBM). The steady state results are compared to measured data available in the published literature. The transient results reveal how the mesoscopic shape of a structure impacts thermal diffusion. With equivalent macroscopic volume fractions, structures with higher mesoscopic volume fractions of high conductivity phases possess higher effective thermal conductivity/diffusivity because there is greater connectivity of the higher conductive material at mesoscopic scale.

1. Introduction

Three dimensional (3D) thermal diffusion in anisotropic heterogeneous media is a challenging problem because of the variation in length scales and material properties of porous media. Anisotropic heterogeneous media include microscopic, mesoscopic, and macroscopic length scales corresponding to the scales of a single material particle, material particle groups, and the minimum external length. The geometric shape can vary with length scale and is not always isotropic [1]. When the particle or grouped particle size of a material phase is much smaller than the macroscopic length scale, thermal diffusion can be considered homogeneous [1]. The effects of the mesoscopic size and shape are insignificant only for material diffusivity ratios between 1 and 3.5 [2,3].

To understand the physical properties of a heterogeneous porous medium, the characteristic length scales and shapes of complex structures must be considered. Several techniques have been proposed to generate 3D pore structures from spatial information derived from 2D images, such as the Gaussian filtering method extended by Quiblier [4] from 2D images to 3D reconstructions. Fourier transforms were later introduced to improve the computational efficiency [5]. More detailed information was added by the pore architecture models and pore analysis tools developed by Wu et al. [6]. To obtain the structure of a porous medium independent of imaging, a simplified statistical based method is necessary. Wang [7] developed a random structure generation-growth method named the quartet structure generation set (QSGS). The QSGS generates a random packed porous medium defined by four parameters: seed probability, self-growth probability, interactive-growth probability, and volume fraction of each phase.

At isotropic growth speed, both the self-growth probability and the interactive-growth probability are related to the Gaussian weighting factors for discrete Gaussian quadrature space and velocity. Thus, determination of both self-growth and interactive-growth probabilities from the discrete Gaussian quadrature space

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Nomenclature

c_p	specific heat capacity, J/kg K
c_s	lattice speed of sound, m/s
c	mesoscopic velocity scale, m/s
$\mathbf{c}$	discrete mesoscopic velocity vector, m/s
g	temperature distribution function, K
k	thermal conductivity, W/m K
L	macroscopic length scale, m
Ma	Mach number
n	phase index
N_{ps}	total phase number
(sh, rg, sc, zs)	shape constraint indexes
t	time, s
T	temperature, K
w	weighting factor
x, y, z	coordinates
x_1, y_1, z_1	coordinates after rotation
$\mathbf{x}$	coordinates in vector form

Greek symbols

ΔT	temperature scale, K
Δt	time scale, s
$\Delta x, \Delta y, \Delta z$	lattice size in x, y, z direction, m
α	thermal diffusivity, m^2/s
θ	rotation angle
ϵ	shape overlap ratio
ξ	a volume ratio geometry factor
η	a surface ratio geometry factor
ρ	density, kg/m^3
τ	relaxation time, s
ϕ	volume fraction
ℓ	mesoscopic length scale, m

Subscripts

eq	equilibrium state
f	fluid
$high$	higher value
(i, j, k)	index of coordinates
a	index of discrete volcity directions
m	mixture of solid and liquid
od	opposite direction
ℓ	mesoscopic length scale
low	lower value
L	macroscopic length scale
ref	reference
s	solid
w	wall
0	initial time value

Superscripts

$\overline{n}$	phase index
$-$	space averaged value
$*$	dimensionless variables

and velocity are required to reveal the underlining physics of material growth. Also a seed probability should be determined as opposed to using an arbitrary number as was used in QSGS [7]. Additionally, shape constraints have to be introduced to describe the mesoscopic shapes and sizes of the material particle groups to accurately model anisotropic heterogeneous porous media. To address the requirements discussed above, we developed a generalized Controllable Structure Generation Scheme (CSGS) to generate both random isotropic homogeneous and shape-constrained anisotropic heterogeneous multiple-phase structures.

In the present study, the new CSGS based on discrete Gaussian quadrature space and velocity is presented. The 3D thermal diffusion for different types of structures is simulated by the Non-Dimensional Lattice Boltzmann Method (NDLBM) [8–10] based on the same discrete space and velocity set. The results provide a uniform tool for the investigation of thermal diffusion in porous media.

2. Discrete Gaussian quadrature space and velocity

Simulations of porous media are based on discrete space with a lattice mesh. To speed up the computation, discrete velocity fields are applied [11,12]. Based on the dimensionality of the space, there are a variety of discrete Gaussian quadrature space and velocity sets with corresponding Gaussian weighting factors. Here, we discuss the discrete Gaussian quadrature space and velocity sets in two-dimensional (2D) and three-dimensional (3D) spaces, referred to as D2Q9 [15,16] and D3Q27 [17], respectively. Other discrete Gaussian quadrature space and velocity sets such as D2Q5 and D3Q19 are subsets of 2D and 3D spaces respectively [13,14]. In 2D space, the dimensionless discrete velocity set for the D2Q9 lattice mesh is

$$\mathbf{c}_a^* = \begin{cases} (0,0) & a = 0, \\ (\pm 1, 0), (0, \pm 1) & a = 1\text{–}4, \\ \sqrt{2}(\pm 1, \pm 1), & a = 5\text{–}8. \end{cases} \quad (1)$$

and the corresponding Gaussian weighting factors are

$$w_a = \begin{cases} 4/9, & a = 0, \\ 1/9, & a = 1\text{–}4, \\ 1/36, & a = 5\text{–}8. \end{cases} \quad (2)$$

In 3D space, the dimensionless discrete velocity set for the D3Q27 lattice mesh is

$$\mathbf{c}_a^* = \begin{cases} (0,0,0) & a = 0, \\ (\pm 1,0,0), (0,\pm 1,0), (0,0,\pm 1), & a = 1\text{–}6, \\ \sqrt{2}(\pm 1,\pm 1,0), \sqrt{2}(\pm 1,0,\pm 1), \sqrt{2}(0,\pm 1,\pm 1), & a = 7\text{–}18, \\ \sqrt{3}(\pm 1,\pm 1,\pm 1) & a = 19\text{–}26. \end{cases} \quad (3)$$

and the corresponding Gaussian weighting factors are

$$w_a = \begin{cases} 8/27, & a = 0 \\ 2/27, & a = 1\text{–}6, \\ 1/54, & a = 7\text{–}18. \\ 1/216, & a = 19\text{–}26. \end{cases} \quad (4)$$

The structure generation scheme and the non-dimensional lattice Boltzmann method are based on the above discrete Gaussian quadrature space and velocity sets. The sets are combined smoothly through physically meaningful dimensionless governing parameters.

3. Controllable structure generation scheme

If a space is filled by N_{ps} materials, the volume fraction of material phase n at the position $\mathbf{x}(x, y, z)$ is

$$P_{(\mathbf{x})}^{(n)} = \frac{V_{(\mathbf{x})}^{(n)}}{\sum_{m=1}^{N_{ps}} V_{(\mathbf{x})}^{(m)}}. \quad (5)$$