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Energy conservative dissipative particle dynamics simulation of mixed convection in eccentric annulus

Zhi-Hong Cao, Kang Luo, Hong-Liang Yi *, He-Ping Tan *

School of Energy Science and Engineering, Harbin Institute of Technology, 92 West Dazhi Street, Harbin 150001, PR China

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ABSTRACT

Dissipative particle dynamics with energy conservation (eDPD) is a potentially effective mesoscopic approach in simulating complex convection heat transfer phenomena. The eDPD is applied to model mixed convection heat transfer in eccentric annulus. We propose a numerical strategy for dealing with irregular geometries in DPD system and by which the application of DPD (or any other particle simulation method) can be extended to mimic hydrodynamics in arbitrarily complex geometries like ones with moving surface or free surface which cannot be defined by mathematical functions. The eDPD results for convective heat transfer are compared to the finite volume solutions and the experimental data, and a good agreement is achieved. The results by eDPD are also compared well with those by lattice Boltzmann method (LBM). From the comparisons we find that the forced, natural and mixed convection flow and heat transfer in complex geometries are correctly predicted using eDPD model. Finally, the effect of eccentricity on heat transfer at various locations is examined at $Ra = 2 \times 10^4$ and $Re = 200$, and the streamlines and temperature distributions as well as Nusselt number are obtained. The results show that the average Nusselt number increases when the inner cylinder moves downward regardless of the radial position.

1. Introduction

Dissipative particle dynamics (DPD) is a particle-based mesoscopic simulation method introduced first by Hoogerbrugge and Koelman [1] in 1992. Hydrodynamic behavior of fluid flow is captured using DPD without the need to solve Navier–Stokes equations. The computational efficiency of DPD is much higher than molecular dynamics (MD) as each DPD particle represents a group of actual molecules. Besides being a particle-based method, DPD is truly mesh free and shows great advantages for flow simulations in complex geometries without spacial discretization. One of the drawbacks of classic DPD, as it was originally formulated, is that the total energy of the system is not conserved in the interaction between particles. This has been remedied independently by Español [2] and Avalos and Mackie [3]. They introduced an internal energy variable and a temperature for each particle in the DPD system. This DPD model with energy conservation is known as eDPD in the literatures. The new model opens up the possibility of investigation of thermal processes in complex fluids with a mesoscopic simulation technique. Since its introduction, the eDPD approach has been applied to model several problems of heat transfer. Ripoll et al. [4] used the eDPD to solve a one-dimensional heat conduction problem. The model showed correct equilibrium fluctuations and agreed with Fourier's law. Qiao and He [5] and He and Qiao [6] applied the eDPD to study of heat conduction in nanocomposite materials and nanofluids. Chaudhri and Lukes [7] extended the eDPD formulation to multicomponent systems and applied it to the 1D and 2D heat conduction problem. Abu-Nada [8] examined 2D heat conduction problems using eDPD, and the Neumann and Dirichlet boundary conditions were considered. Toru Yamada et al. [9] simulated diffusive-ballistic heat transfer in thin films using eDPD. Still, improvement is needed to extend the application of eDPD.

Firstly, up to now, the eDPD studies available in literatures that simulate convective heat transfer are still limited. To the best of our knowledge, there are a few groups applied eDPD to convection heat transfer. Mackie et al. [10] applied the eDPD to simulate natural convection in a box with differentially heated enclosure. Although they were successful in demonstrating part of the basic features of natural convection at low Rayleigh numbers, the results in this study were not compared with experimental or finite-element/finite-volume (FV) solutions. Abu-Nada [11–13] performed

* Corresponding authors. Tel.: +86 451 86412674; fax: +86 451 86221048.
E-mail addresses: yihongliang@hit.edu.cn (H.-L. Yi), tanheping@hit.edu.cn (H.-P. Tan).

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Nomenclature

r	distance
r_c	cut-off radius
R_{list}	radii used in linked lists
R_o, R_i	radii of the inner and outer cylinders, respectively
rr	radius ratio, R_o/R_i
l	distance between the centers of the two cylinders
H	height of solution domain
v	velocity
$v_{\max}$	the maximum velocity of particles
m	mass of DPD particle
n	the total number of DPD particles
N	steps of the simulation
f	force
g	gravity vector
T	temperature
T_h	hot temperature
T_c	cold temperature
T_r	reference temperature
a	repulsion force parameter
e	unit vector
q	heat flux
t	time
Δt	time step
w	weight function
W	the total number of multiplications involved the neighbor and linked lists
C^v	heat capacity at constant volume
k_B	Boltzmann constant
k_o	parameter controlling the thermal conductivity of DPD particle
D	thermal diffusivity
Re	Reynolds number
Ra	Raleigh number
Nu	Nusselt number
Pr	Prandtl number
d	the dimension of simulation domain

Greek symbols

ζ^e	random number for the energy
ζ	random number for the momentum
ρ	density
ξ	dimensionless radial position, $l/(R_o - R_i)$
φ	tangential direction
κ	collisional heat flux parameter
σ	random force parameter
γ	dissipative force parameter
α	random heat flux parameter
ε	eccentricity, $\varepsilon(\xi, \varphi)$
η	dynamic viscosity
ν	kinematic viscosity
θ	dimensionless temperature

Subscripts

i, j	indices
ave	average
c	cold
h	hot
r	reference

Superscripts

C	conservative
D	dissipative
R	random

simulations of natural convection using eDPD. In his works, a 2D Rayleigh–Benard problem and a problem with differentially heated enclosure were modeled. We can see that the results they got are not so satisfactory. In the work of Cao et al. [14], eDPD is used to simulate natural convection in eccentric annulus over a wide range of Rayleigh numbers. In addition, Yamada et al. [15] investigated forced convection in parallel-plate channels with boundary conditions of constant wall temperature and constant wall heat flux by using eDPD. There is no published work reporting mixed convective heat transfer using the eDPD. Because of the universality, importance and complexity of convective heat transfer in engineering applications and relevant theoretical research, it is very necessary to apply eDPD to fundamental problems of thermal convection to promote the eDPD scheme as a powerful tool that could solve various problems of convective heat transfer very well.

Secondly, so far, the eDPD method has been only used to simulate convection heat transfer in simple geometries, 1D channel or 2D rectangular enclosure. In fact, simple enclosures such as straight microchannels were included in most of the works on fluid flow using DPD. However, in real engineering and industrial applications, convection phenomenon often occurs in complex geometries. As a very effective computational tool that can tackle complex fluid behaviors at mesoscale, it is very important that eDPD acquires flexibility in dealing with irregular geometries. While in fact, there were a few studies that applied eDPD to heat transfer in complex geometries. Haber et al. [16] used the DPD to simulated the flow in a system comprised of a fluid occupying the space between two cylinders rotating with equal angular velocities. Abu-Nada et al. [17] explored fluid flow in a two-dimensional convergent–divergent nozzle by means of DPD combined with non-orthogonal transformation. In the work, they transformed an irregular domain into a simple rectangular domain to solve the problem caused by irregular geometries. But the advantage of the DPD as one of particle-based methods is not maximized by this treatment of complex geometries as done in Ref. [17]. Furthermore, the method is not applicable for arbitrarily complex geometries like ones with moving surface or free surface which cannot be defined by mathematical functions. There are at least six issues when the eDPD method is applied to simulate the flow and heat transfer in complex geometries. We will discuss the issues detailed in Section 3. So, more direct and effective solutions to the problems are much needed to develop in application of DPD or eDPD to complex geometries.

Thirdly, the flow and heat transfer in convection has received increased attention in mesoscopic approaches recently, such as LBM [18], eDPD [11–13,15] and multiparticle collision dynamics (MPCD) [19] which is another mesoscopic method which has shown to be able to reproduce heat transport. It is mainly due to the urgent need of more robust simulation tools that could explain and predict mechanisms of convection heat transfer in the mesoscopic level. LBM and eDPD are widely used. However, up to the best knowledge of the authors, there are no detailed works about the comparison between the two methods.

Finally, the implement of no-slip boundary condition in DPD system are also important and need more attention.

Therefore, the present work is to extend the eDPD to model fluid flow and heat transfer in enclosures with more complex boundaries. We take horizontal eccentric annulus as the flowing zone to apply eDPD to the simulation of force, natural and mixed convection. We introduce the eDPD governing equations in Section