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

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ABSTRACT

In this paper, an efficient numerical approach, the dissipative particle dynamics with energy conservation (eDPD), is used to simulate natural convection in eccentric annulus over a wide range of Rayleigh numbers. A numerical strategy is presented for dealing with irregular geometries in DPD system. The eDPD results are compared to the finite volume solutions and the experimental data, and it is found that the temperature and flow fields for the natural convection in complex geometries are correctly predicted using eDPD. The effect of eccentricity on heat transfer at various locations is examined at $Ra = 10^4$, 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]. Hydrodynamic behavior of fluid flow is captured using DPD without the need to solve the Navier–Stokes equations. The first idea of DPD is that soft and finite interactions are considered into standard molecular dynamics (MD) [2]. The scales of time and space that can be reached in DPD are much larger than those in MD. The second idea of DPD is that the soft and finite interactions have dissipative and stochastic contributions, as well as a weak conservative term. The introduction of these dissipative and random interactions between particles can be understood if each DPD particle is representing a group of fluid molecules instead of one molecule [3]. Therefore, DPD is a coarse-grained version of MD, so the computational efficiency is much higher. Besides being a particle-based method, DPD is truly mesh free and shows great advantages for complex flow simulations without spacial discretization. Since its introduction in 1992, DPD has been applied to simulate the behavior of various complex fluids [4,5].

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 limitation precludes the use of DPD in the study of heat transfer in complex fluids. In many problems of interest, either fundamental or applied, the investigation for the transport properties of heat at the mesoscopic level is very important. Thus the incorporation of thermal effects into a DPD algorithm is necessary for its further applications to problems of relevance. This has been remedied independently by Español [6] and Avalos and Mackie [7]. They introduced an internal energy variable and temperature to DPD system. This DPD system with energy conservation is known as eDPD in the literatures. The new model opens up the possibility of studying 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. [8] used eDPD for solving a one-dimensional heat conduction problem. The model showed correct equilibrium fluctuations and agreed with Fourier's law. Qiao and He [9] and He and Qiao [10] applied eDPD to heat conduction in nanocomposite materials and nanofluids. Chaudhri and Lukes [11] extended the eDPD formulation to multicomponent systems and applied it to the 1D and 2D heat conduction. Abu-Nada [12] examined 2D heat conduction problems by using eDPD, and the Neumann and Dirichlet boundary conditions were considered.

Up to now, the eDPD studies available in literatures that simulate convective heat transfer are still limited. 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. Recently, the flow and heat transfer in convection has received

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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
V_w	the velocity of the wall at the collision point
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
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
v	kinematic viscosity
θ	dimensionless temperature

Subscripts

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

Superscripts

C	conservative
D	dissipative
R	random

increased attention from mesoscopic approaches, such as lattice Boltzmann techniques [13] and eDPD method [14–17]. This 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. To the best of our knowledge, there are two groups applied eDPD to convection heat transfer. Mackie et al. [18] applied eDPD to simulate natural convection in a differentially heated enclosure. Although they were successful in demonstrating part of the basic features of natural convection at low Rayleigh numbers, such as prediction of single circulation cell in the enclosure, the results in this study were not compared with experimental or finite element/finite volume (FE/FV) solutions, and the implementation of eDPD model were not described in detail. The other work involved simulation of natural convection using eDPD was done by Abu-Nada [14,15,17]. In his works, a 2D Rayleigh–Benard problem and a differentially heated enclosure problem were modeled. In addition, Yamada et al. [16] investigated forced convection in parallel-plate channels with boundary conditions of constant wall temperature and constant wall heat flux by using eDPD.

So far, the eDPD method has been only used to simulate convection heat transfer with 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, natural convection phenomenon often occurs in complex geometries, such as geometry of the horizontal annuli which is commonly found in underground electric transmission cables, vapor condenser for water distillation and food process. Numerical simulation of natural convection in concentric and eccentric circular cylinder has been reported in the literatures [19–24]. Kuhen and Goldsein [25,26] conducted an experimental and theoretical investigation of natural convection in concentric and eccentric horizontal annuli. Their experimental data is commonly used to validate most of the recent numerical solutions. 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 DPD to complex geometries. Recently, Abu-Nada et al. [27] explored fluid flow in a two-dimensional convergent–divergent nozzle by means of DPD combined with non-orthogonal transformation. In their work, they transformed an irregular domain into a simple rectangular domain to solve the problem caused by irregular geometries. There are two problems when the eDPD method is applied to simulate the flow and heat transfer problems with complex geometries. First, the treatment of boundary conditions becomes more difficult. Second, the optimization algorithms used to improve calculation efficiency are no longer applicable. Solutions to the problems are much needed to develop in application of eDPD method to complex geometries.

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 natural convection. The effect of eccentricity at various locations on flow and heat transfer will be discussed. The present results obtained by eDPD will be