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Dissipative particle dynamics simulation of natural convection using variable thermal properties☆

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ABSTRACT

Dissipative particle dynamics with energy conservation (eDPD) was used to investigate the effect of variable thermal properties on natural convection in liquid water over a wide range of Rayleigh Numbers. The problem selected for this study was a differential heated cavity. The eDPD results were compared to the finite volume solutions and the eDPD method predicted the effects of temperature-dependent conductivity and viscosity on temperature and flow fields throughout the cavity properly. The eDPD temperature-dependent model was able to capture the basic features of natural convection, such as development of thermal boundary layers, and development of natural convection circulation cells within the cavity. The eDPD results experienced some degree of compressibility at high values of Ra numbers ($Ra = 10^5$) and this problem was resolved by tuning the speed of sound of the eDPD model.

1. Introduction

Dissipative particle dynamics (DPD) is a coarse-grained version of the molecular dynamics method, which was introduced by Hoogerbrugge and Koelman [1] to capture larger time and spatial scales when compared to the molecular dynamics (MD) scales. The DPD method is a mesh-free based simulation method, where any fluid is considered as a group of randomly scattered interacting particles that are governed by the conservation of mass and momentum. Many microfluidics and nanofluidics applications were investigated recently by the DPD approach to reveal the essential information about the microscopic structure of the physical processes encountered in these applications [2–7].

The major advantages for using the DPD technique over the conventional continuum methods (e.g., finite volumes and finite elements methods) first is the inherent inclusion of thermal fluctuations in the DPD model. These fluctuations enable a correct imitation of important physical phenomena encountered at micro- and nanoscales, such as heat diffusion, mass diffusion, and momentum diffusion. Practical examples that include thermal fluctuations are the thermal transport in polymeric solutions, colloidal suspension, and phase change applications. Second, the DPD dominates over the conventional methods when the spatial scales vary considerably across the physical domain and span a wide range from macro- to nanoscales. Such resilience in adaption to wide range of scales is inherent in DPD model and in contrast is considered as a major drawback of conventional continuum models.

The DPD approach was extended by Español [8] and Avalos and Mackie [9] to handle thermal transport by adding internal energy to each DPD particle. This version of DPD is shown to conserve energy and it is known as energy conservative dissipative particle dynamics (eDPD) [8]. Since its introduction, the eDPD method was applied to several heat transfer applications by various researchers. Ripoll et al. [10] and Ripoll and Español [11] studied one-dimensional heat conduction and they showed that the method was able to model heat conduction accurately. The method was extended to two-dimensional (2D) heat conduction by Chaudhri and Lukes [12]. The method was further applied to heat conduction in nanocomposites by Qiao and He [13] and heat conduction in nanofluids by He and Qiao [14] and Yamada et al. [15]. Abu-Nada [16,17] implemented various types of boundary conditions to 2D heat conduction. Also, more recently, Li et al. [18] considered the mass diffusivity and viscosity of the eDPD model to be temperature dependent where they simulated a Poiseuille flow and steady heat conduction to validate their temperature dependent model for mass diffusivity, Schmidt and Prandtl numbers.

In regard to convective heat transfer applications of the eDPD model, Mackie et al. [19] applied the eDPD approach to heat flow in a differentially heated cavity. Abu-Nada [20,21] studied natural convection via two basic heat transfer problems, which are differentially heated enclosures and Rayleigh–Bénard convection. The eDPD method was tested over a wide range of Rayleigh numbers using several quantitative benchmarks against finite volume solutions. Yamada et al. [22] studied forced convection heat transfer in parallel plate channels by the eDPD approach. The application of eDPD to other geometries was conducted by Cao et al. [23]. Moreover, Abu-Nada [24] extended the eDPD approach to handle liquids by increasing the eDPD viscosity and producing higher Prandtl numbers that mimic natural convection in water. Also,

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Nomenclature

a	repulsion parameter
C_v	specific heat at constant volume, J/kg·K
c_s	speed of sound
e	unit vector
f	force, N
g	gravity vector
H	cavity height, m
K	Thermal conductivity function, W/m·K
k	thermal conductivity, W/m·K
k_B	Boltzmann constant
k_o	parameter controlling the thermal conductivity of the eDPD particle
n	normal vector
p	dimensional pressure, N/m^2
Pr	Prandtl number, $\mathrm{Pr} = \nu_C/\alpha_C$
q	heat flux, W/m^2
r	position vector
r_c	cut-off radius
Ra	Rayleigh number, $Ra = g\beta(T_H - T_C)H^3/(\nu_C\, \alpha_C)$
T	dimensional temperature, °C
t	time, s
U_{ref}	reference velocity, m/s
v	velocity vector
w	weight function
W	width of the cavity, m
x, y	dimensional coordinates, m
X, Y	dimensionless coordinates, $\mathrm{X} = x/H$, $\mathrm{Y} = y/H$
α	thermal diffusivity, m^2/s
α_{ij}	random heat flux parameter
β	thermal expansion coefficient, 1/K
γ	dissipative force parameter
ζ	random number for the momentum equation
ζ^e	random number for the energy equation
θ	dimensionless temperature, $\theta = (T - T_C)/(T_H - T_C)$
κ	collisional heat flux parameter
λ	random heat flux parameter
μ	dynamic viscosity, N·s/m^2
ν	kinematic viscosity, m^2/s
ρ	eDPD number density
σ	amplitude of the random force
Ω	temperature dependent weight function

Subscripts

C	cold
H	hot
i, j	indices
ref	reference

Superscripts

C	conservative
D	dissipative
R	random
cond	conduction
visc	viscous

more recently, Cao et al. [25] and Abu-Nada [26–28] applied eDPD to several mixed convection applications.

Based on the above-mentioned review, it is very important to extend the application of the eDPD method to more fundamental problems in convection heat transfer. Actually, in emerging fields of convective heat transfer applications, such as natural heat transfer enhancement using nanofluids, the temperature range in the flow domain could be substantially large and the assumption of constant thermal properties becomes questionable. Therefore, to apply the eDPD approach to such convective applications it is very essential to consider the temperature dependency of the thermal properties in the eDPD model. Consequently, the aim of the current work is to investigate natural convection in water by considering the effect of temperature-dependent properties of thermal conductivity and viscosity. This gives more insight on the thermal transport in natural convection, which will help to advance eDPD applicability to simulate nanoscale thermal transport applications such as heat transfer enhancement using nanofluids. The problem considered in this study is natural convection in a differential heated cavity having water as the working fluid. The eDPD model will be assessed over a wide range of Rayleigh numbers.

2. eDPD governing equations

The eDPD method is a particle technique, which is based on pair-wise interactions between neighboring particles within a cut-off radius. The eDPD particles are coarse-grained particles where each eDPD particle represents a group of real fluid molecules. The motion of the particles is governed by conservation of mass, momentum and energy and is described by the following set of equations, by employing the Boussinesq approximation [20,24]:

$$\frac{d\vec{r}_i}{dt} = \vec{v}_i \tag{1}$$

$$\frac{d\vec{v}_i}{dt} = \left(\vec{f}^{\,C}_{ij} + \vec{f}^{\,D}_{ij} + \vec{f}^{\,R}_{ij}\right) + \vec{g}\beta(T - T_o) \tag{2}$$

$$C_v\frac{dT_i}{dt} = \left(q^{\mathrm{visc}}_{\mathrm{ij}} + q^{\mathrm{cond}}_{\mathrm{ij}} + q^{\mathrm{R}}_{\mathrm{ij}}\right) \tag{3}$$

where β is the thermal expansion coefficient and $\vec{g}$ is the gravity vector. The heat flux vectors $q^{\mathrm{cond}}_{\mathrm{ij}}$, $q^{\mathrm{visc}}_{\mathrm{ij}}$, and $q^{\mathrm{R}}_{\mathrm{ij}}$ that appear in Eq. (3), accounts for viscous, collision, and random heat fluxes respectively. The conservative force $\vec{f}^{\,C}_{ij}$, dissipative force $\vec{f}^{\,D}_{ij}$ and random force $\vec{f}^{\,R}_{ij}$ are expressed as [2]:

$$\vec{f}^{\,C}_{ij} = \sum_{j \neq i} a_{ij}\, w(r_{ij})\, \vec{e}_{ij} \tag{4}$$

$$\vec{f}^{\,D}_{ij} = \sum_{j \neq i} -\gamma_{ij} w^D(r_{ij})\left(\vec{e}_{ij}\cdot\vec{v}_{ij}\right)\vec{e}_{ij} \tag{5}$$

$$\vec{f}^{\,R}_{ij} = \sum_{j \neq i} \sigma_{ij}\ w^R(r_{ij})\ \zeta_{ij}\ \Delta t^{-1/2}\ \vec{e}_{ij} \tag{6}$$

where $r_{ij} = r_i - r_j$ and $v_{ij} = v_i - v_j$; e_{ij} is the unit vector pointing in the direction from j to i. The parameter a_{ij} (in Eq. (4)) is a repulsion parameter between the eDPD particles. This parameter affects the interaction between the particles and accordingly controls the equation of state and compressibility of the eDPD system. Also, the parameters γ_{ij} and σ_{ij} in Eqs. (5) and (6) are the strength of dissipative and random forces, respectively. The random number ζ_{ij} that appears in Eq. (6) is a random number with a zero mean and unit variance which has the property $\zeta_{ij} = \zeta_{ji}$ to ensure the conservation of the total momentum of the eDPD system [3–7].

The weight function w for the conservative force decreases monotonically with particle–particle separation distance. It becomes zero beyond the cut-off length. In the present study, we followed the work of Fan et al. [7] by using two different weighting functions, one for the conservative force and the other one for the dissipative and random forces.