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Assessment of dissipative particle dynamics to simulate combined convection heat transfer: Effect of compressibility☆

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ABSTRACT

The current study explored the capability of a discrete particle method known as dissipative particle dynamics with energy conservation (eDPD) to simulate combined convection heat transfer in a vertical lid driven cavity. The study investigated two cases of aiding and opposing buoyancy mechanisms in the lid driven cavity. The eDPD results were compared against the finite volume solutions for the range of Richardson number, $10^{-2} \leq Ri \leq 10^{2}$. The method showed good comparison for the range of Richardson number $10^{-2} \leq Ri \leq 10^{1}$. However, the eDPD method showed deviation from the FV solutions for a high value of Richardson number, $Ri = 10^{2}$, and this deviation is attributed to the compressibility of eDPD system experienced at such high value of Richardson number. Parametric study on the influence of the Richardson number (Ri) on the eDPD compressibility was conducted and presented via temperature isotherms, streamlines, velocity contours, velocity vectors, temperature and velocity profiles.

1. Introduction

Dissipative particle dynamics (DPD) was introduced by Hoogerbrugge and Koelman [1] as a coarse-grained version of molecular dynamics method that could capture larger time and spatial scales compared to molecular dynamics scales. This feature has attracted various researchers to mimic fluid flow physics encountered at micro scale and nanoscale applications since its emersion [2–7]. Español [8] and Avalos and Mackie [9] extended the applicability of the DPD approach to tackle thermal energy transport by adding internal energy for each DPD particle. Such insertion of internal energy in the DPD model was shown to conserve energy and this version of DPD is known in literature as energy conservative dissipative particle dynamics (eDPD) [8]. Fundamentally, each eDPD particle is prescribed by internal energy in addition to other quantities found in the classical DPD models (position, velocity, and mass).

Over the past fifteen years, the application of the eDPD approach to heat transfer was investigated by various researchers. Ripoll et al. [10] and Ripoll and Español [11] focused on the application of eDPD to one-dimensional heat conduction and it was found that the method is capable of modeling heat conduction precisely. The method is extended to model heat conduction in nano composites by Qiao and He [12] and heat conduction in nanofluids by He and Qiao [13]. Chaudhri and Lukes [14] applied the eDPD method to 2D heat conduction. Abu-Nada [15,16] implemented different types of boundary conditions to 2D heat conduction domain using the eDPD method and benchmarked the eDPD results against analytical and finite difference solutions. Recently, Yamada et al. [17] applied eDPD to model conduction in nanofluids.

On the other hand, the application of eDPD approach to convective heat transfer problems was limited. For example, Mackie et al. [18] applied the eDPD approach to heat flow in differentially heated enclosure. Abu-Nada [19,20] extended the application of eDPD to model convective heat transfer. He focused on natural convection applications and tested the approach over a wide range of Rayleigh number where he carried a critical quantitative benchmark in natural convection via two basic heat transfer problems which are differentially heated enclosures (DHE) and Rayleigh–Bénard convection (RB) problem [19,20]. Yamada et al. [21] 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. [22]. Recently, Abu-Nada [23] extended the eDPD approach to handle liquids by increasing the eDPD viscosity and producing higher Prandtl numbers that mimic water convection in relatively high values of Rayleigh numbers. Most recently, Abu-Nada [24] conducted a study on a horizontal lid driven cavity where the working fluid is air. Based on the previous review, it is very important to apply eDPD to more fundamental problems of convection heat transfer to advance the eDPD applicability as a robust tool that could mimic convective heat transfer applications. The method will be assessed under a wide range of combined convection applications ranging from approximately purely natural convection to almost purely forced convection. Besides, the method will be tested under a rigorous condition by

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Nomenclature

a	repulsion parameter
C_v	specific heat at constant volume, J/kg.K
e	unit vector
f	force, N
Gr	Grashof number, $Gr = g\beta(T_H\text{-}T_C)H^3/(\nu_C^2)$
H	cavity height, m
k	thermal conductivity, W/m.K
k_B	Boltzmann constant
k_o	parameter controlling thermal conductivity of the eDPD particle
m	mass of the eDPD particle
n	normal vector
p	dimensional pressure, N/m^2
P	dimensionless pressure, $P = p/(\rho U_p^2)$
Pr	Prandtl number, $Pr = \nu_C/\alpha_C$
q	heat flux, W/m^2
r	position vector
r_c	cut-off radius
Ra	Rayleigh number, $Ra = g\beta(T_H\text{-}T_C)H^3/(\nu_C\,\alpha_C)$
Re	Reynolds number, $Re = U_pH/\nu_C$
Ri	Richardson number, $Ri = Gr/Re^2$
T	dimensional temperature, °C
t	dimensional time, s
t'	dimensionless time, $t' = (t/(H/U_p))$
u, v	dimensional x- and y-component of velocity, m/s
U, V	dimensionless x- and y-component of velocity, $U = u'/U_p$, $V = v'/U_p$
w	weight function
x, y	dimensional coordinates, m
X, Y	dimensionless coordinates, $X = x/H$, $Y = y/H$
α	thermal diffusivity, m^2/s
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, $\theta = (T\text{-}T_C)/(T_H\text{-}T_C)$
κ	collisional heat flux parameter
λ	random heat flux parameter
ν	kinematic viscosity, m^2/s
ρ	mass density, kg/m^3
σ	amplitude of the random force

Subscripts

C	cold
H	hot
i, j	indices

Superscripts

C	conservative
D	dissipative
R	random
cond	conduction
visc	viscous

changing the rotational direction of natural convection flow currents relative to forced convection flow currents by adjusting the thermal boundary conditions in the cavity. Basically, two types of thermal boundary conditions are employed to simulate aiding and opposing flow in the lid driven cavity. These tests will assess the suitability of the eDPD method to mimic mixed convective heat transfer problems and will test the compressibility of eDPD method under such rigorous conditions.

2. Governing equations of eDPD model

The eDPD method is a particle method based on pairwise interactions between adjacent particles within a cut-off radius. The eDPD particles are coarse-grained particles where each eDPD particle represent a group of real fluid molecules. The movement of eDPD particles is governed by conservation of mass, momentum and energy and is described by the following set of equations by employing the Boussinesq approximation [19,23]:

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

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

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

where β is the thermal expansion coefficient and $\vec{g}$ is the gravity vector. The $\vec{f}^{C}_{ij}$, $\vec{f}^{D}_{ij}$ and $\vec{f}^{R}_{ij}$ represent conservative, dissipative, and random forces, which can be written as [2,7,23]:

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

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

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

The weight function w decreases monotonically with particle–particle separation distance. It becomes zero beyond the cut-off radius and given as [19],

$$w\left(r_{ij}\right) = \begin{cases} \dfrac{5}{\pi}\left(1 + 3\dfrac{r_{ij}}{r_c}\right)\left(1 - \dfrac{r_{ij}}{r_c}\right)^3 & \left(r_{ij} < r_c\right) \\ 0 & \left(r_{ij} \geq r_c\right). \end{cases} \tag{7}$$

The heat flux vectors q^{cond}_{ij}, q^{visc}_{ij}, and q^{R}_{ij} account for conduction, viscous, and random heat fluxes respectively and are given as [10,11,13,19,23]:

$$q^{cond}_{ij} = \sum_{j\neq i} \kappa_{ij} w^2\left(r_{ij}\right)\left(\frac{1}{T_i} - \frac{1}{T_j}\right) \tag{8}$$

$$q^{visc}_{ij} = \sum_{j\neq i}\frac{1}{2C_v}\left(w^{D}\left(r_{ij}\right)\left[\gamma_{ij}\left(\vec{e}_{ij}\cdot\vec{v}_{ij}\right)^2 - \frac{\sigma^2_{ij}}{m}\right] - \sigma_{ij} w^{R}\left(r_{ij}\right)\left(\vec{e}_{ij}\cdot\vec{v}_{ij}\right)\zeta_{ij}\right) \tag{9}$$

$$q^{R}_{ij} = \sum_{j\neq i}\alpha_{ij} w^{R}\left(r_{ij}\right)\Delta t^{-1/2}\;\; \zeta^{e}_{ij} \tag{10}$$

where $r_{ij} = r_i - r_j$ and $v_{ij} = v_i - v_j$.

The parameter a_{ij} is the repulsion parameter between the eDPD particles and the parameters γ_{ij} and σ_{ij} in Eqs. (5) and (6) define the strength of dissipative and random forces, respectively [2]. Furthermore, the parameters κ_{ij} and α_{ij} appearing in Eqs. (8) and (10) adjust the strength of the collisional and random heat flux, respectively [10, 11]. The random number ζ_{ij} that appears in Eq. (6) is a random number