SIMULATION OF HEAT TRANSFER ENHANCMENT IN NANOFLUIDS USING DISSIPATIVE PARTICLE DYNAMICS

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ABSTRACT

The current work develops a computational heat transfer model based on Dissipative Particle Dynamics (DPD) approach to study thermal transport in natural convection using nanofluids. The present work tests the role of nanoparticles on heat transfer enhancement in nanofluids, which gives a better understanding of the energy transport between base fluid particles and the suspended nanoparticles in nanofluids. It was found that the heat transfer deteriorates by increasing the volume fraction of nanoparticles.

NOMENCLATURE

a	[-]	repulsion parameter
C_v	J/kg.K	specific heat at constant volume
f	N	force
g	m/s^2	gravity vector
H	m	cavity height
h	W/m^2.K	heat transfer coefficient
k	W/m.K	thermal conductivity
k_B	J/K	Boltzmann constant
k_o	[-]	parameter controlling thermal conductivity of the eDPD particle
Pr	[-]	Prandtl number, Pr= ν/ α
q	W/m^2	heat flux,
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	ºC	dimensional temperature
t	s	Time
u,*v*	m/s	dimensional *x*- and *y*-component of velocity
w	[-]	weight function
U, V		Non-dimensional velocity, U=uH/ α, V=vH/ α
x, *y*	m	dimensional coordinates
X, Y	[-]	dimensionless coordinates, X=*x*/H, Y=*y*/H
α	m^2/s	thermal diffusivity
β	1/K	thermal expansion coefficient
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
ν	m^2/s	kinematic viscosity
ρ	[-]	eDPD number density
σ	[-]	amplitude of the random force

Subscripts

C	cold
H	hot
i, j	indices
nf	nanofluid

Superscripts

bf	Base fluid
C	conservative
D	dissipative
R	random
cond	conduction
visc	viscous

INTRODUCTION

Enhancement of heat transfer in thermal systems is very essential from the industrial and energy saving perspectives. The low thermal conductivity of heat transfer fluids, such as water, is considered a primary limitation on the enhancement of the performance and the compactness of the thermal systems. In recent years, heat transfer enhancement using nano-scale particle dispersed in a base fluid, known as nanofluid, has been used to enhance heat transfer. In fact, there is still a debate in literature

on the role of presence of high thermal conductive nanoparticles on the heat transfer enhancement, especially in natural convection applications. Most theoretical studies in literature reported an enhancement in heat transfer due to the presence of high thermal conductive nanoparticles in contrary to what observed experimentally.

Examples of controversial results are found in the results reported theoretically by [1, 2] where they reported an enhancement in heat transfer due to the addition of nanoparticles in contradictory to what observed experimental findings by Putra et al. [3] and Wen and Ding [4]. The numerical study of Abu-Nada et al. [5] related such deterioration in heat transfer, observed experimentally, to the increased level of viscosity of nanofluids by the presence of nanoparticles which tend to decrease the convection heat transfer. Although such explanation is in agreement with the experimental findings of Putra et al. [5] and Wen and Ding [6], however it lacks the complete picture how the thermophysical properties of nanofluids are related to nanoscopic details of particles interaction in the base fluid. Besides, it does not illuminate the energy mechanisms encountered at nanoscale in nanofluids.

Conceptually, the mentioned theoretical studies relied on using the continuum models to study nanoparticles energy transport in base fluids. The major concern is whether on the scale of several nano meters, the continuum assumption is still valid. Actually, the mean free path of base fluid particles is in the same order of magnitude of the nanoparticles size and the continuum assumptions become questionable. Therefore, a more robust numerical discrete approach is needed to tackle such problem.

In fact, the time and spatial scales of the heat transfer within nanofluids are larger than the complete discrete models such as molecular dynamics (MD) and smaller than the conventional continuum models such as Navier-Stokes Equations (NES). Such intermediate spatial and time scales can be captured using mesoscopic particle-based methods by means of coarse graining where each simulated particle represents a group of actual fluid molecules. The most recent promising coarse grained technique is the dissipative particle dynamics (DPD) method.

Dissipative particle dynamics (DPD) method is a coarse grained version of MD introduced by Hoogerbrugge and Koelman [5], where each DPD particle represents a group or packet of actual molecules. The DPD particles are randomly distributed in the flow domain and particle interaction obeys conservation of mass, momentum and energy. Español [6] and Avalos and Mackie [7] launched energy conservative DPD version appropriate for studying heat transport by adding internal energy to the DPD system. The energy conservative DPD version is known in literature as energy conservative dissipative particle dynamics (eDPD). Since its introduction, the eDPD approach was limited to relatively few heat transfer studies on convective heat transfer problems. Chaudhri and Lukes [9] recently conducted a comprehensive review of the eDPD investigations in literature. Actually, all eDPD conducted studies in convective heat transfer are only limited to pure fluids and it is very important to extend the eDPD approach to mimic convective heat transfer in nanofluids. Therefore, the scope of the present proposal is to extend the applicability of eDPD to investigate the mechanisms of heat transfer, within nanofluids,

DPD MODEL

The time progress of eDPD particles is governed by conservation of momentum and energy and is described by the following set of equations by absorbing the Boussinesq approximation:

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

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

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

where β is the thermal expansion coefficient and $\vec{g}$ is the gravity vector. The conservative force $\vec{f}_{\mathrm{ij}}^{\,\mathrm{C}}$, dissipative force $\vec{f}_{\mathrm{ij}}^{\,\mathrm{D}}$ and random force $\vec{f}_{\mathrm{ij}}^{\,\mathrm{R}}$ are expressed as [10]:

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

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

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

The weight function w for the conservative force is given as,

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

The weighting function for the dissipative and random forces is given as

$$w^D\left(r_{ij}\right) = \left(w^R\left(r_{ij}\right)\right)^2 = \begin{cases} \left(1 - \frac{r_{ij}}{r_c}\right)^S, & (r_{ij} < r_c) \\ 0, & (r_{ij} > r_c) \end{cases} \tag{8}$$

In the present study, the value of S is set to S= ½ and the cut-off radius is set to 1.1. For more details on the selection of S and r_c the reader is referred to Abu-Nada [11].

The heat flux vectors q_{ij}^{cond}, q_{ij}^{visc} q_{ij}^{R} accounts for viscous, collision, and random heat fluxes respectively and are given by [11]:

$$q_{ij}^{cond} = \sum_{j \neq i} \kappa_{ij}\, w^2(r_{ij})\left(\frac{1}{T_i} - \frac{1}{T_j}\right) \tag{9}$$

$$q_{ij}^{visc} = \sum_{j \neq i} \frac{1}{2C_v}\left(w^D(r_{ij})\left[\gamma_{ij}\left(\vec{e}_{ij} \cdot \vec{v}_{ij}\right)^2 - \frac{\sigma_{ij}^2}{m}\right] - \sigma_{ij} w^R(r_{ij})\left(\vec{e}_{ij} \cdot \vec{v}_{ij}\right)\zeta_{ij}\right) \tag{10}$$

$$q_{ij}^{R} = \sum_{j \neq i} \alpha_{ij}\, w^{R}(r_{ij}) \Delta t^{-1/2}\, \zeta_{ij}^{e} \tag{11}$$

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} is a repulsion parameter between the eDPD particles. Also, the parameters γ_{ij} and σ_{ij} account for the strength of dissipative and random forces, respectively. Also, the parameters κ_{ij} and α_{ij} control the strength of the collisional and random heat flux, respectively.

The random number ζ_{ij} is a random number that has a zero mean and unit variance and the random number ζ_{ij}^{e} is non-symmetrical random number with zero mean and unit variance. The relation between the parameters γ_{ij} and σ_{ij} is governed by the Fluctuation-Dissipation theorem [11],

$$\gamma_{ij} = \frac{\sigma_{ij}^{2}\left(T_i + T_j\right)}{4 k_B T_i T_j}, \tag{11}$$

$$\alpha_{ij} = \sqrt{2 k_B \kappa_{ij}} \tag{12}$$

where k_B is the Boltzmann constant. The parameter κ_{ij} is given as,

$$\kappa_{ij} = \frac{C_v^{2} k_o \left(T_i + T_j\right)^{2}}{4 k_B} \tag{13}$$

where k_o is interpreted as heat friction that controls thermal conductivity and, C_v is the heat capacity at constant volume for eDPD particle.

PROBLEM DESCRITIPTION AND MODEL VALIDATION

Figure 1 shows a schematic diagram of the problem geometry selected to investigate the heat transfer enhancement using nanofluids. The cavity is filled with CuO-water nanofluid. The height of the cavity is defined by H and the width of the cavity is defined by W. The aspect ratio (i.e., W/H) is kept constant for the present study and is set to 1. The left wall is maintained at a hot temperature T_H whereas the right wall is kept at a cold temperature T_C. The top and the lower walls are considered adiabatic. The standard Boussinesq model is used to approximate the density variation of the nanofluid.

The problem of natural convection in hand is characterized by two important non-dimensional numbers, which are Prandtl number (Pr) and Rayleigh number (Ra), which are given as:

$$\mathrm{Pr} = \frac{\nu_C}{\alpha_C}; \qquad Ra = \frac{g\beta(T_H - T_C)H^{3}}{\nu_C \alpha_C} \tag{14}$$

Here we defined these dimensionless numbers based on cold wall temperature.

The eDPD parameters (i.e., a_{ij}, γ_{ij}, σ_{ij}, κ_{ij} and α_{ij}) are related to non-dimensional numbers *Pr* and *Ra* via the thermal diffusivity and kinematic viscosity. The Prandtl number considered in this study is fixed to the value of water, *Pr* = 6.55. We need to link this value with the kinematic viscosity and the thermal diffusivity of the eDPD system.

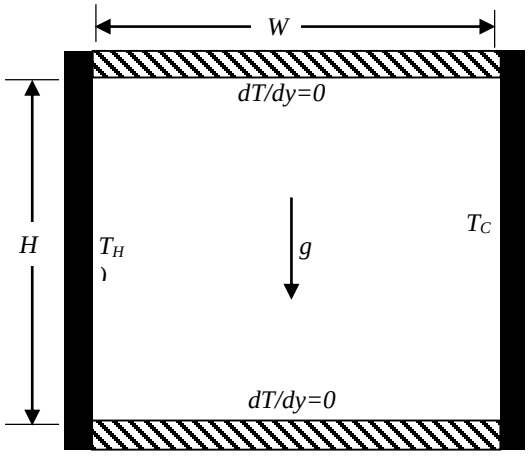


Figure 1 Schematic of the problem geometry

The kinematic viscosity of the eDPD system is assigned by running a Poiseuille flow between two parallel plates. Then, the value of the thermal diffusivity of the eDPD system is simply calculated based on the prescribed value of the Prandtl number (i.e., $\alpha=\nu/Pr$). The value of the thermal diffusivity of the eDPD system is measured by comparing the eDPD results to the analytical solution of a transient heat conduction in a square heated slab. In terms of the eDPD model, the parameter that controls the thermal diffusion is k_o. The value of k_o in the eDPD model is tuned until the analytical solution agrees with the eDPD solution. The values of eDPD kinematic viscosity and thermal diffusivity are measured to be 1.1078 and 0.169, respectively. For full details for measuring the kinematic viscosity and thermal diffusivity of the eDPD system the reader can refer to the work of Abu-Nada [11].

Similarly, the value of Rayleigh number of the eDPD model is assigned by the ratio of the buoyancy forces to the viscous forces The viscous force is assigned by fixing the height of the domain (*H*). In the current study, *H* is fixed to 24. As for the buoyancy force, its value is assigned by fixing the temperature difference between the cold wall and the hot wall, i.e. ΔT , in addition to the value of the body force term ($g\beta$). In the current study, the temperature difference is fixed to $\Delta T=0.4$ and the body force term ($g\beta$) is changed to prescribe the value of buoyancy force and accordingly the value of the Rayleigh number. For full details for assigning the Rayleigh number of the eDPD system the reader can refer to the work of Abu-Nada [11].

In the current study, the Groot-Warren version of velocity-Verlet integration scheme is used to solve the eDPD governing equations. Full details of the integrations scheme used in this paper is found in [11].

The no-slip boundary condition at the four walls of the cavity was used by means of allocating extra wall layers of frozen particles. To avoid the penetration of fluid particles across the solid walls, the particles are bounced back.

With regards to the temperature boundary condition at the hot and cold walls, it is assumed that any particle hitting a wall will

acquire the same temperature of that wall. However, for the adiabatic walls, the conduction heat flux is simply set equal to zero. This condition is applied at top and bottom insulated walls in the cavity, see Fig. 1.

Nanofluid Physical Properties

The effective thermal conductivity of the nanofluid is calculated by the Chon et al. model [13] as:

$$\frac{k_{nf}}{k_{bf}} = 1 + 64.7\varphi^{0.7640}\left(\frac{d_{bf}}{d_p}\right)^{0.3690}\left(\frac{k_{bf}}{k_p}\right)^{0.7476} Pr_T^{0.9955}\, Re^{1.2321} \quad (15)$$

where Pr_T and Re are given respectively as:

$$Pr_T = \frac{\mu_f}{\rho_f \alpha_f} \quad (16)$$

$$Re = \frac{\rho_f k_b T}{3\pi\mu_f^2 l_f}, \quad (17)$$

In the above equations, *f* stands for the base fluid, which is water in this study, k_b is the Boltzmann constant, 1.3807×10^{-23} J/K, and l_f is the mean path of base fluid particles given as 0.17 nm [13]. The correlation for dynamic viscosity of CuO-Water nanofluid is derived using available experimental data of Nguyen et al. [14]. In a previous study, we have derived a correlation and a two-dimensional regression on the experimental data reported in Nguyen et al. [14]. This correlation for CuO-water nanofluids is defined as [5]

$$\mu_{CuO}(cp) = -0.6967 + \frac{15.937}{T} + 1.238\varphi + \frac{1356.14}{T^2} - .259\varphi^2 - 30.88\frac{\varphi}{T} - \frac{19652.74}{T^3} + .01593\varphi^3 + 4.38206\frac{\varphi^2}{T} + 147.573\frac{\varphi}{T^2} \quad (18)$$

Validation of the Numerical Model

The eDPD results for natural convection for pure fluid was validated in previous studies of the author against experimental and numerical published data. The validations is given in references [11 and15].In this paper we will also further validate the case of nanofluid against in-house nanofluid finite volume (FV) code developed for studying heat transfer enhancement using nanofluid. This nanofluid FV was validated and benchmarked against experimental results in previous publications of the author [5, 11, 15]. Figure 2 shows such validation and the figure shows a good match between the present nanofluid eDPD results and the in-house nanofluid FV code results.

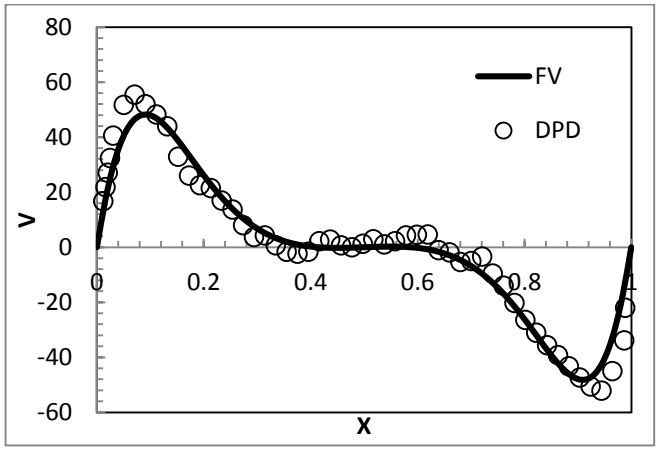
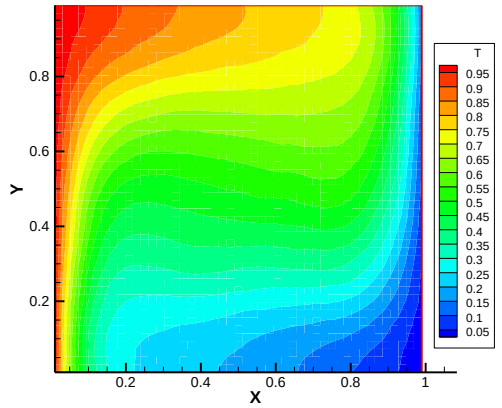


Figure 2 Code Validation: Vertical velocity comparison between current eDPD nanofluid results and FV results at the mid height of the cavity, Y = 0.5 and φ=3%.

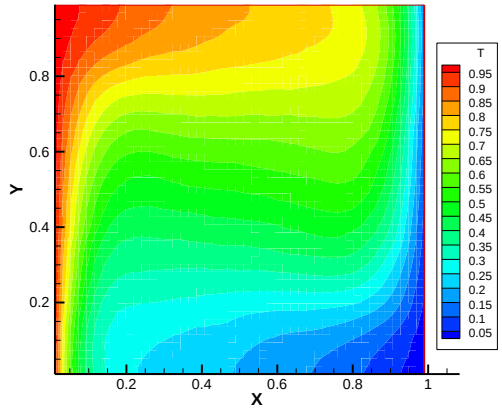
RESULTS AND DISCUSSION

In the current study, the nanofluids considered is CuO-water nanofluid. The volume fractions of nanoparticles considered is φ = 1 and 3 % and the Rayleigh number is fixed to Ra $=5\times10^4$. The thermophysical properties of nanofluid are assumed to vary only with volume concentration of nanoparticles and are independent of the nanofluid temperature. In other words, the thermal conductivity and the viscosity of nanoparticles (given by Eq. (15) and Eq. (18), respectively) are evaluated at a fixed temperature, which is the right wall cold temperature, which is taken as 22 °C in the present study.

Figure 3 presents the temperature isotherms in the cavity. The basic features of heat transfer in differentially heated cavities are captured by the eDPD simulation. For example, the isotherms are more vertical near the hot and cold walls and flatten horizontally in the middle of the cavity due to the dominance of convection. This is a basic feature of natural convection dominated by convection. Figure 3 illustrates some sensitivity of the thermal boundary layer thickness, at to the heated wall, to the concentration of nanoparticles. This sensitivity of thermal boundary layer thickness to volume fraction of nanoparticles is related to the increased viscosity at high volume fraction of nanoparticles. High values of φ increases the nanofluid viscosity which causes the velocity to decrease which accordingly reduces convection. Figure 4 shows the vertical velocity (y-component of velocity) distribution throughout the cavity and it is clear that higher concentration of nanoparticles decreases the fluid velocity in the cavity. The reduction in velocity and convection increases the thermal boundary layer thickness. The increase of thermal boundary layer thickness is responsible for the reduction in temperature gradients at the heated surface, which causes a reduction in Nusselt number.



(a)



(b)

Figure 3 Temperature isotherms (a) φ=3% (b) φ=1%.

Figure 5 (a) shows the local Nusselt number along the heated wall. The local Nusselt number along the heated wall is expressed as:

$$Nu = \frac{hH}{k_{nf}} \tag{19}$$

The heat transfer coefficient (h) is expressed as:

$$h = \frac{q_w}{T_H - T_L} \tag{20}$$

The thermal conductivity is expressed as:

$$k_{nf} = -\frac{q_w}{\partial T / \partial x} \tag{21}$$

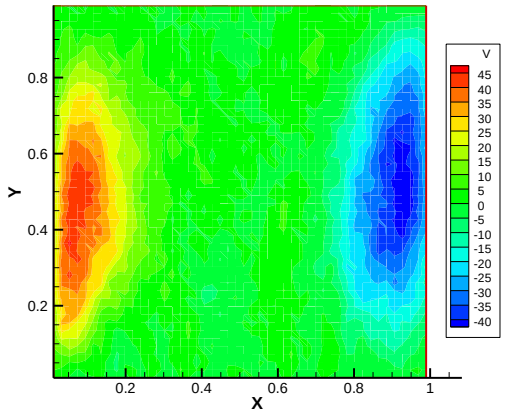
The average Nusselt number is defined as:

$$Nu_{avg} = \int_0^1 Nu(y)dy \tag{22}$$

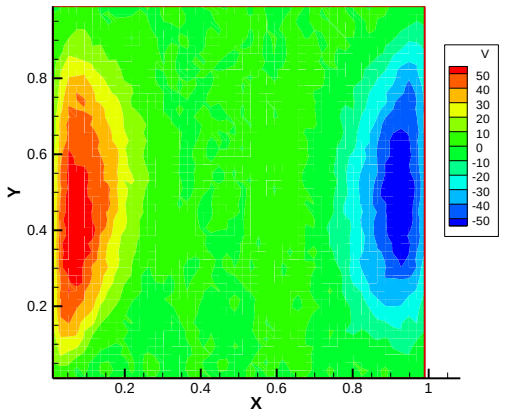
A 1/3rd Simpson's rule of integration is used to evaluate Eq. (22). A normalized Nusselt number is defined as the ratio of Nusselt number at any volume fraction of nanoparticles to that of pure water, and is given as:

$$\overset{*}{Nu}_{avg}(\varphi) = \frac{Nu_{avg}(\varphi)}{Nu_{avg}(\varphi = 0)} \tag{23}$$

The normalized Nusselt number is used as an indicator of heat transfer enhancement where values less than unity correspond to a deterioration in heat transfer. Figure 5(b) shows a decrease in Nusselt number with the increase of volume fraction of nanoparticles. The figure shows that the Nusselt number decreases up to 5 % for volume concentration of φ = 3%. The influence of nanoparticles has two opposing effects on the Nusselt number: a favourable effect that is due to the presence of high thermal conductivity nanoparticles, and an undesirable effect due to the high level of viscosity experienced at high volume fractions of nanoparticles.



(a)



(b)

Figure 4 Y-velocity contours in the cavity (a) φ=3% (b) φ=1%

The heat transfer in natural convection at high Rayleigh numbers is dominated by convection while at low Rayleigh numbers is dominated by conduction. For the Rayleigh number in hand, 5×10^4 , the heat transfer dominated by convection and by the presence of nanoparticles this will cause the nanofluid to become more viscous, which will reduce convection currents and accordingly reduce the temperature gradient and Nusselt number at the heated surface. This is accompanied by some enhancement in heat transfer due to the high thermal conductivity of nanoparticles but, such enhancement is small compared to the deterioration brought by viscosity. This is due to the reduction in the convection currents next to the heated surface, and due to the less pronounced role of Brownian motion, which is due to the

fact that the thermal conductivity of nanofluid is inversely proportional to the viscosity squared as shown in Eq. (17).

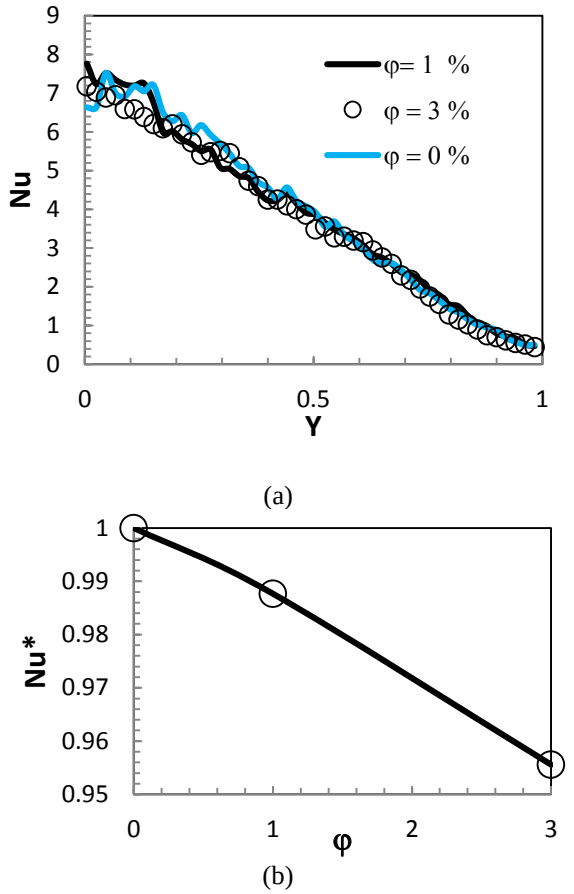


Figure 5 Effect of nanoparticles on Nusslet number (a) Local Nusslet number variation along the left heated wall of the cavity (b) Normalized average Nusslet number at the left heated wall of the cavity

CONCLUSION

Dissipative particle dynamics was applied to investigate the effects of nanoparticles on natural convection in differentially heated cavity. The eDPD simulations were benchmarked against finite volume solutions and it was found that dissipative particle dynamics appropriately predict the temperature and flow fields correctly in the cavity. The heat transfer was found to decrease by increasing the volume fraction of nanoparticles.

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