

# Simulation of heat transfer enhancement in nanofluids using dissipative particle dynamics



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## ABSTRACT

The current paper applied dissipative particle dynamics (DPD) approach to investigate heat transfer within nanofluids. The DPD approach was applied to study natural convection in a differential heated enclosure by considering the viscosity and the thermal conductivity of the nanofluid to be dual function of temperature and volume fraction of nanoparticles. Experimental data for viscosity and thermal conductivity are incorporated in the current DPD model to mimic energy transport within nanofluids. This incorporation is done through the modification of the dissipative weighting function that appears in the dissipative force vector and the dissipative heat flux. For the entire range of Rayleigh number considered in this study, it was found that the DPD results show a deterioration in heat transfer in the enclosure due to the presence of nanoparticles for  $\varphi > 4\%$ . However, some slight enhancement is shown to take place for small volume fraction of nanoparticles,  $\varphi \leq 4\%$ . The DPD results experienced some degree of compressibility at high values of Rayleigh number  $Ra \geq 10^5$ .

## 1. Introduction

The intrinsic low thermal conductivity of heat transfer fluids (HTFs) is considered a major drawback on the heat transfer in thermal systems. Recently, heat transfer enhancement using a suspension of nanoparticles in a base fluid has been used to enhance the intrinsic thermo-physical properties of the HTF. Such suspension is known as a nanofluid and it is shown to enhance heat transfer in forced convection applications. However, there is still a debate on the role of nanofluids on heat transfer enhancement in natural convection applications. Most theoretical nanofluids' studies on natural convection reported an enhancement in heat transfer in contradictory to the experimental findings.

Examples of such discrepancies are found in the early theoretical work reported by [1,2] where they reported an enhancement in heat transfer due to the addition of nanoparticles conflicting with the experimental results of Putra et al. [3] and Wen and Ding [4]. The numerical study of Abu-Nada et al. [5] and Abu-Nada [6] related such experimental deterioration in heat transfer to the high viscosity of the nanofluids colloids by the presence of nanoparticles which affects adversely the convection heat transfer. Also, they showed that the role of nanoparticles had an adverse effect on heat transfer enhancement in natural convection applications. Although such findings explained the reasons for the enhancement reported in early theoretical models. 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.

Abstractly, the mentioned theoretical studies relied on using the continuum models to study nanoparticles energy transport in base fluids. The main concern is whether at the nanoscale particles, the continuum assumption remains valid. In fact, spatial scales and temporal scales of the heat transfer within nanofluids are much larger than the discrete molecules models such as molecular dynamics (MD) and smaller than the conventional continuum models scales such as Navier-Stokes Equations (NES). Such intermediate spatial and time scales can be tackled using mesoscopic methods by means of coarse graining where each meso-particle represents a group of actual fluid molecules.

Dissipative particle dynamics (DPD) method is a coarse-grained version of MD introduced by Hoogerbrugge and Koelman [7], where each DPD particle represents a group of actual molecules. The DPD particles are randomly dispersed in the flow domain and the interaction among them follows conservation of mass, momentum and energy [8,9]. Español [9] and Avalos and Mackie [10] launched a version for energy conservative appropriate for studying heat transport by adding internal energy to the DPD system. Chaudhri and Lukes [11] recently conducted a comprehensive review of the DPD studies conducted in heat transfer. Actually, the DPD conducted studies in convective heat transfer are only limited to pure fluids and it is very important to extend the DPD approach to mimic convective heat transfer in nanofluids. Therefore, the scope of the present proposal is to extend the applicability of DPD to investigate the heat transfer, within nanofluids. The

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**Nomenclature**

$a$	repulsion parameter
$C_v$	specific heat at constant volume, J/kg.K
$c_s$	speed of sound
$d$	nanoparticle diameter, m
$e$	unit vector
$f$	force, N
$g$	gravity vector
$H$	enclosure height, m
$h$	heat transfer coefficient, W/m <sup>2</sup> .K
$K$	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 DPD particle
$Nu$	Nusselt number, $Nu = hH/k_{nf}$
$n$	normal vector
$p$	dimensional pressure, N/m <sup>2</sup>
$Pr$	Prandtl number, $Pr = \nu_c/\alpha_c$
$q$	heat flux, W/m <sup>2</sup>
$r$	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
$v$	velocity vector
$w$	weight function
$W$	width of the enclosure, m
$x, y$	dimensional coordinates, m
$X, Y$	dimensionless coordinates, $X = x/H, Y = y/H$
$\alpha$	thermal diffusivity, m <sup>2</sup> /s
$\alpha_{ij}$	random heat flux parameter
$\beta$	thermal expansion coefficient, 1/K

$\gamma$	dissipative force parameter
$\zeta$	random number for the momentum equation
$\zeta^e$	random number for the energy equation
$\theta$	dimensionless temperature, $\theta = (T-T_C)/(T_H-T_C)$
$\kappa$	collisional heat flux parameter
$\lambda$	random heat flux parameter
$\mu$	dynamic viscosity, N.s/m <sup>2</sup>
$\nu$	kinematic viscosity, m <sup>2</sup> /s
$\rho$	DPD number density
$\sigma$	amplitude of the random force
$\varphi$	volume fraction of nanoparticles (%)
$\Omega$	variable weight function

**Subscripts**

avg	average
bf	base fluid
C	cold
H	hot
i, j	indices
max	maximum
nf	nanofluid
p	particle
ref	reference
s	isentropic

**Superscripts**

C	conservative
cond	conduction
D	dissipative
R	random
visc	viscous

problem considered in this study is natural convection in a differential heated enclosure having CuO-water nanofluid as the working fluid. The bulk physical viscosity and the bulk thermal conductivity of nanofluids, that are both measured experimentally, will be incorporated in our current DPD model to mimic energy transport within nanofluids. The DPD model will be assessed over a wide range of Rayleigh numbers.

**2. Governing equations of the DPD system**

The current work investigates heat transfer enhancement in a differential heated enclosure filled with a CuO-water nanofluid. Fig. 1 shows the problem geometry where the height and the width of the enclosure are defined by  $H$  and  $W$ , respectively. The aspect ratio (i.e.,  $W/H$ ) 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 bottom walls are considered adiabatic and the standard Boussinesq model is used to approximate the density variation of the fluid. A number of coarse-grained DPD particles will be distributed within the enclosure to represent the CuO-water nanofluid. The equations governing for the motion and interaction between nanofluid DPD particles is given by the following set of equations, by adopting the Boussinesq approximation for the buoyancy forces [12–14]:

$$\frac{d\vec{r}_i}{dt} = \vec{v}_i \quad (1)$$

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

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

The heat flux vectors  $q_{ij}^{cond}$ ,  $q_{ij}^{visc}$ ,  $q_{ij}^R$  that appear in Eq. (3), account for conservative, viscous, and random heat fluxes respectively. The conservative force  $\vec{f}_{ij}^C$ , dissipative force  $\vec{f}_{ij}^D$  and random force  $\vec{f}_{ij}^R$  are expressed as [8]:

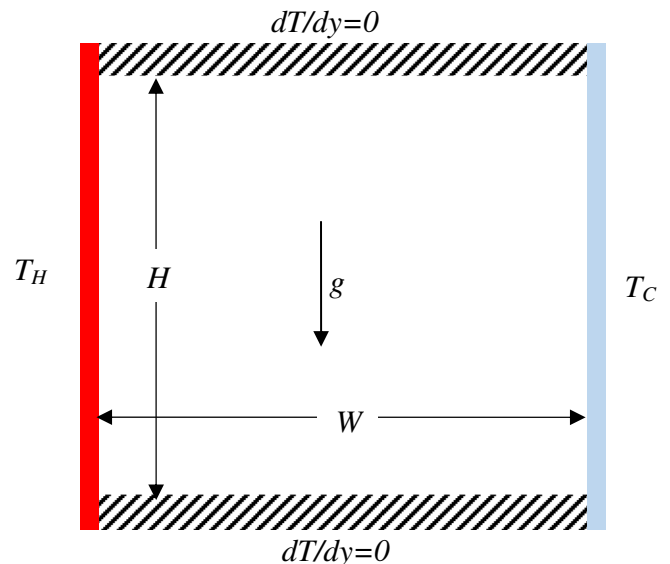


Fig. 1. Schematic of the problem geometry.

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