# NATURAL CONVECTION STUDY OF BROWNIAN NANO-SIZE PARTICLES INSIDE A WATER-FILLED CAVITY BY LAGRANGIAN-EULERIAN TRACKING APPROACH

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## ABSTRACT

In this research Lagrangian method is employed to track the nanoparticles inside a differentially heated walls nanofluid-filled cavity in natural convective flow. The thermo-physical properties of the solid-liquid mixture is also included in Eulerian frame. There are multiple interactions between fluid and particles which turns the simulations for solid-liquid highly complicated. ANSYS FLUENT 15.0 was used in this research to model submicron particles. Moreover, important interaction forces are implemented in the software as a User Defined Function (UDF) to modify the Lagrangian model. Brownian movement of the particles is assumed as a diffusion force acting on each particle during small user defined time step. Pressure gradient, gravity, virtual mass and Thermophoresis forces have also added to the force balance equation. Electrostatic forces are the contributing factors for stability of the nanofluid which they are needed to be present in dynamic equation of the particles. The importance of the forces on distribution of the particles is compared. The results show that the presence of these forces has considerable impact on nanoparticles concentration profiles.

## INTRODUCTION

Some experimental and theoretical analyses of nanoparticles-liquid mixture have shown that nanofluids thermo-physical properties can be treated as highly homogeneous mixture properties [1-3]. On the other hand, the distribution of nanoparticles concentration particularly at the vicinity of the walls cannot be ignored [4, 5]. Considering some important interaction forces could improve the heat transfer results and somehow concentration distribution of solid-liquid flows, but the nanoscale fluid flow is complicated and different than other sizes of particulate flows. Some researchers [6,7] mentioned that Brownian diffusion and thermophoretic forces are the main contributing factors of nanoparticles distribution and other forces are weak, such as non-uniform shear rate, viscosity gradient, gravity and so on. Hwang et al. [7] showed that thermo-physical properties of nanofluids are the most significant parameters in calculation of heat and flow features. Even though, knowing these will not lead to understand the real distribution of nanoparticles inside the flow.

Discrete phase modelling (DPM) could be the useful approach to cover some parts of weaknesses of others [8]. This model specifically considers the effects of each force in force balance equation of the particles. As a result, the influences of other forces such as lift force due to high and non-uniform shear rate and electrostatic forces can be included, which was mentioned by some researchers as the main phenomena happening in nanofluids [4]. Therefore, study of considering other forces specially lift, Brownian diffusion (as a force) and electrostatic forces in DPM is the motivation of this research. Also, the heat and flow features are calculated based on thermo-physical properties of the nanofluid and similar to single phase modelling.

## NOMENCLATURE

| | | |
|---|---|---|
| $A$ | [J] | Hamaker constant |
| $c_p$ | [J/kg.$^o$K] | specific heat |
| $d$ | [m] | diameter |
| $h$ | [m] | Particle to particle distance |
| $h_p$ | [W/m$^2$.K] | heat transfer coefficient |
| $K_B$ | [m$^2$.kg/$^o$K.s$^2$] | Boltzmann constant |
| $k$ | [W/m.$^o$K] | Thermal conductivity |
| $m_p$ | [kg] | particle mass |
| $Nu$ | [-] | Nussult number |
| $Pr$ | [-] | Prandtl number |
| $Ra$ | [-] | Rayleigh number |
| $Re$ | [-] | Reynolds number |
| $V_R$ | [J] | potential energy |
| $V$ | [m/s] | velocity |
| Special characters | | |
| $\alpha$ | [-] | volume fraction |
| $\alpha_0$ | [-] | initial volume fraction |
| $\varepsilon_0$ | [CV$^{-1}$m$^{-1}$] | vacuum permittivity |
| $\varepsilon_r$ | [-] | relative permittivity |
| $\dot{\gamma}$ | [1/s] | shear rate |
| $\kappa$ | [m$^{-1}$] | Debye-Huckel parameter |
| $\mu$ | [kg/m.s] | dynamic viscosity |
| $\rho$ | [kg/m$^3$] | density |
| $\psi$ | [V] | surface potential |
| $\tau_p$ | [s] | particle relaxation time |
| $\tau$ | [Pa] | shear stress |
| $T$ | [K] | temperature |
| *Subscripts* | | |
| $c$ | | Continues phase |
| $nf$ | | nanofluid |
| $p$ | | particle |

## MATHEMATICAL EQUATIONS

Only a few experimental studies of nanoparticles concentration distribution are available in literature. To validate the results of concentration distribution, the results of simulations for concentration distribution close to the wall is compared to the study of Zheng and Silber-Li [4]. They used fluorescent polystyrene 200nm size nanoparticles with density of 1050 Kg/m$^3$. On the other hand, the results of heat transfer are also compared to the experimental study of Ho et al. [9] for Alumina water-filled cavity. Alumina nanoparticles with 129nm size diluted in deionized water were used in their experiments inside a differentially heated vertical walls cavity with size of 25mm ×25mm×60mm. The flow remains in laminar regime in all the simulations. $Al_2O_3$ particle has 3600 kg/m$^3$ density, 765 J/kg K specific heat and 36 W/m.K thermal conductivity.

In DPM approach, nanoparticles are tracked as a large number of particles. The rest of the Navier-Stokes equations are treated as usual for a single phase fluid. A differential form of force balance equation is presented to a particle suspended in the flow to track the trajectory of the particle. It can be done during small chosen time step.

Mass, momentum and energy equation of continues phase:

$$\nabla.(\rho_{nf}\vec{V}) = 0 \tag{1}$$

$$\nabla.(\rho_{nf}\vec{V}\vec{V}) = -\nabla P + \nabla.\tau_{nf} + \rho_{nf} g \tag{2}$$

$$\nabla.(C_{p_{nf}}\rho_{nf}\vec{V}T) = -\nabla.(\vec{q}_{nf}) \tag{3}$$

The available interaction forces between particles and base fluid in Ansys Fluent 15.0 are drag force, pressure gradient, gravity, virtual mass forces. The other forces are needed to be implemented as a User Defined function, including Thermphoretic, mass diffusion, new lift, attractive van der waals and electric double layer repulsion forces. The equation of particle motion is written in unsteady Lagrangian frame as:

$$\frac{dV_p}{dt_p} = \frac{1}{\tau_p}\frac{C_D \,\mathrm{Re}_p}{24}(\vec{V}_c - \vec{V}_p) + \frac{\vec{g}(\rho_p - \rho_{nf})}{\rho_p} + \vec{F}_{pressure} + \vec{F}_{virtual} + \vec{F}_{thermo} + \vec{F}_{diffusion} + \vec{F}_{lift} + \vec{F}_{vdw} + \vec{F}_{EDL} \tag{4}$$

$$\tau_p = \frac{18\mu_{nf}}{\rho_p d_p^2} \tag{5}$$

Particle relaxation time $\tau_p$ is the criterion to choose proper time step, which is more or less $0.1\tau_p$. It can be expected gravity as the important force in natural convection.

Pressure gradient force and virtual mass force per particle mass:

$$\vec{F}_{pressure} = \left(\frac{\rho_{nf}}{\rho_p}\right)V_p \nabla V_c \tag{6}$$

$$\vec{F}_{virtual} = 0.5\left(\frac{\rho_{nf}}{\rho_p}\right)\frac{d}{dt}(V_c - V_p) \tag{7}$$

Thermophoretic force depend on the type of the base fluid and nanoparticles [12,13], and can be expressed as:

$$\vec{F}_{thermo} = -\frac{D_T}{m_p}\frac{\nabla T}{T} \tag{8}$$

$$D_T = 0.78\,\frac{\pi\mu_{nf}^2 d_p}{\rho_{nf}}\frac{k_{nf}}{2k_{nf} + k_p} \tag{9}$$

Nanoparticles mass diffusion force:

$$\vec{F}_{diffusion} = -\frac{K_B T}{m_p}\frac{\nabla\alpha}{\alpha_0} \tag{10}$$

Saffman Lift force, $\dot{\gamma}$ is the shear rate mainly important at the vicinity of the walls [4]:

$$\vec{F}_{lift} = 20.3\mu_{nf}(V_c - V_p)\sqrt{\frac{\dot{\gamma}\rho_{nf}}{\mu_{nf}}}\,\mathrm{sgn}(\dot{\gamma}) \tag{11}$$

Attractive van der waals force [10]:

$$\vec{F}_{vdw} = -\frac{1}{m_p}\frac{A}{6d_p}\frac{1}{x^2(x+1)^3(x+2)^2} \tag{12}$$

$$x = \frac{h}{d} \tag{13}$$

where $A$ and $h$ are Hamaker constant and surface to surface distance of two approaching particles. The amount of Hamaker constant is available [12] for Alumina nanofluid $4.44\times10^{-20}$ J and Polystyrene fluorescent in water $1.3\times10^{-20}$ J

Electrical double layer repulsion force [13]:

$$V_R = \pi d_p \varepsilon_0 \varepsilon_r \psi^2 \exp(-\kappa h) \qquad \kappa d_p < 10 \tag{14}$$

$$V_R = \pi d_p \varepsilon_0 \varepsilon_r \psi^2 Ln[1 - \exp(-\kappa h)] \qquad \kappa d_p > 10 \tag{15}$$

$$F_{EDL} = -\frac{1}{m_p}\frac{dV_R}{dh} \tag{16}$$

The exchanged heat at the surface of a particle is calculated as follows:

$$m_p c_{p_p}\frac{dT_p}{dt} = hA_p(T_c - T_p) \tag{17}$$

Heat transfer coefficient around a spherical particle can be estimated from the following correlation:

$$\frac{hd_p}{\kappa_{nf}} = 2 + 0.6\,\mathrm{Re}_p^{0.5}\,\mathrm{Pr}^{1/3} \tag{18}$$

## RESULTS AND DISCUSSION

To show the accuracy of the method, the concentration distribution of the Polystyrene fluorescent nanoparticles close to the wall is compared to experimental observation done by Zheng and Silber-Li [4] in Figure 1. The fitted average profile presented by Zheng and Silber-Li [4] is illustrated here. The measurements during their tests also revealed oscillation around the average profile similar to the Numerical method in this study with the forces added. As shown in Figure 1, the concentration profile predicted by the method with extra forces added provided better agreement with measurements.

On the other hand, the heat transfer features of the nanofluid-filled cavity in laminar natural convective flow is validated by the results of Ho et al. [9] in Figure 2. The good agreement between numerical simulation and measurements for Nusselt number is observed.

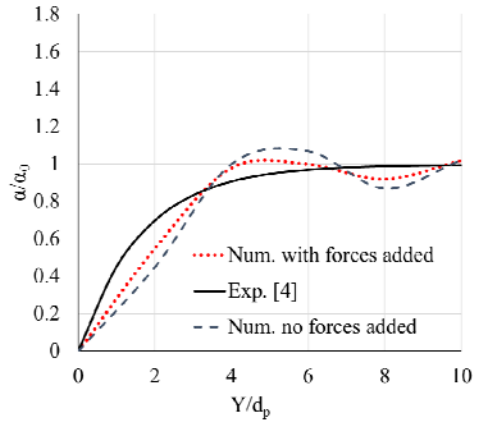



**Figure 1**. Concentration distribution of the Polystyrene fluorescent nanoparticles at the vicinity of the wall. "No forces added" means lack of thermophoretic, mass diffusion, lift and electrostatic forces.

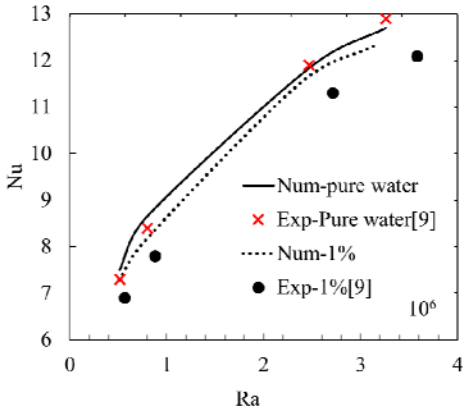
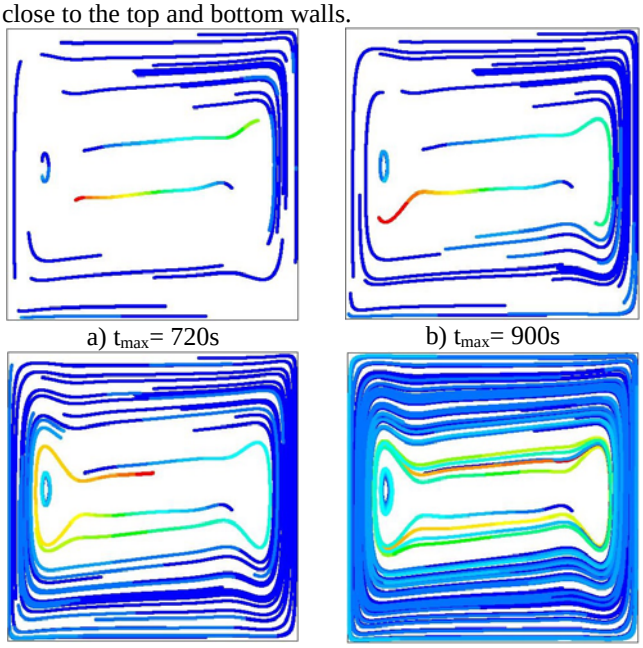



**Figure 2**. Nusselt number in a differentially vertical heated walls cavity with Alumina nanofluid inside.

The Lagrangian frame is used to track nanoparticles in a 2D cavity, some particle streams shown in Figure 3. The particles are tracked from the beginning till the given time is reached. As can be seen, the maximum residence time is initially reached at the middle of the cavity. Velocity with minimum value at the middle is the contributing factor on determination of nanoparticles time as $t=V/x$.

The relative velocity between fluid and particles is shown in Figure 4. Due to driving force in Y direction, the slip mechanism is stronger than X direction. The values on the hot and cold walls indicate that the slip velocity is noticeable inside the boundary layer and cannot be neglected for other simulation methods (such as Mixture model).

The impacts of each forces on the nanoparticles are presented in Figure 5 comparing to drag force. The drag force is clearly induced by the combination of all the forces and has the highest value. It is illustrated that only pressure gradient and virtual mass forces can be safely neglected, but the presence of other forces is essential. It is noted that van der waals and electric double layer forces are highly dependent on particle packing factor and increase in concentration will influence the values. The strongest force is thermophoresis and mainly in X direction, as expected due to high temperature gradient close to the hot and cold walls. The similar logic can be applied to diffusion and lift forces. Stronger lift force in X direction because of shear rate close to the hot and cold walls inside boundary layer and higher concentration gradient in Y direction close to the top and bottom walls.



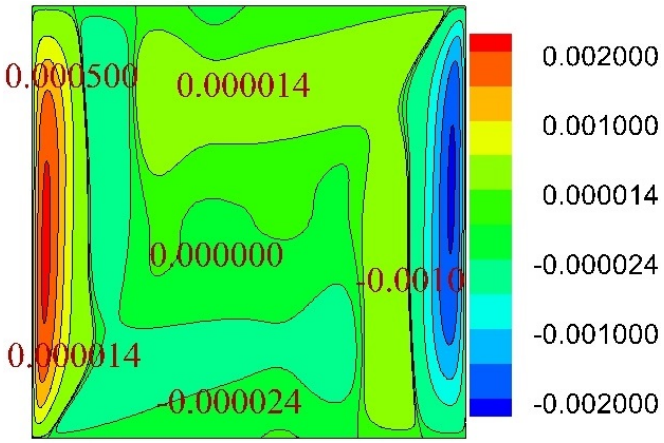
a) $t_{max}$= 720s b) $t_{max}$= 900s

c) $t_{max}$= 1300s a) $t_{max}$= 1900s

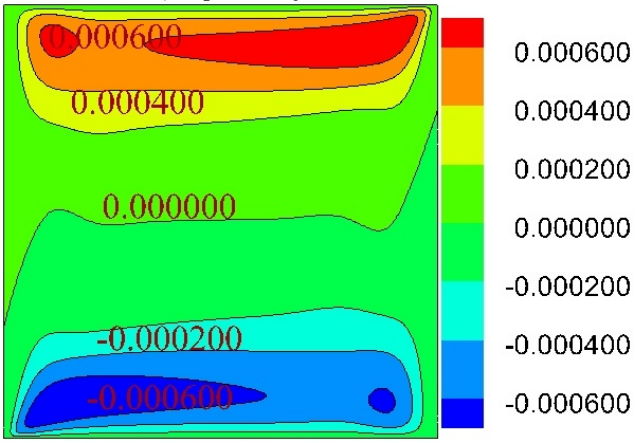
**Figure 3**. Alumina nanoparticles 0.1%vol. tracked inside a cavity colored by particle residence time, the blue and red represent t=0s and maximum time tracked ($t_{max}$), respectively.

## CONCLUSION

The influences of different forces on nanoparticles were investigated by Discrete Lagrangian Method (DPM) in this study. The acting forces included gravitational, pressure gradient, virtual mass, thermophoretic, diffusion, lift, attractive van der waals and repulsive electric double layer forces. The results of concentration profile and heat transfer features were found in good agreement with experimental measurements. The nanoparticles in a cavity natural convection mainly followed the base fluid streamlines almost from the beginning of Lagrangian tracking time frame. The relative velocity between nanoparticles and base fluid was found noticeable and cannot be ignored in simulations by other methods such as homogeneous mixture models. A comparison among all the present forces indicated that all the forces except pressure and virtual mass have considerable effects on the particles, with thermophoresis being the most effective. The simulation of natural convection on Lagrangian method takes long in terms of calculation time. Therefore, it needs smaller time step and also higher number of integral tracking steps for further investigation with increase in nanoparticles volume fraction.




a) slip velocity in Y direction




a) slip velocity in X direction

**Figure 4**. Relative velocity between base fluid and nanoparticles in Y and X direction for Alumina 0.1%vol nanofluid.

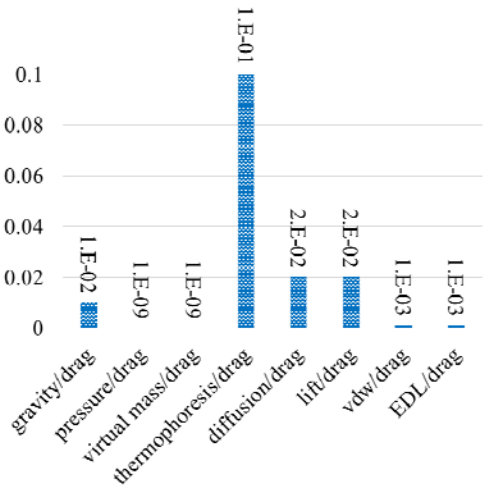



**Figure 5.** Comparing the effective forces on the particles relative to drag force in case of Alumina 0.1%vol in cavity natural convection.

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