

An Investigation on the Dynamic and Thermal Behaviour of Nanoparticulate Suspensions: A Numerical Study

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Abstract-

Nanoparticle suspensions also named nanofluids play a significant role in a wide and different range of applications like thermal and energy applications. In this study, a numerical investigation of the nanoparticle suspensions was carried out, taking into the consideration the interaction between the fluid molecules and the suspended nanoparticles in order to clarify its impact in the flow, heat transfer and transport properties. Also, Diffusion coefficients (Brownian and thermophoresis) were examined. The behaviour of the particulate suspensions was carried out in the term of drag coefficient and particle settling velocity which has a significant effect on the transport properties and thermal behaviour. The results were taken for two types of nanoparticles (Al_2O_3 and TiO_2) with different spherical nanoparticles size (20-50 nm) and with different nanoparticles concentrations (0.1-0.5 vol. %). In addition, to validate the results a comparison with previous results and other models was done, a good agreement was found with those results.

Keywords- Nanoparticle suspensions, buoyancy-driven convection, Brownian motion and Thermophoresis.

I. INTRODUCTION

Nanosuspensions refer to solid particles dispersed in the base fluids, researchers and engineers have been interested in particulate fluids for over a century, there are different applications including such type of fluids. Generally, particulate fluids flow are two-phase flow, in which one phase is the base fluid so called continuous or carrier phase while the another phase refers to a small immiscible particles also named the dispersed phase [1,2]. Nanoparticles are defined as those particles in the size range between 1 to 100 nm. Because of the small size of those particles, they have a high surface to volume ratio, thus high atoms in the surface and the ability to show quantum effects. The resulting innovative and unique properties of nanoparticles cannot be expected those from bulk materials. Nanoparticles exist with great variety in the form of carbon materials, metals, metal oxides ... etc. They also exhibit at different shapes such as spheres, hollow spheres, cylinders, platelets, disks and tubes, etc. [3,4].

In the field of nanosuspensions study, the understandings of dynamic mechanisms for the suspended nanoparticles are necessary to examine and clarify the basic concepts and the behaviour of the nanoparticles in the base fluid. Nanoparticles cannot be correctly characterized and described by applying the molecular or microscopic methods of analysis. Then, a new in-between field pushes a rise to some very unusual physics [5]. This unusual behaviour appears as results of the chemical and physical properties which are depend strongly on the size. At microscopic or macroscopic sizes, one piece of an element has the exact same properties of another piece of the same element. At the molecular level, an atom of an element has the exact same properties of another atom of the same element. But, something happened when the size of an element particle is in the nano range. The mechanical, chemical, physical and electrical properties of these bulk materials are different in the nanometer size. Further, a 10 nanometer particle size has different properties than of the same particle at different size, e.g., 20 nanometers. In order to understand the nanoparticles dynamic mechanisms in the base fluid it is necessary to examine the basic concepts of its behaviour and the forces which act on those nanoparticles [6,7].

Studying the motion and drag on a solid sphere was first observed by Stokes [8]. The problem of the unsteady motion behaviour of a solid sphere was described by Boussinesq and Basset by whom, the theory of the transient particulate flow was first observed [9,10]. Basset introduced an expression for drag on a small sphere with slip velocity in the solid-fluid interface was carried out by [11]. Maxey et al. represented a mathematical analysis for a solid sphere in an arbitrary irregular flow field [12]. Hadamard and Rybczynski studied the problem of a viscous sphere moving in a viscous fluid [13,14]. Schaaf et al. and Crowe et al. described the molecular effects on the heat and mass and momentum exchanges between suspended particles and fluid, In addition, flow regimes of suspended particles and droplets in the gases were specified for the flow [15,16].

With the advances in computational methods the velocities and positions of the suspended particles could be studied for different times. Rapaport showed molecular dynamic descriptions of various time-marching models simulations as well as useful software for their applications [17]. Brownian motion plays a significant role in the motion of suspended particles in nanofluids and it plays an important role in the transport properties of a nanofluid [18,19,20]. Berg studied Brownian dispersion coefficient and the sedimentation coefficient of the nanofluids in order to generate and clarify the specific information about particle aggregation [21]. Puragliesi et al. investigated numerically particle deposition in the buoyancy driven flow of the differentially heated cavity (DHC), three values of the particle diameter

($d_p = 14,25,30 \mu m$) was considered. The Lagrangian model has been chosen for the suspended particles. The forces taken into account are drag, gravity, buoyancy, lift and thermophoresis [22].

In the present work, numerical study was carried out to investigate the effect of fluid Molecules-suspended particles interaction on the dynamic mechanism of nanoparticle suspensions under buoyancy-driven convection. The numerical model is the two-phase model. The study investigated different sizes (20-50 nm) of spherical nanoparticles (Al_2O_3 and TiO_2) with different nanoparticles concentrations ($\phi = 0.1 - 0.5 \text{ vol.}\%$), to observe the impact of these parameters on the behaviour of the particulate suspensions in the presence of temperature gradient. Slip forces (drag, Brownian and thermophoresis) were investigated. Also, particle settling velocity was examined. A good agreement was found between presented work results and those from other models and previous researches.

II. MATHEMATICAL MODELING

The unique approach which is able to account the effect of the slip motion between the suspended nanoparticles and the base fluids is the two-phase approach. Unlike other multiphase flow models, where the phases flow in geometrically different and very complex flow regimes (e.g., bubbly, churn, or plug flow in vapour-liquid systems) the particulate flow systems are composed of suspended particles or clusters of suspended particles within the base fluids [23].

Solving the effect of Brownian diffusion and thermophoresis as a major mechanisms in which the suspended nanoparticles can develop a promote relative velocity with respect to the base fluid (Brownian diffusion occurs from high to low concentrations of nanoparticle, while thermophoresis occurs from hot to cold direction) [24]. Fig. 1 shows the Brownian motion between fluid molecules and suspended nanoparticles which is the most important technique for enhanced thermal behavior and transport properties of nanofluids. The temperature of base fluid, particle size and particle concentration play an important role in the Brownian motion [25].

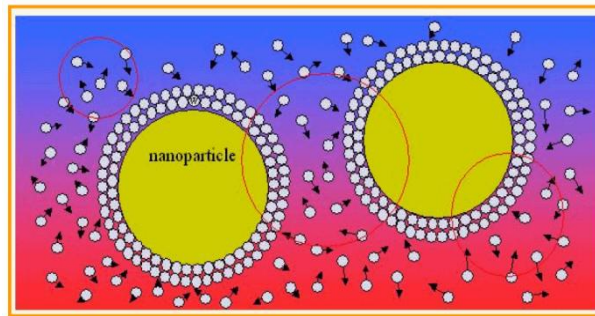


Fig. 1 Brownian motion between fluid molecules and suspended nanoparticles [25]

A. Governing equations

The main assumptions of the model in this study are an enclosure space contains incompressible and laminar flow, without pressure work and viscous dissipation, local thermal equilibrium between suspended nanoparticles and fluid, physical properties of the nanofluid depend on both nanoparticles concentration and temperature. Fig. 2 shows an enclosure geometry include a particulate suspension with one hot side and one cold side while the other sides are assumed to be adiabatic.

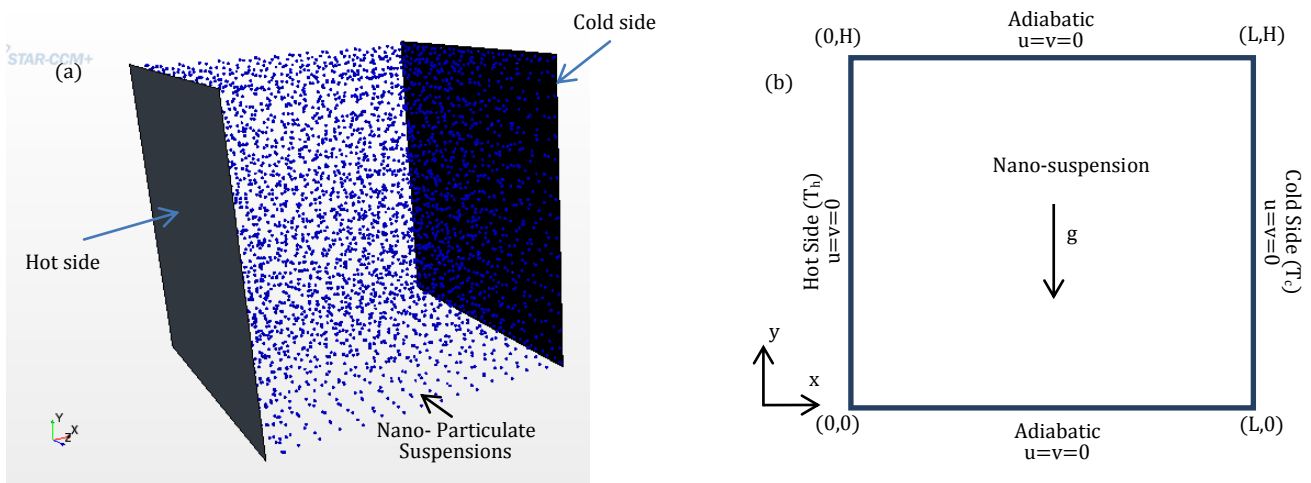


Fig. 2 Enclosure geometry (a) enclosed space contains a particulate suspension (b) coordinate system

Then the governing equations (continuity, momentum, and energy) for the nanofluid, and the continuity equation for the suspended nanoparticles can be written as [23]:

$$\frac{\partial \rho_{nf}}{\partial t} + \nabla \cdot (\rho_{nf} V) = 0 \quad (1)$$

$$\frac{\partial(\rho_{nf}V)}{\partial t} + \nabla \cdot (\rho_{nf}VV) = \nabla \cdot \tau + \rho_{nf}g \quad (2)$$

$$\frac{\partial(\rho_{nf}C_{p,nf}T)}{\partial t} + \nabla \cdot (\rho_{nf}VC_{p,nf}T) = \nabla \cdot (k_{nf}\nabla T) \quad (3)$$

$$\frac{\partial(\rho_{nf}m)}{\partial t} + \nabla \cdot (\rho_{nf}Vm) = -\nabla \cdot J_p \quad (4)$$

Where (V) is the velocity vector, (T) is the temperature, (t) is the time, (g) is the gravity vector, (τ) is the stress tensor, (J_p) is the suspended particles diffusion mass flux, (m) is the mass fraction or nanoparticles concentration ($m = \rho_p\phi/\rho_f$), (ρ_{nf}) is the nanofluid effective density, ($C_{p,nf}$) is the nanofluid effective specific heat at constant pressure, (k_{nf}) is the nanofluid effective thermal conductivity and (μ_{nf}) is the nanofluid effective dynamic viscosity.

The thermophysical properties of the nanosuspension can be defined as following [26,27]:

$$\rho_{nf} = (1 - \phi)\rho_f + \phi\rho_p \quad (5)$$

$$C_{p,nf} = \frac{(1 - \phi)(\rho C_p)_f + \phi(\rho C_p)_p}{(1 - \phi)\rho_f + \phi\rho_p} \quad (6)$$

The thermophysical properties of nanofluids depend not only on the loading of nanoparticles but also on the temperature of nanofluids. Therefore, in the recent numerical researchs, a correlation was developed to obtain the effective thermal conductivity (k_{nf}) and the effective dynamic viscosity (μ_{nf}) of the nanofluids, this correlation was based on an extensive set of experimental results [26,27]:

$$\mu_{nf} = \frac{\mu_f}{1 - 34.87(d_p/d_f)^{-0.3}\phi^{1.03}} \quad (7)$$

$$k_{nf} = (1 + 4.4Re_p^{0.4}Pr_f^{0.66}(T/T_{fr})^{10}(k_p/k_f)^{0.03}\phi^{0.66})k_f \quad (8)$$

Where (ϕ) is the nanoparticles volume fraction, (Re_p) is the nanoparticle Reynolds number, (Pr_f) is the Prandtl number of the base fluid, (T_{fr}) is the freezing point of the base fluid, (k_f and k_p) are the thermal conductivities for the base fluid and nanoparticles respectively, (d_p) is the nanoparticle diameter and (d_f) is the base fluid molecule equivalent diameter.

$$Re_p = \frac{\rho_f v_p d_p}{\mu_f} \quad (9)$$

Where: (v_p) is the nanoparticle Brownian velocity which is calculated as the ratio between (d_p) and the time (t_D) required to cover this distance [28]:

$$t_D = d_p^2/6D_B \quad (10)$$

Where D_B is the Brownian diffusion coefficient, Hence:

$$Re_p = \frac{2\rho_f k_B T}{\pi\mu_f^2 d_p} \quad (11)$$

Where: ($k_B = 1.38 * 10^{-23}$ J/K) is the Boltzmann constant. In the above equations the physical properties are calculated at the nanosuspension temperature (T).

The base fluid molecule equivalent diameter (d_f) can be defined as [29]:

$$d_f = 0.1(6M/N\pi\rho_{fT_0})^{1/3} \quad (12)$$

Where (M) is the molar mass, ($N = 6.022 * 10^{23}$) the Avogadro number, and (ρ_{fT_0}) is the fluid density at reference temperature ($T=293$ K).

By Assuming the nanosuspension as a Newtonian fluid, the stress tensor can be written as [29,30]:

$$\tau = \left(P + \frac{2}{3}\mu_{nf}\nabla \cdot V\right)I + \mu_{nf}[\nabla V + (\nabla V)^t] \quad (13)$$

Where (P) is the pressure, (I) is the unit tensor and the superscript (t) represents the transpose of (∇V).

The diffusion mass flux of the suspended nanoparticles can be calculated as the sum of the Brownian and thermophoretic diffusion terms, for low nanoparticles concentration [31]:

$$J_p = -\rho_{nf} \left(D_B \nabla m + D_T \frac{\nabla T}{T}\right) \quad (14)$$

Where (D_B and D_T) are the Brownian and thermophoretic diffusion coefficients respectively.

By setting the boundary condition at the wall, in addition Dirichlet or Neumann boundary conditions (temperature and no-slip boundary condition of velocity), zero nanoparticles diffusion mass flux ($J_p = 0$).

B. Brownian diffusion

Brownian motion (or molecular diffusion) becomes the dominant collection mechanism for particles less than 50 nm and it becomes more significant as the suspended particles become smaller. The Brownian movement of the suspended particles was first observed by Robert Brown in (1837) and then it was described analytically by Albert Einstein (1905) [32]. The fluid molecules have significantly high velocities and these velocities depend on the temperature of the fluid. In fact, the velocities of fluid molecules define the temperature of fluid as shown in the expression [33,6]:

$$T = \frac{m_m \bar{V}^2}{3k_B} \quad (15)$$

Where (m_m) is the mass of a molecule, (\bar{V}) is the magnitude of the velocity of the fluid molecules.

In the particulate fluids, small suspended particles deflect slightly when fluid molecules impact on them. Furthermore, kinetic energy transfers from the fast moving fluid molecules to the small particle. The diffusivity provides an indication of the extent at which molecular collisions cause very small suspended particles to move in a random manner across the direction of fluid flow. The diffusion coefficient in the equation below represents the diffusivity (D_B) of a particle [33,34]:

$$D_B = \frac{C_c k_B T}{3\pi d_p \mu_f} \quad (16)$$

Where (d_p) is the diameter of the suspended particle, (μ_f) is the dynamic viscosity of the base fluid and (C_c) is The Cunningham Correction Factor and it can be estimated as following [35]:

$$C_c = 1.0 + \frac{(6.21 \times 10^{-4})}{d_p} T \quad (17)$$

C. Thermophoretic diffusion

Thermophoresis is a consequence of the Brownian movement of suspended particles, and from the previous it can be observed that the particle dispersion is higher and the Brownian force become stronger when the local fluid has higher temperature. In the particulate system, when there is a temperature gradient in the flow domain small particles tend to disperse faster in hotter regions and slower in colder regions. This causes the particles migration from hotter to colder regions, the result of the migration is the particles accumulation and higher suspended particles concentrations in the colder regions of the suspension. The phenomenon of thermophoresis was first examined by [36]. Fig. 3 shows the differential dispersion and the resulting thermophoresis, the effect of the Brownian motion on small spherical particles which are suspended in the base fluid with a transverse temperature gradient is also shown.

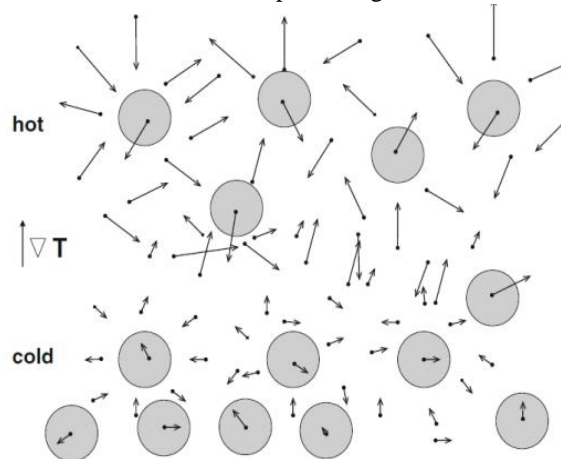


Fig. 3. Collisions with the molecules and the resulting Brownian motion cause the migration of particles [33]

Thermophoretic diffusion coefficient (D_T) is written as following:

$$D_T = \beta \frac{\mu_f}{\rho_f} m \quad (18)$$

Where: (β) is the thermophoresis parameter, for nanofluids containing metal oxide nanoparticles, can be estimated by using the following expression [38]:

$$\beta = \left[(1.519 * 10^4) \left(\frac{k_p}{k_f} \right)^{-3} + 0.95 \right] * [-16.32(\phi)^{2.34} + 0.0193] \quad (19)$$

D. The drag force

The resistive or drag force arises whenever there is a difference in velocity between a suspended particle and its surrounding fluid. Then, the fluid will exert a drag force at the particle. The drag coefficient is related to the velocity of the suspended particles and the flow pattern of the fluid around those particles. While, the Reynolds number (Re_p) of the particle is used as an indication to define this flow regimes. Three regimes were observed from experiments which are laminar (Stokes), transition (intermediate), and turbulent (Newtonian). These three regimes are related to the particle Reynold as [6,33]:

$$\begin{aligned} C_D &= 24/Re_p && \text{Laminar } (Re_p < 2.0) \\ C_D &= 18.5/Re_p^{0.6} && \text{Transition } (2.0 < Re_p < 500) \\ C_D &= 0.44 && \text{Turbulent } (Re_p > 500) \end{aligned} \quad (20)$$

In addition, another empirical drag coefficient model was given by Barnea et al. [39]:

$$C_D = [0.63 + (4.80/\sqrt{Re_p})]^2 \quad (21)$$

Fig. 4 shows the relation between the spherical particle Reynolds number and drag coefficient, the figure divided the flow into three regimes according to the nanoparticle Reynolds number [34].

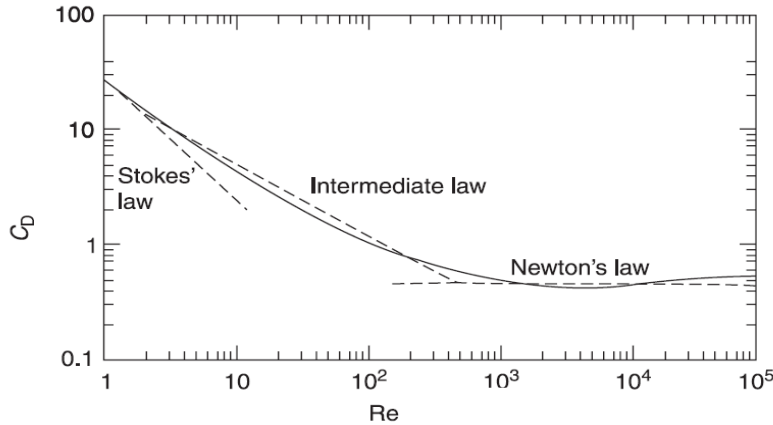


Fig. 4 Drag coefficient for spheres [34]

E. Settling velocity

One of the most important parameter that affects the particle dynamic behaviour is the particle settling velocity. This constant velocity, where all the acting forces on the nanoparticles balance out, is termed as the terminal velocity. In order to calculate this velocity, a dimensionless constant (*K*) is used to determine the proper range of the fluid–particle dynamic laws [6,39].

$$K = d_p(g\rho_p\rho_f/\mu_f^2)^{1/3} \quad (22)$$

Where, the values of *K* in the flow patterns (*K* < 3.3) for Stokes' range, (3.3 < *K* < 43.6) for Intermediate range and (43.6 < *K* < 2360) for Newtons' range. The particle settling velocity is as following:

$$v_t = \frac{gd_p^2\rho_p}{18\mu_f} \quad (\text{Stokes' regime})$$

$$v_t = \frac{0.153 g^{0.71} d_p^{1.14} \rho_p^{0.71}}{\mu_f^{0.43} \rho_f^{0.29}} \quad (\text{Intermediate regime}) \quad (23)$$

$$v_t = 1.74(gd_p/\rho_f)^{0.5} \quad (\text{Newtonian regime})$$

Because the diameter of the spherical nanoparticles is very small, the nanoparticles Reynolds number ($Re_p \ll 1$), and the dimensionless constant ($K \ll 1$). In other words, the nanoparticle suspensions are assumed in the Stokes' regimes low.

III. RESULTS AND DISCUSSION

Numerical investigation was doen by applying the two phase approach using STAR-CCM+ program, two types of nanoparticles (Alumina and Titania) with different spherical nanoparticles size and concentration suspended in the base fluid (water).

Fig. 5 shows the temperature profile in the enclosure which contains the nanosuspension, temperature distributed from the hotter to the colder sides. Fig. 6 shows the velocity vectors and it represents the circulation of the nanosuspension under the effect of the temperature gradient and gravitational force. The motion of the working fluid (nanosuspension) gives an indication about the diffusion of the nanoparticles and the migration from hotter to colder regions. Those figures were taken for the water based TiO₂ nanosuspension ($d_p = 50 \text{ nm}$) and ($\phi = 0.3 \text{ vol. \%}$).

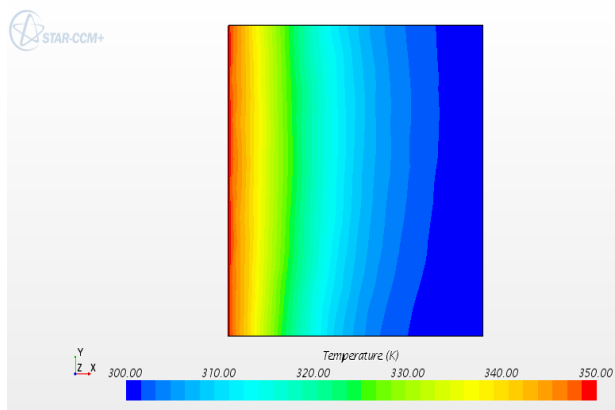


Fig. 5 Temperature distribution of the particulate suspension

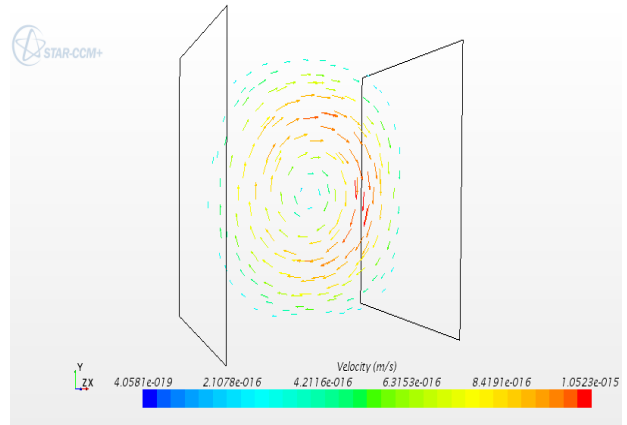


Fig. 6 velocity vector of the particulate suspension

Fig. 7 shows the velocity magnitudes of the nanosuspension inside the enclosure for two types of suspended nanoparticles (Al_2O_3 and TiO_2), particles size ($d_p = 50 \text{ nm}$) with different nanoparticles volume fraction ($\phi = 0.1, 0.3 \text{ and } 0.5 \text{ vol. } \%$), these figures represent the effect of the nanoparticle type on the velocity magnitude distribution because the different physical properties from particle to particle type. Also it can observe that when increasing the nanoparticles concentration (volume fraction) the velocity increases because of the collisions of the nanoparticles in the base fluid or specified limits of volume fraction.

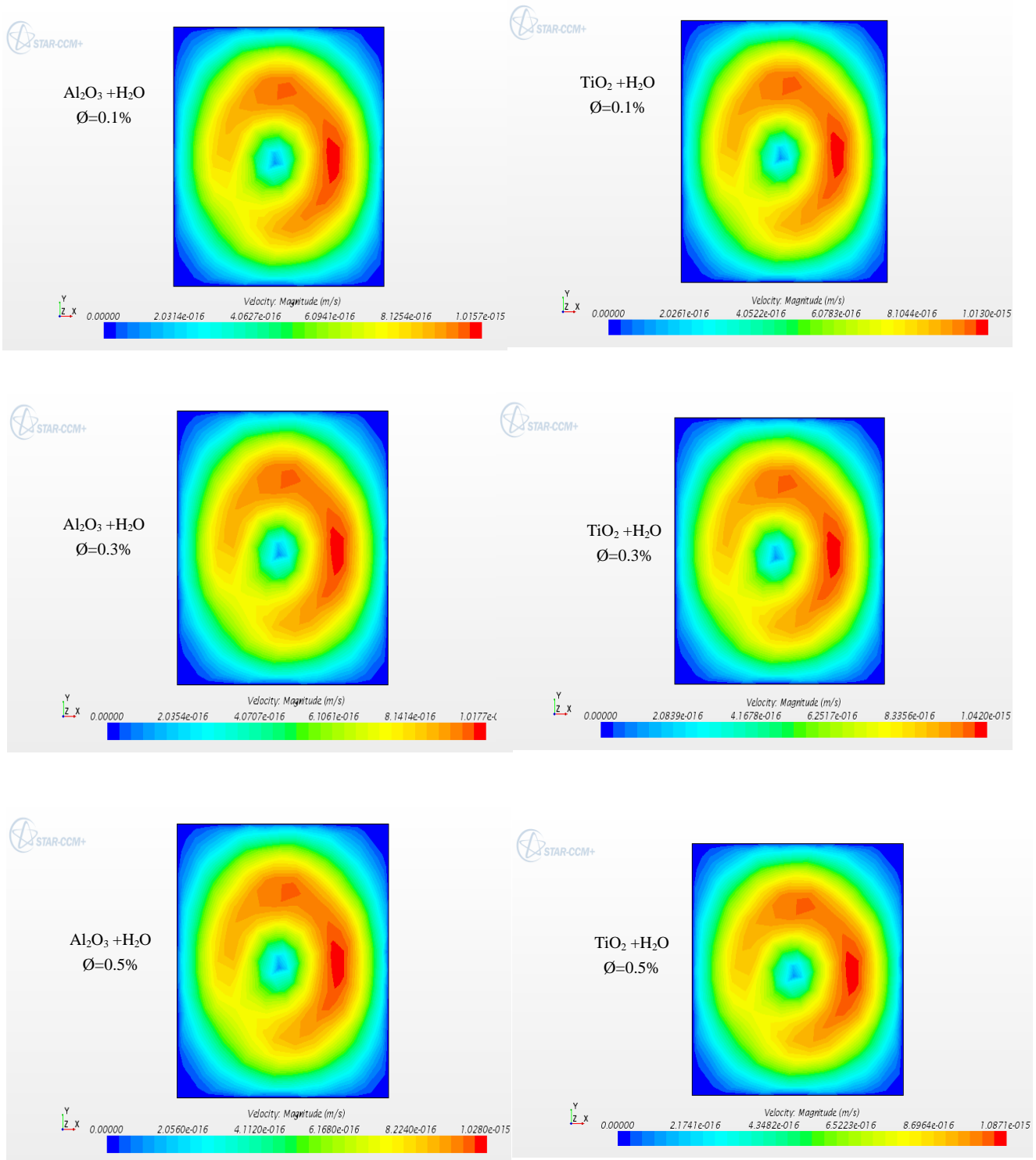


Fig. 7 Velocity magnitude distribution for different nanosuspensions

Fig. 8 shows the relation between the suspended nanoparticle diameters and the Brownian diffusion coefficient. The results were estimated for different average temperature of the nanoparticle suspension, in order to quantify the effect of the temperature on the Brownian diffusion coefficient. Fig 9 shows the effect of the nanoparticles concentration on the thermophoresis parameter for different thermal conductivities ratios (nanoparticles-base fluid thermal conductivity ratio). It shows that the thermophoresis parameter increases with the decreasing of thermal conductivity ratio. And, it decreases with increasing the nanoparticles volume fraction. Figs. 8 and 9 were calculated for (Al_2O_3) nanoparticles.

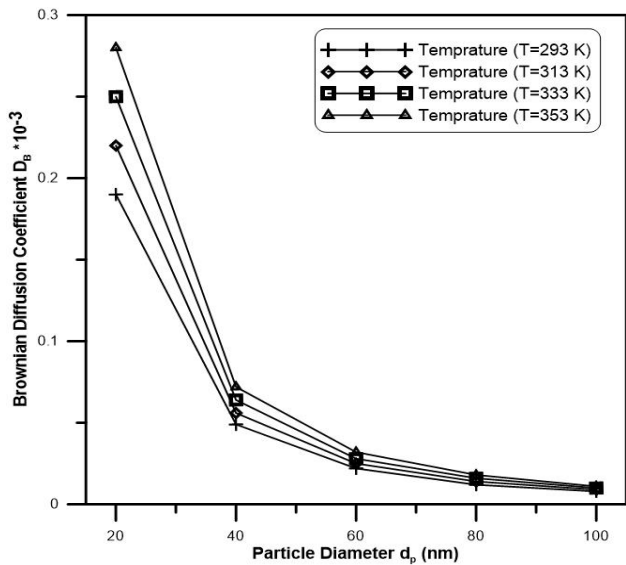


Fig. 8 Suspended particle (Al_2O_3) diameter versus the Brownian diffusion coefficient

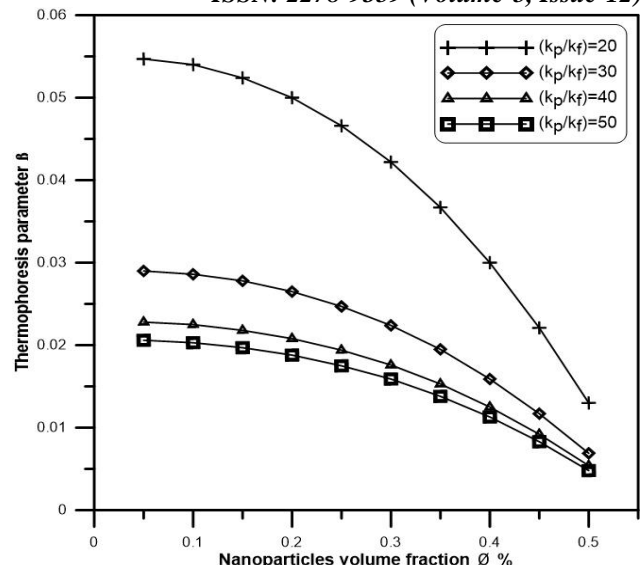


Fig. 9 The relation between nanoparticles (Al_2O_3) volume fraction and thermophoresis parameter

Fig. 10 represents the relation between the nanoparticle Reynolds number and the drag coefficient on the (Al_2O_3) nanoparticles for different nanofluid temperatures. As shown in the figure, because the nanoparticle Reynolds number ($Re_p = f(T, d_p)$) it can be observed that the nanoparticle drag coefficient increases when the nanoparticle size increases while it decreases when the nanofluid temperature increases. In order to validate those results a comparison was done by using another model of empirical drag coefficient which was given by Barnea et al. [35].

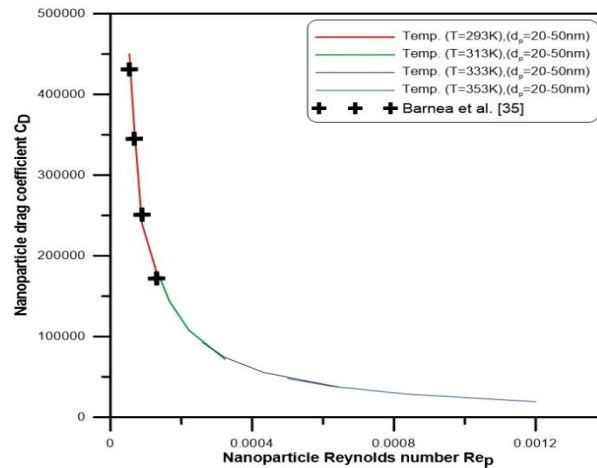


Fig. 10 Nanoparticles (Al_2O_3) Reynolds number versus drag coefficient for different temperature

Fig. 11 shows the relation between the nanoparticles diameter and the nanoparticle settling velocity for the two nanoparticles types (Al_2O_3 and TiO_2), also the obtained results were compared with others from Kim et al. [39].

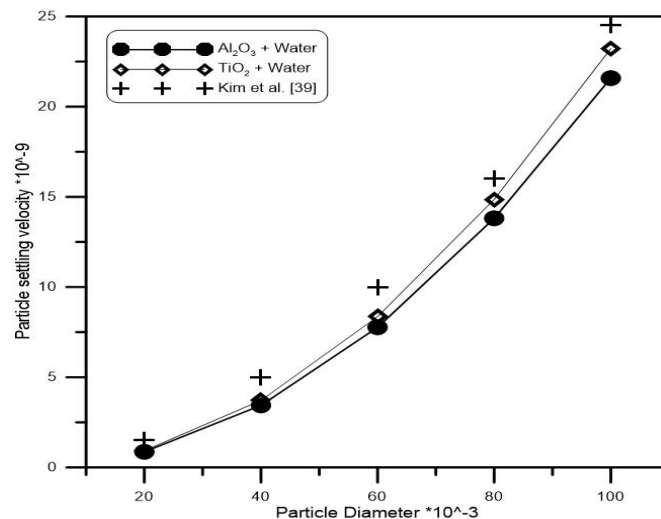


Fig. 11 The relation between Nanoparticles diameter and particle settling velocity

IV. CONCLUSION

The suspended particles dynamic mechanism investigation play an important role in the understanding thermal behaviour and the the energy transport in the particulate suspensions like nanofluids. The fundamentals of energy transport in such types of fluids is the key to develop energy-efficient nanofluids for a wide range of heat transfer applications. Therefore, Brownian motion between suspended nanoparticles and fluid molecules is a key for enhanced energy transport and thermal behavior of nano-particulate suspensions (nanofluids). Fluid temperature, particle size and particle concentration, are closely related to Brownian motion.

An important factor that effects the suspended particles dynamic behaviour is the particle settling velocity (terminal velocity) in the downwards direction, when the density of the particle exceeds the density of the fluid. It is observed that the terminal velocity of the nanoparticles is very low for different particle size. The suspended nanoparticles are not expected to settle even in fluids with low viscosity such as water. Therefore, sedimentation of nanoparticles is not an issue of concern for nanofluids. Nanoparticles settling become an issue if the nanoparticles aggregation take place to form significantly larger clusters, Suspended particle interactions with fluid molecules may cause the formation of aggregates. Clusters and aggregates influence significantly the structure of the particulate suspension and transport properties of nanofluids.

As indicated from the results, the drag force arises when suspended particle moves through fluids. The suspended particles displace the fluid immediately in front of it, this causes momentum transfer to the fluid. The drag force produced is physically equal to the momentum per unit time transferred to the fluid by the suspended nanoparticles. Since the suspended nanoparticle has a velocity a portion of this velocity is transferred by momentum to the fluid (as fluid molecules velocity), the amount of energy transferred from suspended particle to fluid molecular is related to a friction factor which is so called the drag coefficient.

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