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Research Article

# Numerical Study of Viscoelastic Behaviour of Nanofluids

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***Abstract***

*The addition of nanoparticles to the fluids such as water has improved load carrying capacity of such fluids. The key idea is to exploit the viscoelastic properties of nanofluids which can withstand higher loads by adding nanoscale particles in low volumetric fractions to a fluid in order to improve their rheological, mechanical, and thermal properties. The behaviour of shear stress and the viscosity of nanofluids have been studied based on some of the empirical models developed. In this paper an overview of the recent developments in the study of heat transfer using nanofluids is presented. The nonmaterial in base fluid shows some agglomeration in 5µm -8µm, however and the load carrying capacity of the fluid are found to be improved due to the addition of nanoparticles in the base fluid. The viscoelastic properties of the nanofluids are found to be improved with increasing concentration.*

***Keywords:*** *Nanofluid simulations, viscoelastic flows, Molecular dynamics.*

## 1. Introduction

It has been recognized that suspension of nanoparticles in the liquids has improved load carrying capacity in fluids. The key idea is to exploit the rheological properties of nanofluids which can be made by adding nanoscale particles in low volumetric fractions to a fluid in order to improve their rheological, mechanical, and thermal properties. The base fluid can be any liquid such as water, oil, ethylene glycol, or conventional fluid mixtures. Limited available studies on nanofluid viscosity have been reported (R. Prasher et al, 2006), (B. Wang et al, 2004),( P. K. Namburu et al,2007). In most of the research, the behaviour of shear stress and the viscosity of nanofluids have been interpreted. Some of the empirical models developed are limited either to the zero or one dimensional. (N. Casson et al,1959) developed widely used empirical model.

To clearly understand the fluid behaviour at nanoscale two dimensional models could give us the better and meaningful information. (Phuoc et al , 2009, Massoudi et al 2011), obtained the values for suspension viscosity used casson empirical equation and for various nanoparticles and its suspension in the base fluid such as water (E.C.Bingham et alm1922) . It was experimentally proved that the deionized water-nanofluids with poly-ethylene-oxide or poly-vinyl-pyrrolidone as a dispersant, have significantly improved the rheological properties in the fluid, it was experimentally proved but there is not computational model obtained to fully understand the nanofluid behaviour in various conditions.

(Choi. et al,1998), (T. M. Kwon et al, 2000) calculated the intrinsic viscosities of CrO2—ethylene glycol, $\gamma$-Fe2O3, $\alpha$-Fe2O3—EG and Ba-ferrite-EG nanofluids at infinite shear rate and reported a decrease of the viscosity with an increase in the particle volume fraction. This could be problematic, since the intrinsic viscosity should reach the viscosity of the base fluid in case of dilute suspensions or increase as the particle volume fraction increases if the suspension is dense enough. It is important to understand the engineering behaviour and correct nature of the nanofluids and its behaviour under different external forces and boundary conditions to appropriately conclude about the applicability of the nanofluids in engineering applications.

The existing understanding of the effective compressibility and viscous behaviour of the is ineffective and one can take the help of atomic level molecular dynamics approach to know the underlying nanofluids behaviour so that they can be applied to the engineering applications.

In this paper by examined the factors such as stress and strain in $Al_2O_3$ nanofluid molecules by considering rectangular two dimensional wall model and the fluid atoms in the form of clusters in the control area with which can understand the mechanical behaviour of the clustered atoms of nanofluids in the base fluid water (R. G. Larson et al,1998),( R. B. Bird etal,1977), (Bang, I. C. et al, 2005 ), (K. V.Wong et al 2010). Numerical simulations were conducted with micro rectangular container. It is considered that the nanofluids behave in special motions of rotation and translation but also affected by the interactions of nanoparticles. The walls of the cylinder are dynamic and The Lennard-Jones potential

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model is implemented to deal with the interactions between atoms. The behaviour and interaction of nanoparticles at different time through friction process and impact of nano particles could be obtained the nature of nanofluids under load system could be analyzed.

## 2. Molecular Dynamics Modelling

In general, most complex fluid flows, such as nanofluids flow, is nonlinear, since they exhibit unusual and peculiar characteristics such as visco-elasticity, fluctuating yield stress, normal stress differences. It is investigated concentrated nanoparticles suspensions in base fluids. The non-linear time-dependent response of such fluids obeys, Stokes law of drag. To formulate the mathematical equation of nanofluid flow in the micro container it is assumed that the viscous drag is equal to the buoyancy force. It is considered that the slip-flow and creep flow of a nanofluid in a micro container with a radius *a*. The nanofluid is treated as a power-law non-Newtonian fluid of steady and incompressible flow, constant number of atoms in the molecules of fluid with negligible radial velocity and energy dissipation effects.

$$\tau^* = \frac{r^*}{2}\frac{dp^*}{dz^*} = m(-\frac{du}{dr^*})^n \quad (1)$$

$p^*$ the pressure
$u$ the axial velocity
$r^*$the axial location

The values of *m*,*n* are functions of the volume fraction of the nanoparticles. It should be noticed that in our work we consider the nanofluid as a single-phase fluid, so the slip here is only between the nanofluid and the wall of the container with boundary conditions

$$u^*(a) = L_s^0\dot{\gamma_w}\,(1-\frac{\dot{\gamma_w}}{\dot{\gamma_c}})^{-\frac{1}{2}} \quad (2)$$

where *a* is the radius of the micro rectangular container, L a constant slip length, $\dot{\gamma_w}$ the shear rate at the wall of the tube, and $\dot{\gamma_c}$the critical shear rate at which the slip length diverges. Solving the above two equations yields the velocity profile of the nanofluid particles are governed by the equation in the micro-container as given below.

$$u^* = \left(-\frac{1}{2m}\frac{dp}{dz^*}\right)^{\frac{1}{n}}\left|L_s^0 a^{\frac{1}{n}}\left(1-\frac{\dot{\gamma_w}}{\dot{\gamma_c}}\right)^{-\frac{1}{2}} + \frac{n}{n+1}\left(a^{\frac{n+1}{n}} - r^{\frac{n+1}{n}}\right)\right| \quad (3)$$

## 3. Introduction to Molecular Dynamics

One of the major tools in the theoretical study of molecules is the method of molecular dynamics simulations (MD). It calculates the time dependent behaviour of a molecular system, such simulations usually provided complete information on the fluctuations and conformal changes of molecules and atomic clusters. Though MD is an excellent analysis tool will not be able to perfectly model the real world problems using it. At the atomic level, particles obey complex quantum laws; however there are a number of statistical ensembles which closely approximate real particle behavior using classical laws. It is computer simulation technique in which the time evolution of interacting atoms is followed by integrating their equations of motion. That is, at intervals of the time steps, the forces between all pairs of atoms are calculated and accumulated, and then each atom is moved with respect to one another and the calculation will be repeated. Then the data of all the simulation s are processed using statistical analysis tools in regular intervals. For instance, temperature, pressure and potential/kinetic energy drifts are commonly calculated and recorded after each time-step, averaged over large timeframes, can be compared to measured results of real simulations of nanofluids; otherwise it would be impossible for any real experiments to provide detailed information about individual atoms.

The fixed grid, not to be confused with the grid fil, has a fixed number of equal sized cells along each axis, as shown in Figure1. Unlike the other structures, the cell which contains an atom can be determined in constant time by dividing the atom's position by the cell length along each dimension. A fixed grid is typically stored as an array of cells, where each cell contains a pointer to the list of atoms it contains.

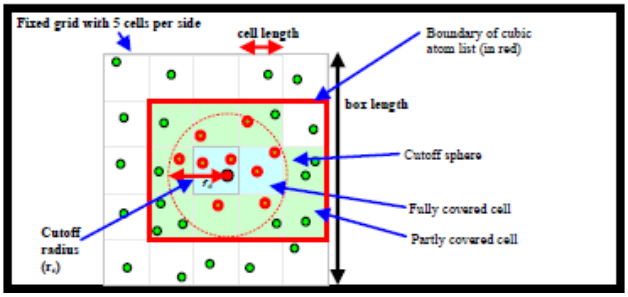


**Figure. 1** Grid of Cluster of atoms

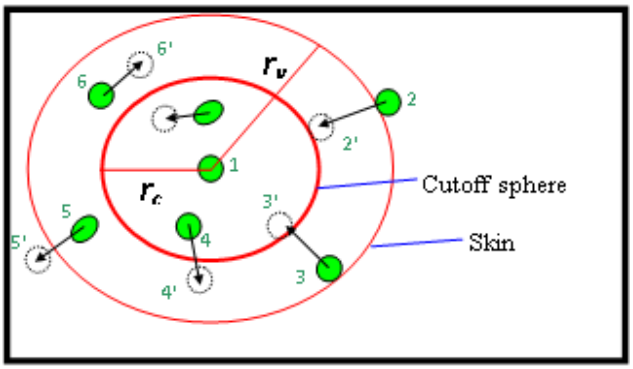


**Figure 2** Spherical boundary around cluster of atoms

The cut-off sphere (with radius $r_c$) around each molecule is surrounded by a larger sphere, called a skin with radius $r_v$. During the first time step a large neighbours list is constructed, containing all pairs of neighbours within $r_v$ of each other, and this list is rebuilt at intervals. Between these intervals, the neighbours list is simply updated by recalculating distances between neighbours and

determining which are within the actual cut-off radius $r_c$. The method is successful because the skin is chosen to be thick enough that no molecule can penetrate through the skin and into the surroundings. For instance, in Error! Reference source not found. **2**, point 2 will never be able to get further than the position 2', and penetrate the cut off sphere before the list is rebuilt.

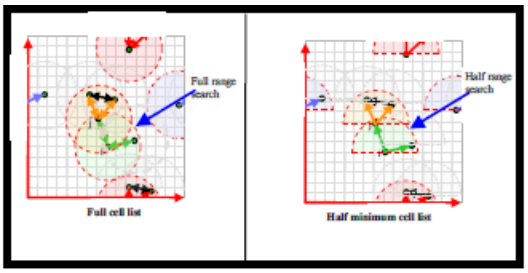


**Figure 3** Full Cell vs. Half Cell with rectangular boundary

## 4. Results and Discussion

The number of time-step and iterations per time step used in simulations is varied four times, since simulating about one hundred atoms in each cluster and four such clusters of molecules could take few seconds per iteration. For this reason, a time limit of about two minute was set for the simulations and terminated even if the desired number of iterations had not completed. The Results of the simulations were appended to a case file, and analysed in Excel.

The techniques used for testing are orderly in a logical sequence, such that the most successful method discovered in one section used in all subsequent runs. It is due to the movement of the wall surfaces close to one another and the atoms are getting compressed to a dense cloud of mixture of base fluid and nanoparticles. Very small load of about 5N is applied on all the faces of the container. The cluster of molecules is monitored for the intermolecular distances and the pressure rise in the control area.

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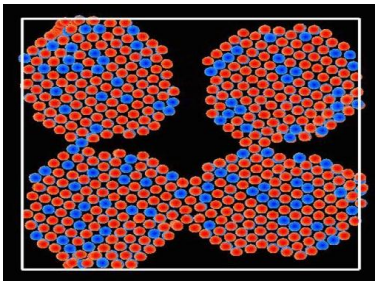

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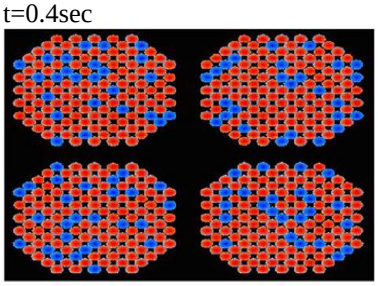

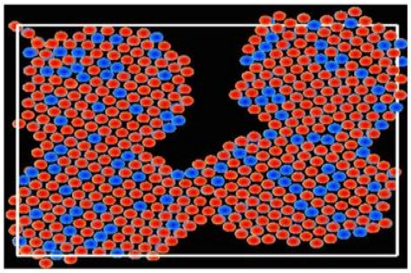

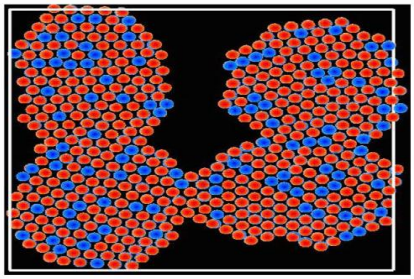

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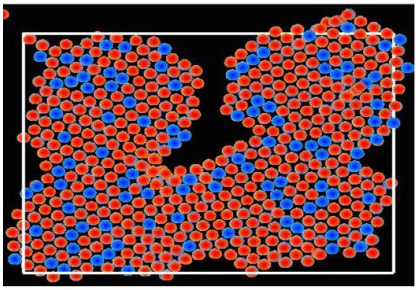

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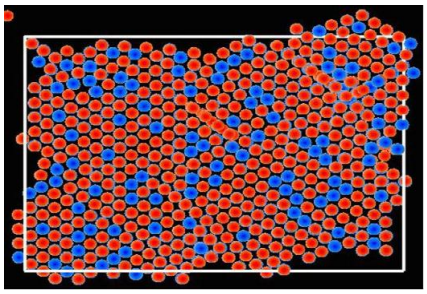

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**Figure 4** Deformation of Cluster under external pressure

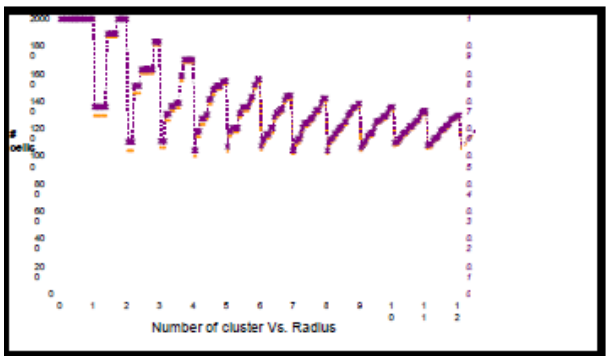


**Figure 5** Pressure vs. Intermolecular fluctuations

The nanofluids are arranged to check the viscous effect at low concentrations It is found 4%-18% step up of the intermolecular viscosity of nanofluids for water with $Al_2O_3$ in the normal temperature range 30–35°C. At a very low loading of 2N $Al_2O_3$ particles start wiggling to occupy the non prominent locations in the clusters. For a loading of 10N at 0.001% of $Al_2O_3$ particles, the improvement of intermolecular viscosity was around 12%-34%. Such interesting phenomena indicate that, except for particle size, there exist important factors related to the motion of particles. Also, the increments in thermal conductivity of the nanofluids were found to be nonlinear with temperature and almost linear with particle volume fraction. Chemical factors such as the need for direct contact of the metal surface with the solvent medium have important effects on the resulting effective thermal conductivity.

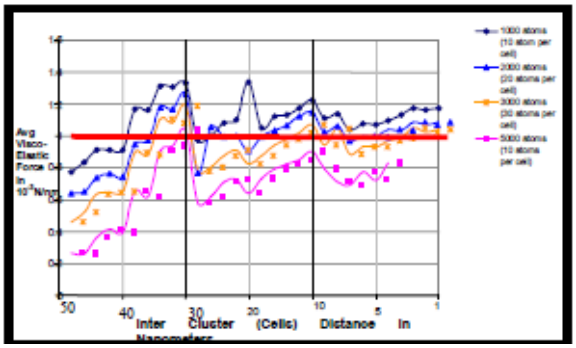


**Figure 6.** Stress distribution vs. Inter Cluster distance

It is noticed from the figure__ that the stress distribution in the rectangular chamber is raising to the maximum when the walls of the container are moved towards the centre by an external means. The viscoelastic forces in the four runs are plotted with respect to inter cluster distance and the cluster of 5000 atoms.

## 5. Conclusions

The following conclusions are drawn from the results presented above:

This paper presents an overview of the recent developments in the study of heat transfer using nanofluids. Many important, complex and interesting phenomena involving nanofluids have been reported in the literature. Researchers have given much more attention to the thermal conductivity rather than the heat transfer characteristics. The use of nanofluids in a wide range of applications appears promising, but the development of the field faces several challenges:

The lack of agreement between experimental results from different groups the often poor performance of suspensions; and lack of theoretical understanding of the mechanisms. Further theoretical and experimental research investigations are needed to understand the heat transfer characteristics of nanofluids and identify new and unique applications for these fields.

1. The nonmaterial in base fluid shows some agglomeration in 5µm -8µm, however and
2. The load carrying capacity of the fluid are found to be improved due to the addition of nanoparticles in the base fluid.
3. The viscoelastic properties of the nanofluids are found to be improved with increasing concentration.

## References

Prasher.R et al (2006), Measurements of nanofluid viscosity and its implications for thermal applications, *Applied Physics Letters*, vol. 89, no. 13, Article ID133108.

Wang.B et al (2004) Viscosity, thermal diffusivity and Prandtl number of nanoparticle suspensions, *Progress in Natural Science*, vol. 14, no. 10, pp. 922–926, 2004.

Namburu P.K et al (2007) Viscosity of copper oxide nanoparticles dispersed in ethylene glycol and water mixture, *Experimental Thermal and Fluid Science*, vol. 32, no. 2, pp. 397–402, 2007.

Choi H. J, et al (2000) Effects of shear rate and particle concentration on rheological properties of magnetic particle suspensions, *Journal of Materials Science*, vol. 35, no. 4, pp. 889–894.

Kwon T. M, et. al (1998) Viscosity of magnetic particle suspension, *Journal of Molecular Liquids*, vol. 75, no. 2, pp. 115–126.

Casson. N, (1959) A flow equation for pigment-oil suspensions of the printing ink type, in *Rheology of Disperse Systems*, C. C. Mill, Ed., Pergamon, New York, NY, USA.

Bingham E. C., (1922) *Fluidity and Plasticity*, McGraw–Hill, New York, NY, USA.

Phuoc. T. X, et.al (2009) Experimental observations of the effects of shear rates and particle concentration on the viscosity of Fe2O3-deionized water nanofluids, *International Journal of Thermal Sciences*, vol. 48, no. 7, pp. 1294–1301

Phuoc T. X, et.al (2011) Viscosity and thermal conductivity of nanofluids containing multiwalled carbon nanotubes stabilized by chitosan, *International Journal of Thermal Sciences*, vol. 50, no. 1, pp. 12–18

Bang, I. C. et.al (2005) Heat transfer performance and phenomena of Al2O3-water nano-fluids from a plain surface in a pool *International Journal of Heat and Mass Transfer*, vol 48, no. 12, 2420–2428

Larson R.G, (1999) *The Structure and Rheology of Complex Fluids*, Oxford University Press, New York, NY, USA

Bird R.B, et.al (1977) *Dynamics of Polymeric Liquids*, vol. 1, John Wiley & Sons, New York, NY, USA.