STATIC AND DYNAMICAL PROPERTIES OF NANOFLUIDS

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Supervisor Dr. Sunita Srivastava
Department of Physics,
Panjab University,
Chandigarh-160014

Panjab University, Chandigarh

Summary and Conclusions

Several exciting features of colloids invite the researcher to explore them further with great interest. Motivation of the Thesis was to study the transport behavior of fluids and to make their applications more specific to industrial purposes. In this work, it has been found that there is an increase in heat capacity with the increase in the size of nanoparticle and temperature of the system. The interfacial layer enhances the overall volume fraction of the nanoparticles, which, in turn, enhances the specific heat of the system. Theoretical model based on the effective medium theory has been proposed for the effective thermal conductivity of nanofluids by considering an interfacial layer around the particle with ellipsoidal shape. It is presumed that after dispersion, some nanoparticles in nanofluids with interfacial layer around them form aggregates while others remain well dispersed. Effective thermal conductivity of nanofluids has been calculated in terms of eccentricity of nanoparticles, thickness of interfacial layer and size for varying particle concentrations in the base fluid. The predictions of the model have been found to be in good accord with the available experimental data. Thus, it has been concluded that the interfacial layer and shape of the nanoparticles in base fluid have significant bearing on the enhancement of thermal conductivity of nanofluids. Aggregates resemble more closely to compact solid like structure which help in better heat conduction by providing an easier path for the carriers of heat, i.e. phonons, to travel when there is temperature gradient. Moreover the interfacial layer and spheroidal shape particles also contribute to the enhancement, which provides larger surface area for heat exchange.

While studying the rheology of nanofluids, inclusion of fractal aggregates and particle sphericity explained the behavior quite well. In this case also, the deviation of the particles from spherical shape is considered which increases the overall surface area and hence viscosity of the nanofluids. The fractal aggregates form chain like structures with a kind of irregularity that results in strong bonding among the particles and stress on the system leading to the enhancement in viscosity of nanofuids.

In addition to nanofluids, the self diffusion coefficient of soft interacting particle with Gaussian core potential has been analyzed at different temperature and densities above 0.35 at which these fluids show diffusion anomaly. For this, the radial distribution functions used

to evaluate the second and fourth frequency moments of VACF were obtained from the molecular dynamics simulation. The phenomenological memory function has been used to investigate sum rules of the Velocity auto correlation function (VACF) of fluid. It has been seen that as temperature is increased, the self-diffusion coefficient also increases and the increase is faster when the triplet contribution is positive and hence results in more value at low density and higher temperature as seen in simple liquids. The results of VACF and self diffusion coefficient compare well with the available molecular dynamics simulation results. Furthermore, contribution due to three body correlations is found to play a significant role in anomalous behaviour of self –diffusion coefficient and velocity autocorrelation functions. Lastly, VACF has been studied for one component fluid under confinement which involves a frequency which gets modifies as a result of confinement. In order to study this, the short time behaviour of VACF involving the modified frequency has also been studied. It is reported in the literature that the triple temperature of GCM is T_t= 0.00873 and that the density of coexisting fluid at the triple temperature is $\rho_t^* = 0.16431$. Therefore, analysis has been done below and upper the freezing transition temperature. At constant value of channel width, (x), $V(t)$ decreases with increasing density and the decay is fast at constant temperature. The self diffusion coefficient has been calculated as function of channel distance for different state points. It is concluded that anomaly in the VACF and self diffusion coefficient of Gaussian core model fluid still persists under the confinement.