# A SYSTEMATIC STUDY OF DYNAMIC PROPERTIES OF NANOFLUIDS

**A THESIS**

**Submitted to the**

**FACULTY OF SCIENCE**

**PANJAB UNIVERSITY, CHANDIGARH**

**for the degree of**

**DOCTOR OF PHILOSOPHY**

**2013**

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# Summary of the Thesis: Ishu Goyal

## A SYSTEMATIC STUDY OF DYNAMIC PROPERTIES OF NANOFLUIDS


The processes on the nanometer scale have implicitly been studied for past several decades in chemistry, physics, biology, materials science, and many areas of engineering. However, in past two decades, advances in technological tools like AFM, STM, ion beam lithographs etc. has accelerated great interest in interdisciplinary research fields of nano science and nanotechnology. Anomalous transport properties of fluids confined to nanoscale has attracted attention of theoretical scientists from numerous disciplines. This unusual behaviour of fluids at nanoscale can be related to the characteristic physical scaling length of the fluid viz. Debye length and hydrodynamic radius to coincide nearly with the dimensions of the nanostructure itself. This new dynamic field has many applications in technology, biology, and medicine.Presentthesis deals with the study of fluids confined to nanochannels. An effort has been made to understand the dynamic properties of fluids like diffusion and viscosity in nano confined geometries using theoretical techniques. The behaviour of the fluid is observed to be of non-Fickian type. In confined situations, viscosity is also found to be quite different from that of bulk. Viscosity is a collective property, has been studied for different widths of the nanochannel in contrast to diffusion which is related to a single particle motion and is a function of the distance from the wall. In the entire work, fluid has been assumed to be confined in z-direction *i.e.* in a direction perpendicular to the flow.The use of auto correlation functions like velocity auto correlation function (VACF) and stress auto correlation function (SACF) has been made to calculate diffusion and viscosity through the use of Green-Kubo formulae.

To calculate diffusion, we have developed a model for Lennard Jones fluid confined in nanoscale space. The fluid under consideration is taken at reduced density and reduced temperature, and is confined to a nanochannel of very small width *i.e.* about 5 atomic diameters. Due to confinement in such a small scale, the layering of fluid has been observed. It forms layers in high and low density regions. The width of layers thus formed is found to control the behaviour of diffusion.

To calculate viscosity, we have considered Lennard-Jones fluid, Ar-Kr binary mixture and isotopic fluid. Longitudinal and volume viscosities have been calculated by confining the fluid to a nanochannel of width twenty times that of the atomic diameter and an enhancement in it is observed near the wall of the channel. To conclude, we find that both the transport properties namely, diffusion and viscosity show anomalous behaviour when confined at nanoscale.