Abstract

Present work mainly comprises of study of transverse dynamics and shear viscosity of two component fluids and a part of the thesis is devoted to these studies for a two component fluid at nano scale. For this the transverse stress auto correlation (TSAC) function for a two component fluid has been studied. Exact expressions for the initial sum rules of the above mentioned TSAC function have been calculated and have been transformed in such a manner that they became suitable for the numerical calculations. The knowledge of TSAC function for a two component fluid, it’s sum rules and a suitable memory function have been used to predict the time evolution of TSAC function and a corresponding transport coefficient namely the shear viscosity for a two component (binary) fluid at a particular density and temperature. The result then has been compared with the molecular dynamics result. This work also includes the study of shear viscosity for an isotopic two component fluid, the mass and concentration dependence of sum rules of TSAC function and also the mass and concentration dependence of shear viscosity of an isotopic fluid. This work also involves the hydrodynamic treatment of transverse dynamics of two component fluids based on a dynamical variable. This involves the study of three transverse correlation functions (i) total current auto correlation function, (ii) total current-mass-concentration current function and, (iii) mass-concentration current autocorrelation function. Also the shear viscosity for a two component fluid has been studied when it is confined in one dimension in a channel of nano size. Further the mass and concentration dependence have been studied for a two component fluid when it is confined to a nanochannel.
This thesis has been divided into following five chapters:

1. Introduction
2. Transverse Stress Auto Correlation (TSAC) Function and Shear Viscosity of Two Component Fluids
3. Isotopic Two Component Fluid: Mass and Concentration Dependence of Shear Viscosity
4. Transverse Dynamics of Two Component Fluids
5. Nanofluidics: Shear Viscosity of Two Component Fluids in Nanochannels.

In chapter 1 today's scenario has been discussed for the shear viscosity, transverse dynamics, and nanofluidics with special attention to two component fluids.

Chapter 2 is based upon the study of transverse stress auto correlation (TSAC) function for a two component fluid. Zeroth, second and fourth frequency sum rules related to the TSAC function have been derived for two component fluids. These sum rules involve two body and three body static correlation functions. The three body correlation function for a one component fluid is estimated by using the superposition approximation, however, in this chapter a new approximation for a two component fluid based upon the old superposition approximation has been proposed as a modified superposition approximation. This modified superposition approximation takes care of the concentration dependence of the triplet correlation function in case of a two component fluid and reduces to the old superposition approximation for a one component fluid. For fourth frequency sum rule only two body contribution is calculated as the three body correlations in this case contribute very less as compared to the two body correlations. The three body contribution for the fourth frequency sum rule has been approximated from the previous knowledge of the same for one component fluids. To study shear viscosity of the two component fluid we have used the time correlation function approach coupled with the Mori-Zwanzig memory function formalism. The memory function can be calculated by using binary collision and...
mode coupling theories. By using Lennard-Jones form of potential as interaction potential for the system, a modeled (secant) memory function, studying the short time behaviour of the TSAC function and Green-Kubo formula, the shear viscosity for a two component fluid has been studied. The expressions for the sum rules involving partial pair and triplet correlation functions are general in nature and can be applied to any two component system. These expressions then have been transformed into a form which is suitable for the numerical computation. In the present work these sum rules have been computed numerically for a two component system involving Ar and Kr. The knowledge of these numerically calculated sum rules has been then applied to calculate the shear viscosity of Ar-Kr mixture. The result obtained is compared with the molecular dynamics (MD) simulations and found to be in good agreement with that. In this chapter some empirical models have also been investigated. These empirical models namely the linear model and the exponential model relate the shear viscosity of a two component fluid with the individual shear viscosities of the two components of the liquid mixture and their respective concentrations in the mixture.

Chapter 3 is devoted to the study of shear viscosity of a two component isotopic fluid and its mass and concentration dependence. In this chapter the zeroth, second and fourth frequency sum rules have been reformed for their use in the study of shear viscosity of an isotopic two component fluid. This chapter also deals with the mass and concentration dependence of these sum rules for an isotopic two component fluid. The sum rules have been modified in such a manner that their dependence on the masses and concentrations of the isotopic constituent of the mixture appear in them. This appearance is in such a way that we can write these sum rules for a two component isotopic fluid in terms of the respective sum rule expressions for one of the constituent of the isotopic two component fluid multiplied by a factor which carries the knowledge of mass ratio and hence mass dependence and the concentration dependence. The mass and concentration dependence of the second and fourth sum rules have been studied separately. The time evolution of TSAC function for different mass ratios has been studied. The short time behaviour of TSAC function in this
section has also been studied for different concentrations of the constituents of a two component isotopic liquid. The mass and concentration dependence for a two component isotopic fluid have been derived from the linear and exponential models mentioned in chapter 2 and then compared with our work.

In chapter 4 the transverse dynamics of a two component liquid has been analyzed. In this chapter special consideration has been given to the behaviour of the three transverse time correlation functions namely, the total current auto correlation function, total current-mass-concentration current function and the mass-concentration current autocorrelation function as these are important in case of the standard hydrodynamic treatment of transverse dynamics of two component fluids. The k dependent zeroth, second and fourth frequency sum rules for each of the above mentioned correlation functions have been calculated with the help of a dynamical variable.

Chapter 5 has been devoted to a branch of the latest development in the field of science and technology termed as nano-science/nano-technology. This branch deals with the various properties of fluids and is popularly called nano-fluidics. In this section a two component fluid has been studied when it is confined to a channel of nano scale dimensions. In particular the behaviour of shear viscosity has been studied in the above mentioned context. For this study a transverse stress auto correlation (TSAC) function has been studied for the two component fluid under confinement which involves a modified frequency as a result of confinement. From the earlier knowledge of zeroth, second and fourth frequency sum rules of the TSAC function for a two component fluid and the knowledge of the above mentioned modified frequency, dependence of shear viscosity of a two component fluid has been studied while it is under confinement in one dimensional channel of nano size (nanochannel). For this the short time behaviour of TSAC function involving the modified frequency has also been studied. The variation of modified frequency with the change in channel width has also been studied in this chapter. This chapter also involves the study of an isotopic fluid under confinement in a channel having nano sized width. For this the earlier knowledge of mass dependence of the sum rules for a two component fluid
has been used from chapter 3. These sum rules (second and fourth) depend upon the mass ratio of two species involved in the isotopic mixture. These sum rules are directly related with the frequency which gets modified with the varying mass ratio and the concentration of one type of species of the isotopic mixture, in addition to the modification experienced by it due to the variation in the size of nanochannel in which the isotopic mixture is confined. The dependence of modified frequency on the mass ratio of isotopic species and their respective concentrations in the isotopic mixture has also been studied. This mass and concentration dependence of the modified frequency also affects shear viscosity of the isotopic mixture confined in a nanochannel. This shear viscosity has been studied for different mass ratios of isotopic species at different concentrations.