

Non-equilibrium Molecular Dynamics Simulation of Transport Properties for Inhomogeneous Fluids

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We present simulation results for the transport properties of inhomogeneous non-equilibrium atomic and polymeric fluids undergoing planar Poiseuille flow. We study systems confined between channels of several atomic diameters width and investigate the dependence of the shear stress, strain rate, density and shear viscosity as functions of channel width, density and field strength. In our simulations, the shear viscosities are computed by applying a new linear hydrodynamic constitutive model for computing the spatially dependent non-local shear viscosity. Our viscosity calculations by using this new model are free from the singularities experienced by applying the commonly accepted local constitutive model and they make no assumption about the overall system density and boundary condition which are needed in the Navier-Stokes viscosity calculation. The non-local constitutive model is simple, general, and has widespread applicability in nanofluidics where experimental measurement of position dependent transport coefficients is currently inaccessible. In principle the method can be used to predict the flow profile of any arbitrary inhomogeneous system. We demonstrate this by predicting the flow profile for a simple fluid undergoing planar Couette flow in a confined channel of several atomic diameters width.