Nonlocal Constitutive Equations for Shear Flow in Fluids with Strongly Inhomogeneous Density and Velocity Profiles

Peter Daivis [C, S], Benjamin Dalton and Kirill Glavatskiy
School of Applied Sciences, RMIT University, Melbourne, Vic, Australia
peter.daivis@rmit.edu.au

Billy Todd
Department of Mathematics and Centre for Molecular Simulation, Swinburne University of Technology, Hawthorn, Vic, Australia

We present new theoretical expressions for the density, strain rate and shear pressure profiles in strongly inhomogeneous fluids undergoing steady shear flow with periodic boundary conditions. The expressions that we obtain take the form of truncated functional expansions. In these functional expansions, the independent variables are the spatially dependent longitudinal and transverse forces that we apply in non-equilibrium molecular dynamics simulations. The longitudinal force is directed along the y-axis, is composed of one or more sinusoidal components that vary in the y-direction and it produces strong density inhomogeneity. The transverse force is directed along the x-axis, varies sinusoidally in the y-direction and it produces shear flow. The functional expansions define new material properties, the response functions, which characterise the system's non-local response to the longitudinal force and the transverse force. We find that the longitudinal force, which is mainly responsible for the generation of density inhomogeneity, also modulates the strain rate and shear pressure profiles. Likewise, we find that the sinusoidal transverse force, which is mainly responsible for the generation of sinusoidal shear flow, can also modify the density. These couplings between density inhomogeneity and shear flow are also characterised by non-local response functions. We conduct non-equilibrium molecular dynamics simulations to calculate all of the response functions needed to describe the response of the system for weak shear flow in the presence of strong density inhomogeneity up to the third order in the functional expansion. These response functions are then substituted directly into the truncated functional expansions and used to predict the density, velocity and shear pressure profiles. The results are compared to the directly evaluated profiles from molecular dynamics simulations and we find that the predicted profiles from the functional expansions give excellent agreement with the directly computed density, velocity and shear pressure profiles.