

Abstract Submitted
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Rheological and statistical characteristics of the Lennard-Jones fluid undergoing planar Couette flow and second-law violations¹
BHARATH RAGHAVAN, MARTIN OSTOJA-STARZEWSKI, Univ of Illinois - Urbana — We use Non-equilibrium Molecular Dynamics (NEMD) simulations to investigate the rheological and statistical properties of molecular fluids interacting via a Lennard-Jones potential undergoing planar Couette flow. From kinetic theory and the Boltzmann equation, we obtain a rheological equation of state that captures the stress-deformation responses exceptionally well. We obtain a shear-rate dependent model for the viscosity, similar to the Cross model, and demonstrate how this model arises naturally from the Boltzmann equation, possessing an inherent scaling parameter that unifies the rheological properties of the LJ fluid. Using thermo-mechanics, we formulate a dissipation function modeling the LJ fluid as a quasilinear fluid. We explore the statistical properties of the shear-stress under isothermal conditions and the tendency to violate the second-law of thermodynamics, from the probability density function obtained using Information theory. We examine the autocorrelation function (ACF), and power spectral density (PSD) of the shear stress, and their dependence on the fluid state-points and applied strain rates to draw inferences regarding the causes of shear-thinning frequently observed in such systems, and provide insight into the structure of the flow.

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Bharath Raghavan
Univ of Illinois - Urbana

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