Elucidating the prediction of an asymmetric stress tensor and couple stresses from a NET perspective (theory and molecular simulations)

It has been almost exclusively assumed that the stress tensor employed in Fluid mechanics is symmetric, which implies that there is no interchange between macroscopic and molecular angular momenta.[1] Such a consideration assumes that matter is continuously distributed throughout the body. Although this stands as a reasonable basis for analyzing the behavior of materials at the macroscale level, it fails to do so in cases where the microstructure size-dependency cannot be neglected, such as polymeric systems or suspensions. In fact, the micro-rotation of freely suspended particles in fluid suspensions gives rise to an antisymmetric stress, known as couple stress.[2] It is more likely that couple stresses arise in fluids with very large molecules.[3,4] A comprehensive theory in this regard is the one developed by Stokes.[4] Couple stress theory (CST) is found to be quite useful in the description of various types of lubricants, blood, and polymeric suspensions.[5] The CST has been utilized in many biomedical applications, such as blood flow in the microcirculation, pulsatile systolic hemodynamics, and even swimming of microscopic organism in micro-continuum fluids.[2]

In the present work, we first aimed to verify whether the above-mentioned modification of classical fluid mechanics is thermodynamically admissible by using non-equilibrium thermodynamics.[6,7] We have generalized previous work,[6] dealing with isothermal systems, to the case wherein both the mass density and the entropy density (or temperature) are state variables (this work will soon be submitted for publication[8]). Secondly, we provided the theoretical work for developing the CST for non-Newtonian fluids. As a structural variable, we employed the conformation tensor, [6,7] which is coupled with the rotational motion of polymer chains.[9] Finally, we have performed non-equilibrium molecular dynamics (NEMD) simulations using atomistic detail. We first conducted such simulations on polymer melts, that bear a rotational contribution when a shear flow is applied. This work has culminated in the publication of a paper in Dynamics,[10] wherein we generalized a previously derived constitutive model[11] by considering a variable non-affine or slip parameter. We have also conducted NEMD simulations of dilute solutions of linear DNA fragments that are known to exhibit a rod-like conformation,[12] since rod suspensions are known to exhibit an asymmetric contribution to the stress tensor.[13]

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