**Rheological characterisation of viscoelastic polymer solutions by mesoscale modelling**

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**Abstract**

This work demonstrates a novel mesoscale modelling framework based on many-body dissipative particle dynamics (mDPD) that can be used to simulate chemically specific dilute polymer solutions. Macroscopic properties such as deformation response, storage and loss moduli, relaxation times of many such liquids are difficult to be obtained using a full-atomistic MD or united-atom MD, given the expensive computational schemes for long-chain polymer solutions and low signal-to-noise ratio. Moreover, estimation of certain rheological properties such as first normal stress difference are beyond the scope of such simulation scales. Given the technical challenges associated with experimental methods in the dilute polymer regime, and the requirement of satisfactory constitutive equations to model such liquids in continuum scale simulations, an alternative approach for modelling such liquids is required. The work here simulates polymer solutions at mesoscales with experimental Schmidt numbers (> 103). The simulations showcase how sensitive features of mild viscoelastic fluids, such as first normal-stress difference and viscosity are modelled under non-equilibrium conditions appropriately for these liquids. The computation of storage (G’) and loss moduli (G”) provides the individual contribution of the viscous and elastic components. It is shown that the addition of polymer increases both G’ and G”. Using this framework, it is possible to see the changes happening with respect to polymer radius of gyration and terminal relaxation time as functions of temperature. A combination of density-dependent conservative force parameters, and systematically derived dissipative force cut-off and angle stiffness energies. The reported relationships between the mDPD (reduced) units and real (SI) units make the model accessible for direct comparison with results from macroscopic experiments of industrially important viscoelastic liquids.