RESEARCH INTERESTS OF THE MD GROUP AT ROYAL HOLLOWAY COLLEGE

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LINEAR AND NON-LINEAR RESPONSES OF DENSE LIQUIDS

In the modern world it is increasingly necessary to make things in the shortest possible time. This often involves applying extreme conditions to a material which, for example, could be used as an interface between other materials [1-3] or be moulded into a desired shape. To achieve the best results it is useful to understand the mechanism by which these materials respond to rapidly changing conditions. For example, the rheological properties of fluids are of particular importance to chemical and lubrication engineers who frequently encounter non-newtonian flow phenomena such as shear thinning (a decrease in shear viscosity with increasing shear rate), shear thickening (an increase in shear viscosity with increasing shear rate) and the behaviour of other non-newtonian materials, such as exhibited by the class of compounds known as Bingham plastics.

It would be interesting to discover what factors are needed in the characteristics of a molecule to produce the observed behaviour in these fields.

It has been shown [4-6] that there is a remarkable similarity between the response of many complex materials, such as glasses, lubricants at high pressure, polymer solutions and melts and those of simple model liquids to sudden changes in applied conditions. It has been revealed that even the Lennard-Jones (LJ) liquid exhibits many features in common with the above more complex materials and it is currently being used in MD to provide a mechanistic framework on which to base analytical representations of polymer, glass and pressurised-lubricant non-linear viscoelastic behaviour. Provided appropriate normalisation with respect to internally derived characteristic timescales is made, these disparate systems manifest very similar reductions in relative shear viscosity when shear rate increases. The effect of shear straining implemented during MD, or in an integral equation formulation, has already gone part way towards establishing the theoretical ground-rules which bring about these common features [1-6]. In particular, a coupling of shear and 'bulk' structural distortions from the equilibrium structure seems essential to account for certain fascinating viscoelastic properties.

It is hoped that such simulation and theoretical treatments will be useful in interpreting a wide variety of technologically important roles for liquids both in the linear [7-8] and non-linear regimes [1-6].

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