Rheology of complex fluids from Molecular Dynamics

E.O. Castrejón-González
Departamento de Ingeniería Química, Instituto Tecnológico de Celaya.
Av. A. García Cubas 600, Col. Alfredo V. Bonfil, Celaya, Gto. C.P. 38010, México.
omar@iqcelaya.itc.mx

Abstract

Equilibrium and Non-Equilibrium Molecular Dynamics were used to understand the relationship between the molecular structure and the rheological behavior of complex fluids. The analyzed systems were: i) Polymer (chains) solutions with different conformations (e.g. Linear, branched, hyperbranched, dendrimers, etc.), ii) Micelles consisting in surfactant molecules immersed into two types of solvent (oil and water like) and iii) Associative polymers.

Some potentials were used, since simple FENE and Lennard-Jones [1] (for coarse-grained molecular models) until more complicated such as: COMPASS and PCFF [2] (for atomistic simulations).

The equations of motion were solved for shear flow with SLLOD equations of motion integrated with Verlet's algorithm [3]. A multiple time scale algorithm extended to non-equilibrium situations was used as the integration method.

The structural properties include Static Structure Factor, Radius of Gyration and Anisotropy Factor.

By other hand, the rheological parameter was mainly the shear viscosity as a function of shear rate; in this case we have observed three regions in the rheological response: i) Newtonian behavior, ii) Shear Thinning and iii) Shear thickening [4], depending on the system under study.

All the simulations were performed using both Medea [5] and LAMMPS [6] softwares, as well as programming code developed in C++ and FORTRAN.

References

[1] O. Castrejón-González, J. Castillo-Tejas, O. Manero and J. F. J. Alvarado (2013). Structure factor and rheology of chain molecules from molecular dynamics, *J. Chem. Phys.*, **138**, 184901-1-11.

[2] H. Sun (1998). COMPASS: An *ab Initio* Force-Field Optimized for Condensed-Phase Applications Overview with Details on Alkane and Benzene Compounds, *J. Phys. Chem. B*, **102**, 7338-7364.

[3] J. Haile (1992). *Molecular Dynamics Simulation*, John Wiley & Sons.

[4] E.O. Castrejón-González, V.E. Márquez Baños, J.F. Javier Alvarado, V. Rico-Ramírez, J. Castillo-Tejas and H. Jiménez-Islas (2014). Rheological model for micelles in solution from molecular dynamics. *Journal of Molecular Liquids*, **198**, 84-93.

[5] MedeA® 2.13, Materials Design Inc., Angel Fire, NM, USA (2012).

[6] S. Plimpton (1995). Fast parallel algorithms for short-range molecular dynamics. *Journal of computational physics*, **117**, 1-19.