

Simple Models for Shear Viscosity and Self-Diffusion of Liquid Metals

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In this work, we are using the smooth hard-sphere theory to correlate and predict self-diffusion and shear viscosity of dense fluids, specifically liquid metals. We are employing a recent density correction for shear viscosity [1] and the Speedy's density correction for self-diffusion [2]. The corrections for density effects were generated using molecular dynamics data for hard-spheres. In the case of shear viscosity, which is a collective property, data from large systems were employed, although for self-diffusion, as shown by Sigurgeirsson Heyes [3], Speedy's correction provided similar results for large systems. It should be stressed that density corrections play a very important role for transport properties, mainly at high densities. Both models employed very simple algebraic expressions with just one adjustable parameter.

In addition, we are studying the role of effective hard sphere diameters applied to correlate and predict shear viscosity and self-diffusion of liquid metals.

- [1] L.A.F. Coelho, *Journal of Supercritical Fluids* **34**, 243 (2005).
- [2] R.J. Speedy, *Molecular Physics* **62**, 509 (1987).
- [3] H. Sigurgeirsson and D. M. Heyes, *Molecular Physics* **101**, 469 (2003).