Modified Residual Entropy Scaling of Transport Properties

Presented by
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Abstract
The domains of thermodynamics and transport properties (here, viscosity, thermal conductivity and self-diffusion) have been moving towards each other in recent years, and the thermodynamic property residual entropy has been found to be intimately connected to appropriately scaled transport properties. Furthermore, we have in recent works identified a novel scaling approach, which we denote “modified residual entropy scaling”, that has the desired behavior in the liquid phase and in the dilute gas limit. We demonstrate the suitability of this novel scaling approach for a number of model fluids, including the hard sphere, inverse-power-law, and especially the Lennard-Jones 12-6 model potential. We close with a discussion of how the lessons learned from the model potentials can be applied to real molecular fluids.

Biography
Ian Bell received his PhD from Purdue University in 2011 in mechanical engineering, followed by a post-doctoral appointment at the University of Liege, in Liege, Belgium, with an emphasis on open-source computational tools for compressors, heat pumping systems, and thermophysical properties. Since 2015, he has been at the National Institute of Standards and Technology in Boulder, Colorado and is part of the REFPROP development team.