The Boltzmann gas equation in relation to Onsager–Stefan–Maxwell diffusion for Lennard-Jones gas mixtures

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The Enskog method is an asymptotic method that provides solutions of the Boltzmann equation close to local equilibrium. The method predicts kinetic properties of gases, such as Stefan–Maxwell diffusivities, in terms of certain collision integrals. We describe a method to compute collision integrals, and a method of molecular dynamics simulation of Stefan–Maxwell diffusivities based on Onsager's regression hypothesis. We investigate how analytical predictions compare with molecular dynamics simulations for mixtures of Lennard-Jones gases and experiments with mixtures of monatomic gases. We apply the Enskog method to derive continuum-level model equations. Within the limitations of Enskog's method, these results identify with a set of multi-species transport equations that Goyal and Monroe recently derived using the alternative theory of irreversible thermodynamics.