Abstract Submitted
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Stefan-Maxwell diffusivities of gas mixtures, and Onsagers regression hypothesis[1] MAXIM ZYSKIN, CHARLES MONROE, University of Oxford — Stefan-Maxwell diffusivities play an important role in continuum multi-species transport theories (Goyal and Monroe, JES 2017 ; Goyal and Monroe, Electrochem. Acta 2021), and in the modelling of electric batteries in particular. These diffusivities in general depend on composition, temperature and pressure, leading to a nonlinear system of transport equations, with nonnegative entropy production rate, controlled by the Stefan-Maxwell diffusivities and other kinetic parameters, including thermal diffusivity and viscosity. It is therefore important to develop robust computational methods to determine Stefan-Maxwell diffusivities, as these are not predicted by the continuum modelling framework. In the case of gas mixtures, analytic methods, and molecular dynamics method bases on Onsagers regression hypothesis (Monroe, Wheeler and Newman, IECR 2015) are available. We carefully compute scattering integrals that determine kinetic parameters and investigate StefanMaxwell diffusivities, including higher-order corrections, within Lennard-Jones gas mixtures. We perform molecular dynamics simulations based on Onsagers regression hypothesis, paying attention to the role of the thermostat, and compare molecular dynamics simulations, analytical results, and available experimental data.

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