Thermophysical Properties of Molten Salts Using Atomistic Simulations

Haimeng Wang [S], Ryan S. DeFever and Yong Zhang
Department of Chemical and Biomolecular Engineering, University of Notre Dame, Notre Dame, IN, U.S.A.

Fei Wu, Shobha Sharma, Matthew S. Emerson and Claudio J. Margulis
Department of Chemistry, The University of Iowa, Iowa City, IA, U.S.A.

Edward J. Maginn [C]
Department of Chemical and Biomolecular Engineering, University of Notre Dame, Notre Dame, IN, U.S.A.
ed@nd.edu

Molten salts reactors (MSRs) are considered as a leading candidate of the next generation of nuclear reactors for their potential reliability, safety, and commercial advantages. Fundamental understanding of the thermodynamic and transport properties of molten salts is important to their applications in MSRs. In this study, we performed molecular dynamics (MD) simulations to investigate the melting points, self-diffusivity, shear viscosity, and other transport properties of monovalent and divalent chloride salts. The transport properties were calculated using equilibrium molecular dynamics simulations. Melting points were calculated using two distinct methods, a direct method called the solid-liquid direct coexistence method, and a free energy-based method called the pseudo-supercritical path method. Results obtained from both methods are compared and the benefits of the different methods are discussed in relation to computational performance and accuracy. Several classical force fields were selected for the MD simulations, including an induced dipole model, a Drude model, and a fixed charge model. Furthermore, a deep neural network-based potential was also introduced and benchmarked with other classical models. Overall, we discuss how the models of various levels of complexity affect the accuracy of computing melting points and transport properties of molten salts.