Thermal Properties of a LiF-ThF4 Molten Salt Fuel

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Molten salt reactors have seen an insurgence of interest and studies because of their high efficiency and their relatively compact design when compared to traditional reactors such as boiling water reactors. Moreover, their low operating pressure is considered to enable safer nuclear reactors. Molten Salt Reactors had a large amount of research interest in the 1970s-1980s but began to fade until recently. In the present research study, we explore the thermodynamic properties of LiF-ThF4, a representative Molten Salt Reactor (MSR) fuel at micro/nanoscale to increase the knowledge of properties of pertinent fuels. Various important thermodynamic and/or thermal transport properties such as thermal conductivity, thermal diffusivity, and heat capacity are estimated by the help of molecular dynamics simulations; transport properties are estimated by utilizing non-equilibrium molecular dynamics while diffusion properties are evaluated by using equilibrium molecular dynamics that involves velocity and/or flux auto-correlation. These simulations are conducted using LAMMPS, an MDS (Molecule Dynamics Simulator) with differing simulation sizes and found an average value of thermal conductivity at 1.4497 W/(m-K). It is anticipated that the results obtained in the present study can be employed by experimentalists to choose the composition that can optimize the thermal transport efficiency of MSRs, accelerating the advance in future ‘inherently safe’ nuclear reactors.