

Thermal Transport in Molten Salt Reactor Fuels

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In this research study, we explore the thermal transport property of Molten Salt Reactor (MSR) fuels by using molecular dynamics simulations. MSR has been drawing attention from researchers recently since it can run at high temperatures, yielding high energy production efficiency at relatively low amount of fuel mass. Its low operating pressure reduces the risk of a large break and loss of coolant significantly. Among different possible MSR fuels, LiF-ThF₄ is selected to examine the thermal transport property of MSR fuels. Reverse Non-equilibrium molecular dynamics is employed to estimate the thermal conductivity of LiF-ThF₄ at various temperatures, ranging from 300 K to 1200 K. In addition, different mole fractions of LiF and ThF₄ are selected to find the optimized composition of MSR fuels that enable efficient energy transfer. The simulation results indicate that thermal transport in MSR fuels is already diffusive and is not affected by the size of the simulation structure. However, the thermal conductivities of MSR fuels show a moderate degree of dependency on temperature; at high temperatures, the increased momenta of molecules induced by high temperatures are expected to increase the scatterings of molecules, enhancing the propagation of phonon energy. The thermal conductivity of 75 % LiF – 25 % ThF₄ is shown to be 1.36 W/m-K at 300K but is increased to 1.46 W/m-K as the operating temperature is increased to 1200 K. The authors believe that the results obtained in the present research will provide a microscopic understanding on the thermal transport property of MSR fuels and contribute to the development of more advanced MSR.