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Molecular Dynamics Simulation of the Transport Properties of Molten Transuranic Salt Mixtures AUSTIN BATY, PETER MCINTYRE, AKHDIYOR SATTAROV, ELIZABETH SOOBY, Texas A&M University — The Accelerator Research Laboratory at Texas A&M is proposing a revolutionary design for accelerator-driven subcritical fission in molten salt (ADSMS), a system that destroys the transuranic elements in spent nuclear fuel. The transuranics are the most enduring hazard of nuclear power, since they contain high radiotoxicity and have half-lives of a thousand to a million years. The ADSMS core is fueled by a homogeneous chloride-based molten salt mixture containing the chlorides of the transuranics and NaCl. Knowledge of the density, heat capacity, thermal conductivity, etc. of the salt mixtures is needed to accurately model the complex ADSMS system. There is a lack of experimental data on the density and transport properties of such mixtures. Molecular dynamics simulations using polarizable ion potentials are used to determine the density and heat capacity of these melts as a function of temperature. Green-Kubo methods are employed to calculate the electrical conductivity, thermal conductivity, and viscosity of the salt using the outputs of the model. Results for pure molten salt systems are compared to experimental data when possible to validate the potentials used. Here we discuss potential salt systems, their neutronic behavior, and the calculated transport properties.

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