Preliminary Work for Nonproliferation Monitoring for Molten Salt Reactors

Jacob Tellez, Ph.D. student, Colorado School of Mines, jtellez@mines.edu
Nicole Hege, Ph.D. student, Colorado School of Mines, nicolehege@mymail.mines.edu
Will Smith, Ph.D. student, Washington State University, william.t.smith@wsu.edu

Advisor: Jen Shafer

Abstract: Nonproliferation monitoring of next-generation molten salt reactor (MSR) designs requires strict monitoring of fuel salt compositions to ensure safe and secure operation. This project explores online monitoring capabilities for the uranium (III) chloride salt in the KCl-LiCl eutectic via experimental and computational approaches. The experimental portion of this project involved construction of a molten salt furnace for the eutectic salt. The techniques used to determine the speciation inside the furnace include Raman spectroscopy, UV-Vis spectroscopy, and differential pulse voltammetry. The furnace was designed to study the uranium (III) chloride composition in the eutectic over a range of temperatures from 650 - 1125 K. Preliminary modeling of the uranium (III) chloride salt aided in verification of the force field implementation as well as understanding the structural and kinetic properties of the salt such as density, coordination number, radial distributions, diffusion coefficients, and network formation. The force field consists of a modified Born-Mayer-Huggins pair potential and is implemented with the molecular dynamics software, GROMACS. Snapshots from the equilibrated classical molecular dynamic trajectory were used as starting coordinates for the Ab Initio Molecular Dynamics (AIMD) simulation. The AIMD simulations done using CP2K, employed the Scalar-relativistic norm-conserving Goedecker–Teter–Hutter medium-core pseudopotentials for uranium and chlorine with 14 ([Xe 4f14 5d10] 6s2 6p6 7s2 5f3 6d1) and 7 ([He] 2s2 2p5) valence electrons, respectively, and the molecularly optimized double-zeta basis set (MOLOPT-DZVP-GTH). The IR/Raman spectrum was calculated from Wannier centers at every fifth time-step in the trajectory.