Investigation of Fission Product Influence on the UCl_3-LiCl-KCl Eutectic

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Abstract:

Post-processing of used nuclear fuel and on-line processing schemes for salt-cooled nuclear reactors rely on electro refiners making use of metal chloride solutions containing a variety of solvated fission products. These molten salt solutions contain numerous radioactive isotopes and must be held at elevated temperatures making experimental inquiry challenging. This work employs classical molecular dynamics simulations to investigate the nanoscale structure and thermophysical properties of systems containing multiple trivalent metal chlorides in the LiCl-KCl eutectic salt. The interaction potential is implemented with CP2K and based on a Born-Mayer-Huggins polarizable model. Systems are validated against a combination of simulation results, x-ray diffraction data, and extended x-ray absorption fine structure data. Preliminary investigations evaluate the effect of La^{3+} on the coordination and mobility of U^{3+} in solution.

Validation efforts reproduce coordination of all ions and activation energies of the U^{3+}-Cl^- pair compared with simulation results and XRD data for pure UCl_3 and 5% UCl_3 in LiCl-KCl. The simulated bulk density of pure UCl_3 is significantly higher than experimental results; however, calculations of the crystal volume for UCl_3 and $LaCl_3$ agree with experimental and calculated values. Self-diffusion coefficients of uranium and chloride ions in pure UCl_3 agree with previously simulated values. An investigation of the effects of the presence of La^{3+} in a uranium-containing solution remains ongoing.