Graduate Student Seminars
Wednesday, November 18
4pm
Hill Hall 202

Beamline Improvements to the MInes NEutron Radiography (MINER) Facility

Clinton Wilson
King Research Group
The Colorado School of Mines

Abstract. The MInes NEutron Radiography (MINER) facility provides students and researchers at the Colorado School of Mines with the capability to perform neutron imaging at the Geological Survey TRIGA Reactor (GSTR). The current beamline consists of a 1.5 inch inner-diameter aluminum pipe routed from the reactor up to an experiment station in the reactor bay. There are several limitations associated with the current beamline, including a relatively small beam diameter which limits the size of objects which can be successfully imaged, and a tendency toward beamline misalignment, resulting in non-uniform fluxes and high radiation levels in the reactor bay. A second generation beamline, currently under construction as the focus of this project, is intended to overcome these drawbacks and improve the overall performance of the MINER facility. MCNP analysis has been performed throughout this project to aid with beamline design. Part of this analysis has shown that the addition of a pre-collimator (intended to accommodate various beam filters) greatly reduces the fraction of scattered neutrons at the imaging plane, and eliminates the need for a neutron absorbing liner inside the collimator.

Use of molecular dynamics to evaluate tributyl phosphate and diamylamyl phosphonate containing systems

Michael Servis
Braley Research Group
TheColorado School of Mines

Abstract. Solvent extraction is utilized by the nuclear energy industry as a separations technique for reprocessing used nuclear fuel. In the industry standard PUREX (Plutonium URanium EXtraction) process, an amphiphilic extractant molecule like tributyl phosphate (TBP) selectively transfers metal ions of interest, such as uranium or plutonium or thorium, from a dissolved aqueous solution into a dodecane organic phase. It has been shown that the aggregation chemistry of similar extractant molecules varies drastically despite similar molecular structure. This difference in behavior is evident in third phase formation, an undesirable phenomenon that occurs at high extracted metal ion concentrations. TBP is more prone to this phenomenon than the similar extractant diamyl amyl phosphonate (DAAP). This study examines the structure and interaction of post-extraction TBP-metal ion complexes in their organic diluent using molecular dynamics (MD) simulations. Initial studies involve the development of an MD model of TBP more accurate than those commonly used in the literature. To ensure a realistic and robust model, comparison to relevant experimental properties was performed. The MD parameter adjustments applied to the TBP model were implemented for DAAP and those extractants were simulated in dodecane and octane organic diluents to analyze self-aggregation behavior. Aggregates were characterized by graph

theory analysis and the dimerization constant and interaction mean free energies were assessed. Water and nitric acid extraction by TBP in dodecane was also simulated to analyze the resulting hydrogen bonding networks that define extraction complex structure. This methodology will be applied to metal ion-containing systems that correspond to third phase systems.