Combining Experiments and Simulations of Extraction Kinetics and Thermodynamics in Advanced Separation Processes for Used Nuclear Fuel

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ABSTRACT:

The proposed research is aimed at investigating extraction systems for used nuclear fuel. We propose to study how the kinetics and thermodynamics of metal ion extraction can be described by molecular dynamic (MD) simulations and how the simulations can be validated by experimental data. Furthermore, the project includes the applied separation by testing the extraction systems in a single stage annular centrifugal contactor and coupling the experimental data with computational fluid dynamic (CFD) simulations. The project would address important challenges in aqueous separations processes currently under development for used fuel treatment. Chemical speciation and complexation could be better understood and successful simulations could have broad impacts on several different processes including advanced TALSPEAK, ALSEP and GANEX. These processes all rely on combinations of several organic extraction reagents and/or aqueous hold-back reagents making the kinetics of extraction a challenging problem. The work proposed here have the potential to increase the confidence and accuracy of computer modeling of the metal ion extraction as well as improve the connection between batch and contactor extraction kinetics.

Specific objectives of the proposed research are as follows:

1. Study and establish a rigorous connection between MD simulations based on polarizable force fields and extraction thermodynamic and kinetic data.
2. Compare and validate CFD simulations of extraction processes for An/Ln separation using different sizes (and types) of annular centrifugal contactors.
3. Provide a theoretical/simulation and experimental base for scale-up of batch-wise extraction to continuous contactors.

The total budget of $799,938 is requested to support this 3 years collaborative research effort between 2 PIs at the University of California, Irvine and 3 PIs at US DOE National Laboratories. An international partner from FZ Jülich, Germany, is included as non-funded consultant for the duration of the project.