



U.S. Department of Energy

Advanced Characterization of Molecular Interactions in TALSPEAK-like Separations Systems

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ABSTRACT

The NEUP Program Supporting Fuel Cycle R&D Separations and Waste Forms (FC-1) program requests long-term R&D projects focusing on streamlining separation processes for advanced fuel cycles. A clear example of important streamlining would be a process that combines the functions of the TRUEX process for partitioning of lanthanides and minor actinides away from PUREX raffinates with the TALSPEAK process that aims to subsequently separate transplutonium actinides from fission product lanthanides. It has been shown (in the laboratory) that these processes can be made to work in series as consecutive unit operations in advanced processing. But even operating in series, the combination is challenging because the processes require different classes of extractant solutions and different aqueous phases operating under very different conditions of acidity. Each process requires either phase modifiers in the extractant phase or concentrated buffer solutions in the aqueous phase for the process to work. The use of multiple reagents brings the probability for complex and potentially unexpected interactions. The predictability of such processes in sequential operation will be much improved with increased understanding of the interactions between aqueous and organic component molecules. Even greater economies and improvements in system performance could be achieved if more complete understanding of molecular interactions allowed multiple processes to be collapsed into a simpler suite of separation operations. In our earlier experience in characterizing the TALSPEAK process, we have determined that modern analytical and computational tools provide an unprecedented opportunity to understand such phenomena and thus develop more robust separation processes. This proposal targets the application of titration calorimetry, NMR spectroscopy and complementary optical methods of analysis to the development of lanthanide-actinide aqueous separation methods based on TALSPEAK-like chemistry. The research team has significant previous experience in cooperative research projects on this and similar topics. The work is to be conducted principally at Washington State University with collaborative interactions with two DOE National Labs for high activity work and the unique facilities available there. Short duration assignments of graduate student and Postdoctoral Associate researchers at the DOE lab facilities broadens the scope of the research, while providing opportunities for young investigators to experience the professional workplace environment. The project also features non-funded consultation arrangement with a French scientist well acquainted with the methods to be investigated and familiar with both the issues in the science and with similar processes being developed in Europe.