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Development of Integrated Process Simulation System Model for Spent Fuel Treatment Facility (SFTF) Design

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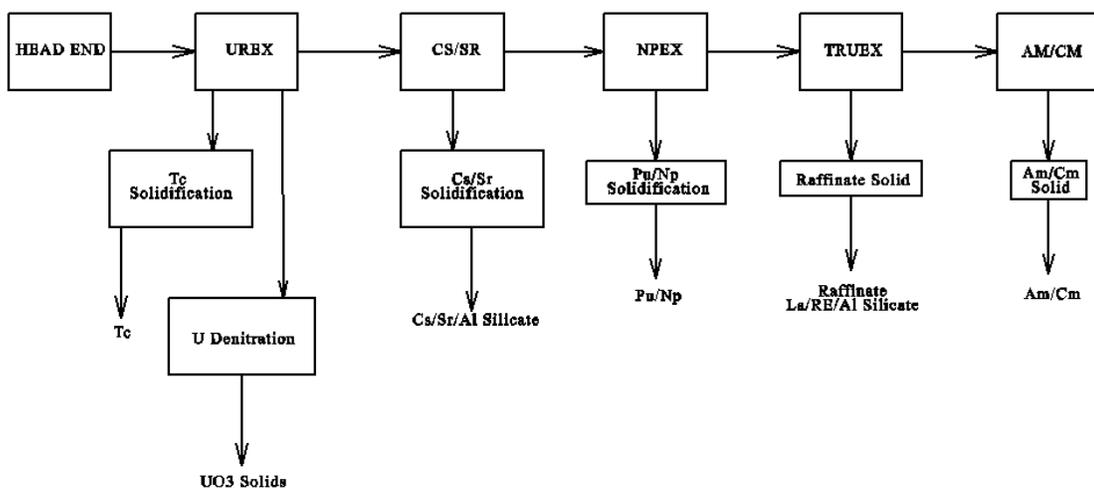*Y. Chen and S. Hsieh*

BACKGROUND

Simulating Spent Fuel Treatment Facility (SFTF) processes is the major focus for this project. The approach is to combine commercial process simulation software, ASPEN-Plus with the chemical separation calculation from the ANL's AMUSE code. Based on the current System Engineering Model package, TRPSEMPro (developed by UNLV), the project objective is to create a system framework that interacts with both programs and provides analyzed results useful for SFTF design that provides functionality of receiving, temporarily storing, and preparing spent nuclear fuel for leaching.

The SFTF has many individual processes that make up the overall separations process. Each individual process contains numerous operations that are responsible for the chemical separation. UREX is often the first removal process in the overall scheme of spent fuel recycling. After extracting U and Tc from the spent fuel, the washed and rinsed effluents (Cs/Sr raffinate) move on to the next separation process.

A key concept in the SFTF plant design is the recycling of nitric acid. The purpose of the nitric acid recycle system is to concentrate the spent nitric acid to a desired molarity that in turn can be recycled back into the process. The spent nitric acid streams from many processes are collected and sent to a distillation column where it is separated from the impurities collected in the various separation processes. The feed to the separation column contains acetic acid and water as well as the desired nitric acid.

RESEARCH OBJECTIVES AND METHODS

The overall goal of this project is the creation of a framework that combines all the strengths of AMUSE's complicated calculations, well-established commercial system process packages, and TRPSEMPro's flexible parameter optimization modules. Development of the process simulation code can be done using the solvent extraction process at Argonne National Laboratory in collaboration with the UNLV Nevada Center for Advanced Computational Methods.

The major objectives are the following:
- Develop a framework for simulating the Spent Fuel Treatment Facility (SFTF) process using AMUSE code, commercial process package, such as ASPEN-PLUS, and system engineering model.
- Develop a middleware package that can communicate between the AMUSE code and any selected commercial packages.
- Extend the existing system engineering model for the optimization process that includes process simulation results.
- Include a scenario-based database system that efficiently reports required information as chart output using web-based programming, and Microsoft Visual Basic (MS VB).

RESEARCH ACCOMPLISHMENTS

- Completed the feasibility study of the nitric acid recycle process using the ASPEN-Plus system process package.
- Completed the "skeletal backbone" study of the NPEX process using the ASPEN-Plus system process package.
- Integrated the ASPEN-Plus process model with the TRPSEMPro system engineering modeling package, developed by the UNLV team.

Process Simulation of Nitric Acid

ANL is interested in understanding the feasibility of applying tower separation for nitric acid, acetic acid and water separation, with nitric acid leaving as bottoms product with a higher concentration of 4.5M from 0.6M. The purpose of the simulation is to validate the feasibility of using tower design. An arbitrarily assigned molar flow rate was chosen in an effort to test the hypothesis. Two parametric studies were conducted for this distillation simulation. The first parametric study was to observe the effects of varying the reflux ratio on the outlet flow rates while the second one examined the effect of varying the number of stages on outlet flow rate.

With the temperature, pressure, feed concentration, distillate rate and number of stages held con-

Overall process flow sheet.

stant it was desired to study how changing the reflux ratio in the column affects product flow rates. Increasing of reflux ratio gives an overall decrease of nitric acid flow rate and increase of acetic acid and water flow rate in the bottom streams. In the second parametric study, molar flow rate of nitric acid from the bottom streams continuously decreases along with the increasing of the number of stages and is gradually stabilized after number of stages larger than 6.

While the studies performed have shown that the manipulation of both reflux ratio and number of stages affects the separation of feed components, the changes are minimal and can be considered negligible. The simulation showed that it is not feasible to design a tower that removes nitric acid as a bottoms product from a feed of nitric acid, acetic acid and water. If it is desired to separate and obtain a high purity nitric acid stream; having the nitric acid leave the column as distillate is an option. Under such a circumstance, it is no longer necessary to have a rigorous separation model. AS-PEN Plus can calculate the number of stages and reflux ratio based on the engineer's desired separation efficiency.

The new ASPEN Plus flow sheet for this second separation simulation will concentrate a 0.6M feed of nitric acid (in water) to a 4.5 M solution (in the tops stream). The ASPEN Plus simulation data indicates a possible optimized number of stages is around 15 with the reflux ratio of 0.60.

Process Simulation of NPEX Process

The NPEX process is used by ANL scientists to remove plutonium and neptunium from spent fuel. The work conducted in this project is the simulation of the process following the removal of

the plutonium/neptunium strip product. The simulation is intended to construct a "skeletal backbone" of the plutonium metal production process due to the difficulty of acquiring the plutonium metal production process simulation parameters.

Interface to ASPEN-Plus through the TRPSEMPro Package

To generate the middleware interface between TRPSEMPro and ASPEN Plus, element types of "Streams" and "Blocks" from AS-PEN-Plus package need to be clearly identified. Streams can be further divided into input and output parts while blocks store system-related information. The currently developed interface shows the essential functions of file selection, data processing and file storage. The major role of the developed TRPSEMPro package is to perform the optimization process using both ASPEN-Plus system process engineering and chemical separation process. The data communication and result presentation from these two programs can be valuable for the SFTF design. Since the AMUSE code has been integrated with the TRPSEMPro package, the current internal database is integrated with those results generated from the ASPEN-Plus simulation. While the development of the data communication and processing tool is the major focus, optimization criteria development will be provided or developed by researchers from the ANL.
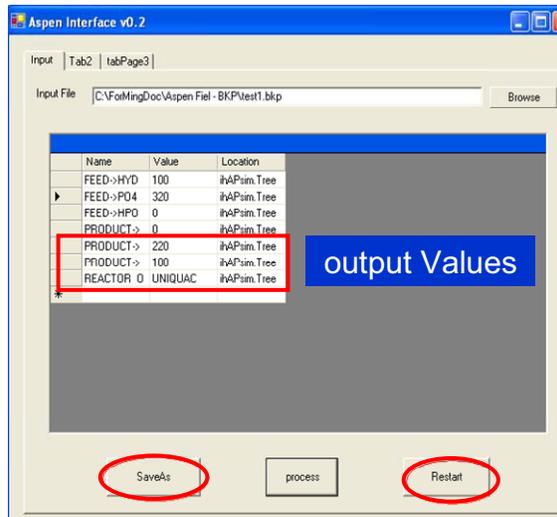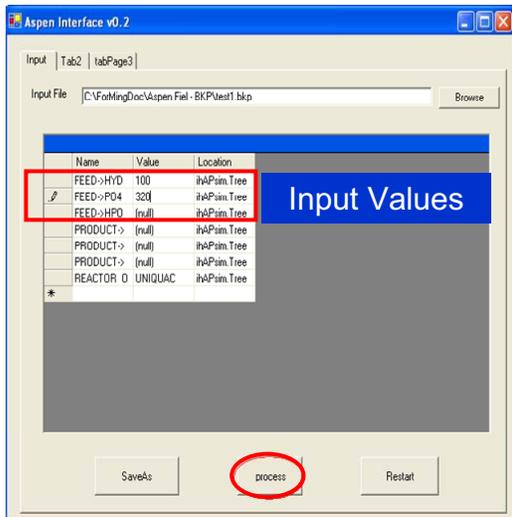
FUTURE WORK

• Complete the feasibility study of the nitric acid recycle process using the ASPEN-Plus system process package.
• Complete the "skeletal backbone" study of the NPEX process using the ASPEN-Plus system process package.
• Integrate the ASPEN-Plus process model with the TRPSEMPro system engineering modeling package developed by the UNLV team.

Interface for accessing ASPEN Plus package.

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