

## Task 24

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

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## BACKGROUND

The UNLV Transmutation Research Program is developing technology for the transmutation of nuclear waste to address long-term disposal issues. Integrating and enhancing the Argonne Model for Universal Solvent Extraction (AMUSE) code that contains a great part of chemical separations processing, is the major part of a previous 3-year project. Simulating the Light Water Reactor (LWR) Spent Fuel Treatment Facility (SFTF) processes is the major focus for this three-year project. The approach is to combine commercial process simulation software, ASPEN-Plus, with the chemical separation calculation from the AMUSE code. Based on the current Integrated System Optimization Program, ISOPro, 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 the functionality of receiving, temporarily storing, and preparing spent nuclear fuel for leaching.

The spent fuel treatment facility has many individual processes that make up the overall separations processes. As illustrated in the overall process flow sheet below, each block represents a unique process that carries out an individual chemical separation. Each individual process block contains numerous operations that are responsible for the chemical separation. By removing the primary constituent, U, from spent fuel enables more waste to be stored at geologic repositories. The Uranium Extraction Process (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 major objectives described below will lead to a creation of framework that combines all the strengths of AMUSE's complicated calculations, well-established commercial system process package and ISOPro'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 research team from Mechanical

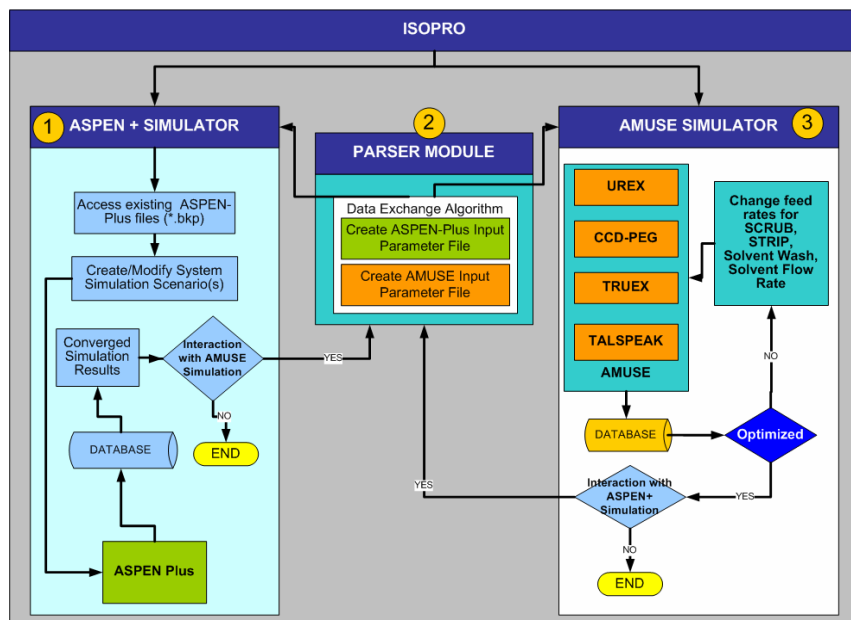
Engineering Department at UNLV. The objectives of this project are:

- To develop a framework for simulating the Spent Fuel Treatment Facility process using the AMUSE code, ASPEN-Plus commercial process package and ISOPro system engineering model.
- To develop middleware interfaces that can communicate between the AMUSE code and ASPEN-Plus packages.
- To extend the existing system engineering model for the optimization process that includes process simulation results.
- To 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

- Integrated the ASPEN-Plus process model with the ISOPro system engineering modeling package, developed by the UNLV team.
- Tested the simplified system process integration using the ISOPro package.
- Generated complete version of the ISOPro package user manual and tutorial.
- Made an interface to interact with ASPEN-Plus through the ISOPRO Package

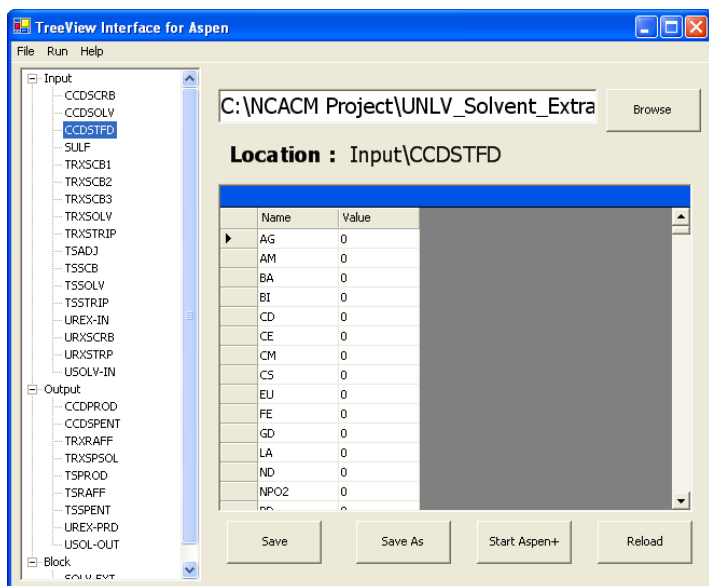
To interact with both the AMUSE and ISOPro packages, the middleware interface based on the ISOPro should provide the capability of interacting with external programs, converting input and



Modified TRPSEMPro system architecture

output data and managing process results. The major task for the year was to complete the interface to the ASPEN-Plus program through the developed ISOPro package. The data communication and result presentation from these two programs are valuable for the SFTF's process design task. The internal MS Access database was developed for storing intermediate and final simulation results from both programs. However, input and output data files originally generated from each individual program are kept intact and are used to populate the initial data sheet within each middleware interface. Although the program integration was completed, the final SFTF's system optimization work is not included in this report due the export control nature of the AMUSE code. The optimization can be completed by the ANL research team by plugging the full AMUSE program into the ISOPro package. The accomplishments for the year are summarized as follows:

- The framework design was revised to improve the performance of the system. It defines the data flow from ASPEN-plus to AMUSE with the data set "parser module" in the middle. Based on the discussion with ANL staff, the UREX+1a process simulation flow chart was updated based on the input and output natures defined in the database storage.
- The middleware for the ASPEN-Plus interacts with the ASPEN-Plus and populates data into a user friendly, tabulated format. It displays the information from streams and its elements. The user can modify the input values and directly run the simulation through the interface. There are sets of standard menu items listed to provide faster access. A "Tree"



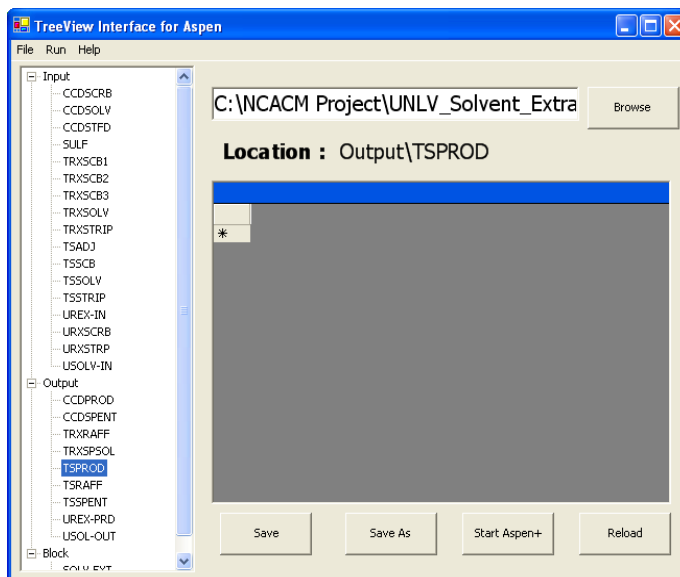
## ACADEMIC YEAR HIGHLIGHTS

- ◆ M. Cheng, M. Hodges, K. Kwan, H.T. Hsieh, and Y. Chen (UNLV); G. Vandegrift, J. Copple and J. Laidler (ANL), "An Object-oriented Systems Engineering Modeling Design for Integrating Spent Fuel Treatment Facility and Chemical Separation Processes," 2006 American Society of Mechanical Engineers, International Mechanical Engineering Congress, Chicago, IL, November 5-10, 2006.

view of the streams is organized into "Input" and "Output" based on the "Blocks" definition retrieved from the Aspen "bkp" file. After each simulation run from the ASPEN-plus, input/output information is updated into the interface. The selected programming algorithm can significantly impact the read/write efficiency of the code, especially loading a large and complicated "bkp" file. A "nested hash" programming technique was used. To accelerate data access, ASPEN-Plus information was stored in two hashes, one for Input streams and one for Output streams.

## FUTURE WORK

Future work will include optimization of the system and chemical separation processes using the ISOPro system engineering modeling package developed by the UNLV team.



Screenshots of the newly updated ISOPRO interface to the ASPEN-Plus; (left) input stream; (right) output stream.

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