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

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## Task 24

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

Y. Chen and S. Hsieh

## BACKGROUND

This effort is a continuation of the work of Task 8 (see page 20), and the same overview applies. The chemical separation process is calculated by the Argonne Model for Universal Solvent Extraction (AMUSE) code, developed in the 1980s, that designs multi-stage countercurrent flowsheets for the TRUEX solvent extraction process. The Generic TRUEX Model (GTM) and AMUSE predicts chemical behavior in solvent extraction processes by calculating component distribution ratios. Further, the countercurrent mass balance algorithm contains terms for stage efficiency and other-phase-carryover for both the aqueous and organic phases. All five process segments of the UREX+ process were programmed into AMUSE code. The currently developed TRPSEMPro (Transmutation Research Project System Engineering Model PROgram) by the Nevada Center for Advanced Computational Methods (NCACM) at the University of Nevada-Las Vegas can be highly integrated with the AMUSE code and commercial packages to calculate the complex interactions between proposed process changes.

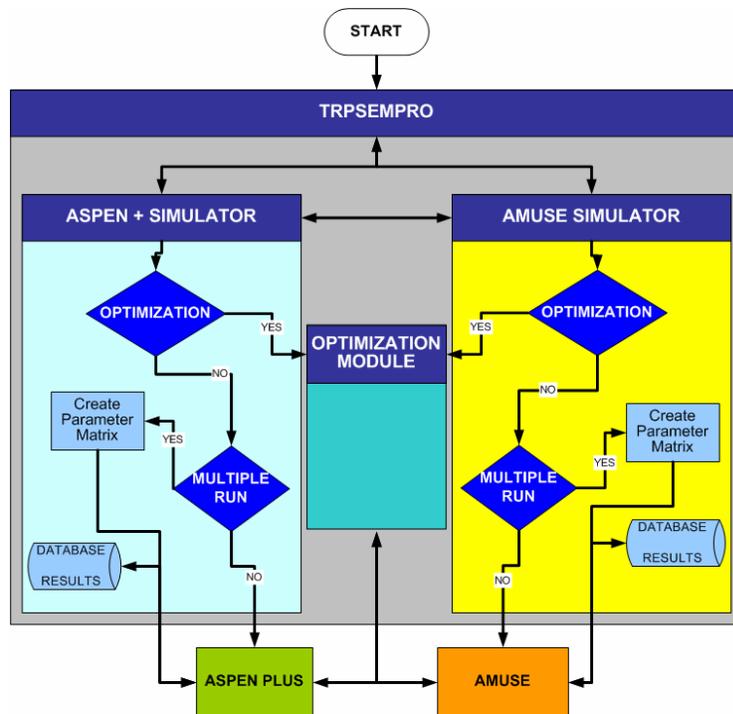
While successfully embedding AMUSE module into a dedicated System Engineering Model (TRPSEMPro), Argonne National Laboratory is interested in further simulating the Light Water Reactor (LWR) Spent Fuel Treatment Facility (SFTF) combining commercial process simulation packages and core calculation of the AMUSE that derived for using with the UREX+ process. The designed SFTF will receive, temporarily store, and prepare spent nuclear fuel for leaching. The leached fuel will then be separated by solvent extraction to recover:

- Uranium, Technetium and Iodine for disposal as low-level waste (LLW)
- Cs/Sr for decay storage and eventual disposal as LLW while Pu/Np for production of mixed-oxide (MOX) fuel
- Am/Cm for short-term storage and eventual use as fast-reactor fuel
- Two raffinates from the UREX+ process containing all soluble fission products but Cs, Sr, Tc, I, and the rare earth elements will be converted to a solid for disposal in the repository.

## RESEARCH OBJECTIVES AND METHODS

The major objective is to create a framework that combines all the strengths of AMUSE's complicated calculations, well-established commercial system process package such as ASPEN-PLUS, HYSYS and PRO/II and TRPSEMPro's flexible parameter optimization modules. Development of the process simulation code can be done using the solvent extraction process experience at Argonne National Laboratory and in collaboration with the NCACM. The major activities of the task are the following:

- Develop a framework for simulating the SFTF process using AMUSE code, commercial process package, such as AS-



The framework design for the chemical separation process.

PEN-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 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).

A comprehensive study of commercial simulation packages has been performed by the Argonne National Laboratory. The three most promising packages identified were ASPEN-PLUS, HYSYS and PRO/II. All these packages require purchasing the aqueous electrolyte package that can incorporate AMUSE as the unit operation for solvent extraction. Since the ASPEN-PLUS provides a greater capability for solids handling, the major task here will create a communication tool between the AMUSE code and the ASPEN-PLUS. ASPEN-PLUS or an alternative, used for the SFTF process simulation, will be thoroughly studied for data parsing capability.

The NCACM team intends to develop a middleware package that can communicate between the AMUSE code and any selected commercial packages. An interface will be developed that incorporates AMUSE as the solvent extraction unit operation and any commercial package as the head-end and back-end processes.

## RESEARCH ACCOMPLISHMENTS

This project identified the parameter correlations and data manipulation channels between the AMUSE code and the selected process simulation software package such as identified AMUSE input/output (from AMUSE Macros) to specify input streams associated with typical spent fuel, determine all inputs and outputs for each process block, select key components to monitor throughout process, and document key individuals or organizations for each process block. Also, AMUSE input/output (from TRPSEMPro package) have been identified to specify input streams associated with typical spent fuel, determine all inputs and outputs for each process block, and select key components to monitor throughout process. The communication protocols from the selected process simulation package have also been identified to specify the possible data manipulation routes, determine the most suitable channel for data transferring, and streamline the discrepancies among AMUSE code, TRPSEMPro and the selected process package such as ASPEN-PLUS, HYSYS and PRO/II.

The middleware for data manipulation among the AMUSE code, system engineering model and the selected process simulation software package has been developed to define Framework Architecture. The middleware has included a database design for temporary data repository. The XML data communication standard has been used for data manipulation. However, some of the process package might not support XML-enabled transfer and will be considered respectively. The middleware implementation – use programming languages, such as MS VB and VB.net, are under development.

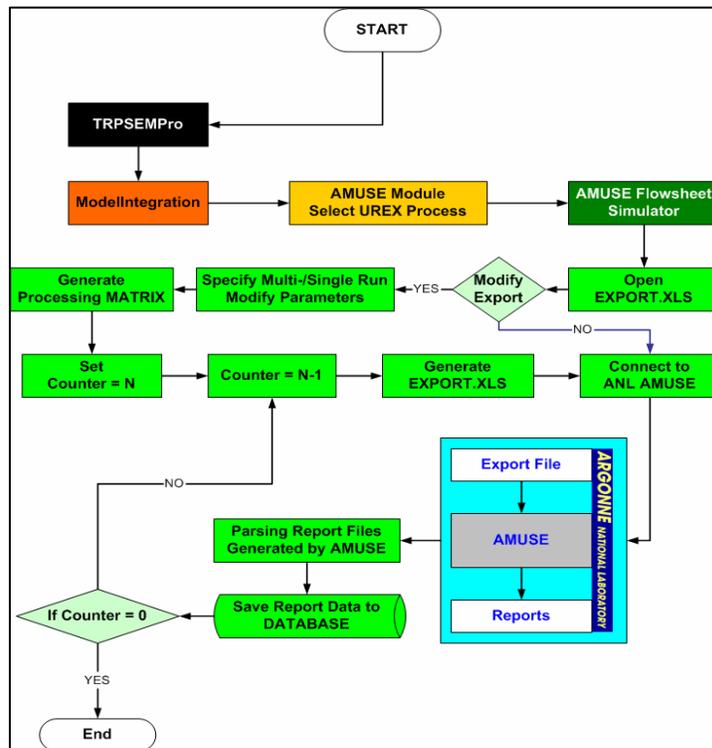
The overall TRPSEMPro system model is evolving as the TRP project continues. UNLV will work to incorporate changes to the overall process as time advances and make changes to the software that allows it to be used as a part of the overall systems engineering model and that allows it to be used as a stand-alone process model. A few modifications need to be studied to allow the optimization of the process. Argonne National Laboratory collaborators will provide the system information to analyze a variety of proposed configurations.

## FUTURE WORK

It could take years before incorporating all of the UREX separation processes into the developed systems engineering model. While waiting for completing the processes, developing more system analysis modules for TRPSEMPro will definitely strengthen its capability on solving complex chemical separation process. Future work also includes increasing the sophistication of the systems engineering model, such as addition of optimiza-

## ACADEMIC YEAR HIGHLIGHTS

- ◆ “Development of Systems Engineering Model for Spent Fuel Extraction Process” was published in the Proceedings of IMECE2004, ASME International Mechanical Engineering Congress, Anaheim, CA, November 13–19, 2004



Middleware design flowchart for the AMUSE Simulator.

tion tools. As optimization constraints are provided, relative comparisons of process options with regard to waste generation, proliferation resistance, throughput capabilities, facility requirements, and cost are possible. The system model will provide engineers and scientists a user-friendly Window-based graphical user interface package. Increased confidence in the models and further refinements render greater objectivity and technical credibility to the decision-making process. Also, three candidate software packages have been identified: Aspen Plus<sup>®</sup>, HYSYS<sup>®</sup>, and PRO/II<sup>®</sup>, which will be coupled or interacted with TRPSEMPro and AMUSE to define actinides and fission product physical-chemical databases, accurately predict aqueous electrolyte systems, and create a thermodynamic package for phase diagrams and coupling of phase diagrams with kinetic process modeling.

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