

Task 24

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

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BACKGROUND

Integrating and enhancing the Argonne Model for Universal Solvent Extraction (AMUSE) code, which contains a great deal of chemical separations processing, was part of TRP Task 8. Simulating the Light Water Reactor (LWR) Spent Fuel Treatment Facility (SFTF) processes is the major focus for this project. This approach combines 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) this project aims to create a system framework that interacts with both programs and provides analyzed results useful for a SFTF design that provides the functionality of receiving, temporarily storing, and preparing spent nuclear fuel for leaching.

A spent fuel treatment facility has many individual processes that make up the overall separation. Each block in the overall process flow sheet represents a unique process that carries out an individual chemical separation, and each block contains numerous operations that are responsible for the chemical separation.

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.

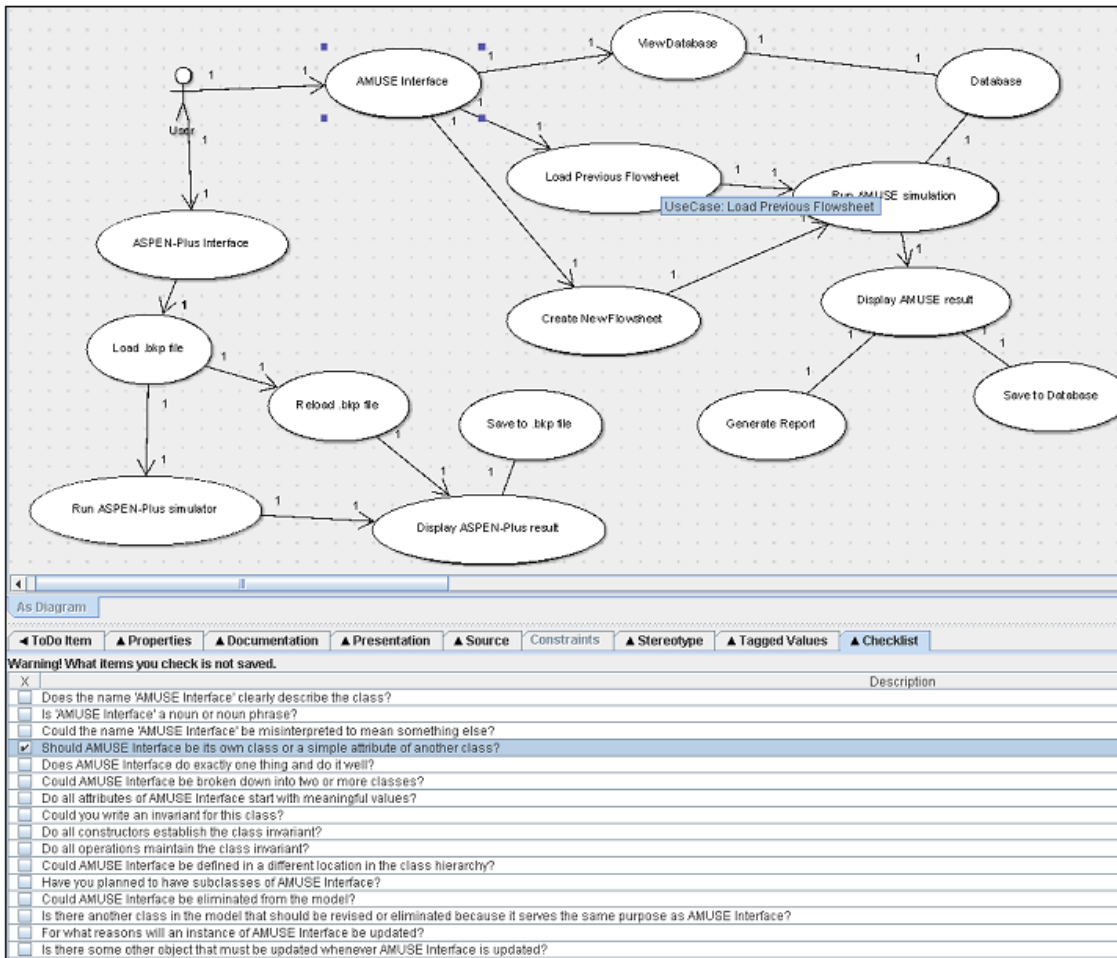
A key concept in the SFTF plant design is the recycling of nitric acid. The purpose of the nitric acid recycling system is to concentrate the spent nitric acid to a desired molarity which, in turn, can be recycled back into the process. The spent nitric acid streams from many processes are collected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

RESEARCH OBJECTIVES AND METHODS

The major objectives will lead to the creation of a framework that combines all the strengths of AMUSE's complicated calculations, well-established commercial system process package, and ISO-Pro'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 the Mechanical Engineering Department at UNLV. The objectives are as follows:

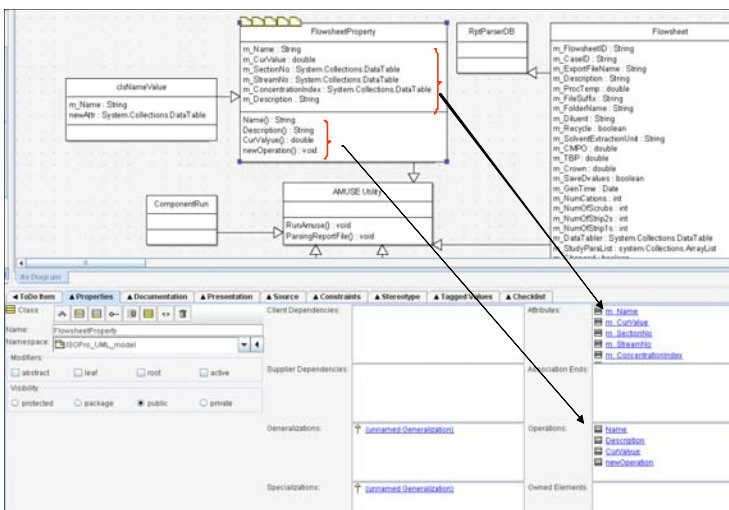
- To develop a framework for simulating the Spent Fuel Treatment Facility process using the AMUSE code, ASPEN-Plus commercial process package and ISOPro system engineering model.
- To develop middleware interfaces that can communicate between the AMUSE code and ASPEN-Plus packages.
- To extend the existing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



Use Case for the updated ISOPro package.

ACADEMIC YEAR HIGHLIGHTS

- ♦ M. Chang, H.-T. Hsieh, Y. Chen, and M. Hodges, "Development of an Integrated Systems Engineering Modeling Package for Chemical Separation Processes under Advanced Fuel Cycle Initiative," *Proceedings, ICAPP '08, Anaheim, CA, USA, June 8-12, 2008, Paper# 8208.* (accepted)



Detailed design factors for the "Flowsheet" module are documented in the property sheet shown at the bottom.

RESEARCH ACCOMPLISHMENTS

- Completed final version of the ISOPro User Manual associated with summarized ISOPro source codes.
- Redesigned and completed use case and design class diagrams (DCD) of the ISOPro package using ArgoUML.
- Improved ISOPro system and AMUSE data flow and re-coding on VB.NET and ActiveX Data Objects (ADO) with improved data reading function.

To better maintain and improve the ISOPro system engineering package, construction of Unified Modeling Language (UML) diagrams was initiated. Unlike the general user manual or tutorial, the UML diagrams are specifically designed for communication among programmers and software engineers with standardized terminology and module definition. The creation of such diagrams provides high flexibility on version control, code comparison and module modification. They can be distributed to different development identities (institutes) in the future for coordinating software improvement and modification efforts. Three major components were developed. They are Use Cases for ISOPro package, Class Diagram for AMUSE middleware interface, and Class Diagram for ASPEN-Plus middleware interface.

Use Case Model

Use cases are about defining requirements needed for the package development. For example, 15 user goals were determined in the current ISOPro system. The user initially decides to execute either the AMUSE or ASPEN-Plus package. Once the package is selected, sequential actions are followed. Each block (goal) is associated with a checklist that guides the code development. Use

cases summarize both functional and non-functional requirements. To improve the package in the future, developers can easily identify existing functional blocks from use cases and effectively modify this package.

Design Class Diagram

Design class diagrams are used to identify the specification for the software classes after determining use cases. Information related to classes, associations and attributes, interfaces, methods, and dependencies was included in the DCD. There are seven classes associated with ExprotFilePaser class. No method was developed under these classes.

Initial design of the ISOPro interface read in a large amount of ASPEN-plus parameters into the system (or database), which slows down the system dramatically. The identified solution was to rewrite the program to read in all parameter fields into database sequentially and flag null parameter fields during reading. An optimized "search" algorithm was implemented to exclude those null data fields during data from the database into the interface. The improvement was completed. UML diagrams were used to evaluate data flow and efficiency for the ISOPro system. The ISOPro interaction with the AMUSE macros was identified as the bottleneck. The proposed UML diagram solution is to change the existing VB programming into a VB.NET architecture, which provides better data access module and easier coding style. The improvement was started by changing AMUSE data flow and re-coding ADO for better extendibility and maintainability. Methods and attributes from complicate classes such as TreeView, Flowsheet, and FlowsheetProperty have been identified. The development of the diagram makes maintenance and modification more effective. Programs or modules from the ASPEN-Plus simulation can be attached into the current diagram effectively.

FUTURE WORK

Future work will include optimization of the system and provide more simulated chemical separation process cases using the ISOPro system engineering modeling package developed by the UNLV team.

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