2004

Development of a Systems Engineering Model of the Chemical Separations Process

Yitung Chen
University of Nevada, Las Vegas, yitung.chen@unlv.edu

Darrell Pepper
University of Nevada Las Vegas, pepperu@nye.nscee.edu

Sean Hsieh
University of Nevada, Las Vegas, hsiehht@nscee.edu

Task 8

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Y. Chen, D.W. Pepper, and S. Hsieh

BACKGROUND

The chemical processing of used nuclear fuel is an integral component of any strategy for the transmutation of nuclear waste. Due to the large volume of material that must be handled in this first step of the transmutation process, the efficiency of the separations process is a key factor in the potential economic viability of the transmutation strategies. The ability to optimize the chemical separation systems is vital to ensure the feasibility of the transmutation program.

Systems analysis, or total systems modeling, is one of the strongest tools available to researchers for understanding and optimizing complex systems such as chemical separations processes. Systems analyses permit researchers to present decision-makers concise evaluations of system options and their characteristic features. The primary goal of this project is to develop a systems model that can be used to parameterize and optimize chemical separations processes.

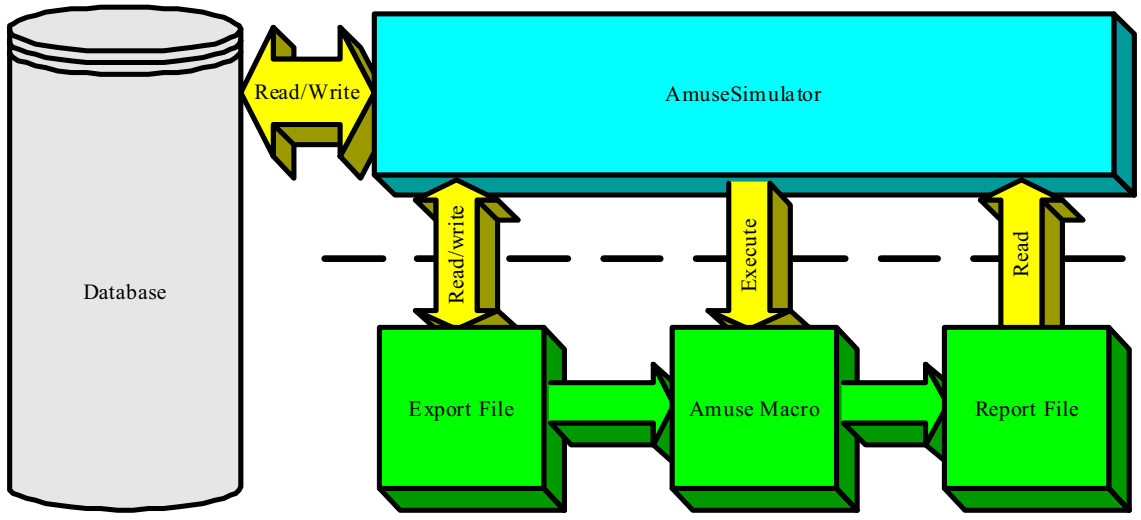
RESEARCH OBJECTIVES AND METHODS

This work includes reviewing and analyzing the AMUSE code structure, examining other possible implementations, defining software activities, developing a verification plan, and modifying and improving the software. This work also involves redefining the graphical user interface (GUI) to increase the utility of the AMUSE code suite as a stand-alone analytical package.

Developing a systems engineering model requires ongoing discussions with Argonne National Laboratory personnel to identify pertinent components of the chemical separations process. Each step requires model development to establish its significance with regards to the overall process. Comprehensive model development involves defining the inputs and outputs from individual models and establishing how each connects to the other within in the chemical separations process.

RESEARCH ACCOMPLISHMENTS

Based on the clearly defined objectives above, this project developed a general-purpose systems engineering model software, TRP System Engineering Model Program (TRPSEMPro) that will be used to improve productivity in the design process. A complete implementation of the systems engineering model requires integration of various chemical separation components. One of the major tasks for the project is to demonstrate the advantage of using a system engineering model concept that integrates with AMUSE chemical separation module. The system model also includes various numerical optimization technologies and Design of Experiments (DOE) study technologies. The framework and environment for a systems engineering model of the chemical separations system is used to establish the baseline model, which will be used as a reference for examining the impacts of any modifications.



The Architecture design for AMUSESimulator

Object-Oriented Analysis and Design was used for developing and implementing the TRPSEMPro system. A graphical notation, Unified Modeling Language, was employed to express object-oriented designs. Microsoft.Net architecture was for system development and Visual Basic.NET was the major programming language behind the system. XML (Extensible Markup Language) is widely used to describe data and sets of elements and attributes that can be defined by researchers. XML Schema was used for describing the structure of the system engineering model. XML Database was used to store all the run-time data for AMUSE module. Since significant experimental data will be generated and require systematic analysis, MS SQL Server 2000 database was selected for housing all run-time parameters and simulation results. The model combines with the commercial software packages, MATLAB OPTIMIZATION toolbox and SIMULINK module from Mathworks.

The system model, TRPSEMPro, considers input simulation modules from multiple disciplines with inconsistent input/output handles. The package with the aid of middleware can communicate with various simulation modules developed by other research groups and create an XML-based model description file. The critical components for the system engineering modeling include System Manager, Model Integration, Study Plan, and Solution Viewer.

The introduction of the middleware design provides flexibility to interface to other simulation modules without significant program modification. The demonstration code from AMUSE macros is kept intact during all system development stages. AMUSESimulator, is the middleware software package which was designed and implemented to serve as a bridge between the AMUSE code, and the systems engineering model, TRPSEMPro. Such an approach can reduce the time-consuming modification on the system model side and keep flexibility on the simulation modules development side.

Object-oriented design is used to identify four major objects. First, the data input interface takes the user input from these blocks and creates an export file. Secondly, an export file serves as the input to the AMUSE code that performs all the chemical extraction calculations. The third component handles result file open and save. The fourth component acts as an optimization tool that continuously interacts with MATLAB commercial components until the optimization objectives are achieved.

HIGHLIGHTS

- "Development of Systems Engineering Model For UREX Process," ANS Accelerator Applications in a Nuclear Renaissance, San Diego, CA, June 1-5, 2003.
- "Development of a Systems Engineering Model for Spent Fuel Extraction Process," AFCI Semi-Annual Review Poster Presentation, Santa Fe, NM, August 2003.
- "Development of Systems Engineering Model For UREX Process," ASME International Mechanical Engineering Congress and R&D Expo, Washington, DC, November 16-21, 2003.
- Lijian Sun completed his M.S. in Mechanical Engineering (December 2003), thesis entitled "Development of a Systems Engineering Model of the Chemical Separation Process."

Further system enhancement allows the user to select various process types. An interface for conducting multiple runs has been created. The GUI includes a list of variables, a range for those variables, all of which provide an envelope of end results.

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 optimization 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®, HYSYS®, and PRO/II®, 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.

Research Staff

Yitung Chen, Principal Investigator; Associate Professor, Mechanical Engineering Department; Associate Director, NCACM
Darrell W. Pepper, Professor, Mechanical Engineering Department; Director, Nevada Center for Advanced Computational Methods
Sean Hsieh, Research Assistant Professor, UNLV Nevada Center for Advanced Computational Methods
Randy Clarksean, Adjunct Professor, Mechanical Engineering Department

Students

Sushma Gujjula, Haritha Royyuru, and Lijian Sun, Graduate Students, Mechanical Engineering Department

Collaborators

James J. Laidler, Senior Scientist, Chemical Technology Division, Argonne National Laboratory
George F. Vandergrift, III, Senior Scientist, Chemical Technology Division, Argonne National Laboratory