AN OBJECT-ORIENTED SYSTEMS ENGINEERING MODEL DEVELOPMENT FOR IMPROVING DESIGN FACTORS OF THE SPENT FUEL EXTRACTION PROCESS

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ABSTRACT

The United States is embarking on a national program to develop accelerator transmutation of high-level radioactive waste (ATW) as part of the Transmutation Research Program (TRP) project at its national laboratories. Through the TRP, the U.S. joins international efforts to evaluate the potential of partitioning and transmutation along with advanced nuclear fuel cycles. The TRP is aiming to develop technology for the transmutation of nuclear waste to address major long-term disposal issues. The Argonne National Laboratory (ANL) researchers have been working on development of the chemical separations scheme as an integral part of the TRP program.

The development of the fuel cycle scheme requires the consideration of complicate process from transuranic elements and long-lived fission products derived by Light Water Reactor (LWR) spent fuel to separation processes involving intermediate critical reactor steps. Any proposed modification to the process can have impacts on the fuel design, amount of waste generated by the process, number of cycles through the reactor, etc. In a nuclear growth scenario, the introduction of advanced thermal reactor designs will almost certainly result in changes in separations system requirements that must be met with optimized systems.

Systems engineering model is a powerful tool for enhancing the ability to improve such tedious refinement process. The separation process, as a model, can be systematically identified into groups of blocks that have specific separation functions. One block's effluent flows into another block as input. Each block has its process target. For a complex process like chemical separation process, the use of modularized systems engineering model approach can speedup the design and process refinement.

Under the guidance from the Chemical Engineering Division, Argonne National Laboratories (ANL), the Nevada Center for Advanced Computational Methods (NCACM) at University of Nevada-Las Vegas (UNLV) is developing a systems engineering model that provides process optimization tool through the automatic adjusted input parameters, such as feed compositions, stage numbers and flow rates, to improve the countercurrent solvent-extraction process on treating high-level liquid waste, such as U and Tc. Major objectives of the paper are to introduce the design concepts of the systems engineering model and to demonstrate the completed multiple-run module.

INTRODUCTION

The United States is embarking on a national program to develop accelerator transmutation of high-level radioactive waste (ATW) as part of the Transmutation Research Program (TRP) project at its national laboratories. Through the Program, the U.S. joins international efforts to evaluate the potential of partitioning and transmutation along with advanced nuclear fuel cycles. Transmutation means nuclear transformation that changes the contents of the nucleus. The TRP is a developing technology for the transmutation of nuclear waste to address many of the long-term disposal issues. An integral part of this program is the proposed chemical separations scheme. Figure 1 shows a block diagram of the current process as envisioned by Argonne National Laboratory (ANL) researchers [1], [2], [3].

Nearly all issues related to risks to future generations arising from long-term disposal of such spent nuclear fuel are attributable to ~1% of its content that includes plutonium, neptunium, americium, and curium (the transuranic elements) and long-lived isotopes of iodine and technetium. While removing transuranics from discharged fuel destined for disposal, the toxic nature of the spent fuel drops below that of natural uranium ore within a timeframe of several hundred years. Figure 1 depicts the fuel cycle scheme in which the transuranic elements and long-lived fission products from Light Water Reactor (LWR) spent fuel are sent directly to an accelerator-driven sub-critical reactor for transmutation. Other schemes under consideration involve intermediate critical reactor steps; this would result in major changes in the design, development and analysis of separations systems. Systems engineering would enhance the ability to respond with such changes.

The complete process considers existing LWR spent fuel, separation processes, fuel fabrication, transmutation, disposal as a low-level waste (LLW), and the reprocessing of fuel after transmutation. This is an involved process that can be varied in a number of ways. Any proposed change to the process can have impacts on the fuel design, amount of waste generated by the process, number of cycles through the reactor, etc. In a nuclear growth scenario, the introduction of advanced thermal reactor designs will almost certainly result in changes in separations system requirements that must be met with optimized systems.

As indicated in Figure 1, the separation process can be systematically identified as a group of blocks that have specific separation functions and parameters. One block's effluent flows into another block as input. Each block has its process target. For a complex process like chemical separation process, constructing a systems engineering model is critical for design optimization and process refinement. The objective of this research to develop a systems engineering model software that integrates existing separation modules from various agencies for analyzing and improving chemical separation process in a systematic and optimized ways. Due to the availability of the process modules, this research only demonstrates the systems engineering model using Argonne Model for Universal Solvent Extraction (AMUSE) module from Uranium Extraction (UREX) process. The system design concept and developed interface will be discussed in the paper.
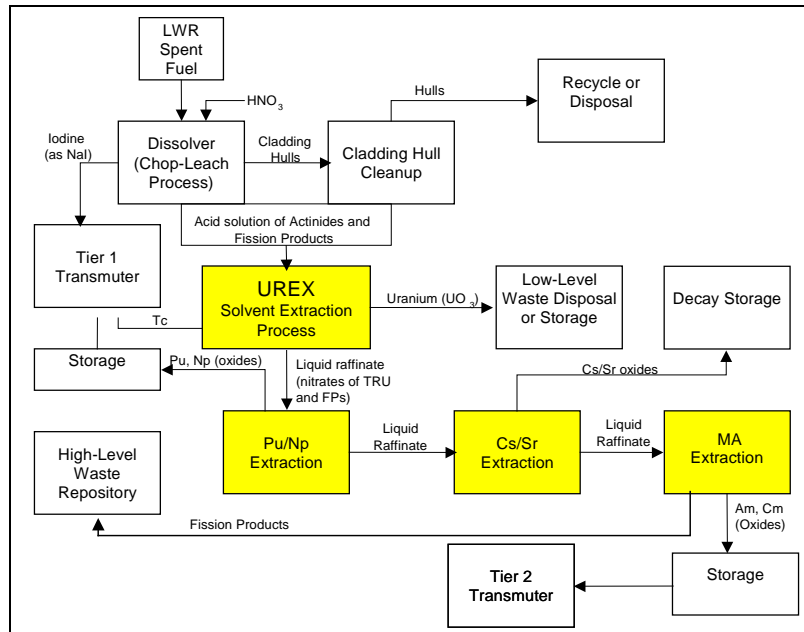
Fig. 1. Chemical separations system for TRP program.

Methodology

This research is primarily concentrated on prototyping system engineering model for solving complicate chemical separation process. It is appropriate to provide insights about systems engineering, design of study and optimization.

System Engineering

System Engineering Model consists of defining and implementing an approach to solving problems, while managing complexity and communicating over the entire lifetime of a project [4]. Such model can be generally divided into two parts [5]: modeling and optimization. The model usually performs requirements definition, conceptual design, subsystem partitioning, and system validation. The chemical separation process can be identified as blocks that have specific separation functions and attributes. All blocks are linked to each other where one block's effluent flows can be another block's input. Each block has its process target. Since all separation processes were developed individually from the ANL side, each process block shown in Figure 1 usually calculated by a set of equations or relationships to model its mass transport through the process. No standard input or output convention can be followed from those developed software (package). Along with the growth of system complexity, the process can become difficult and hard to analyze mathematically. Therefore, research here is to design and develop a system model with the capability to bridge the existing codes to the systems engineering model.

A few critical components are required during the system modeling: input/output parameters, execution sequence of extraction processes, system analysis, and process monitoring. Therefore, the designed system model defines four components:

- System Manager - the main interface for setting up and executing problems.
- Model Integration – the interface to couple simulation programs with system engineering model and specify its execution sequence. It can also create model description files using XML.
- Study Plan – the module provides a convenient means for detailed problem formulation information that defines all the design parameters. Techniques such as optimization and design of experiments are included, too.
- Solution Viewer - provides various tabulated and graphical interface for monitoring the optimization process as it moves through the design space.

Design of Experiment (DOE) and Optimization

Design of Experiment (DOE) is the method generally used for setting parameter values in a set of experiments. Several techniques about DOE study, such as Full-Factorial, Parameter Study, Data File, Orthogonal Arrays, Central Composite and Latin Hypercubes, have been studied [6], [7]. More details can be found through the provided references.

Qualitatively optimization implies multiple decision choices that implicitly recognize the necessity of choosing among alternatives. Quantitative description of the solution requires a quantitative description or mathematical model of the problem itself. Optimization presupposes the knowledge of the design rules for the specific problem, primarily the ability to describe the design in mathematical terms. These terms include design variables, design parameters, and design functions. Design variables are entities that identify a particular design. In the search for the optimal design, these entities will change over a prescribed range. The values of a complete set of these variables characterize a specific design. Design Parameters, in this thesis, identify constants that will not change as different designs are compared, while design functions define meaningful information about the design. Those functions establish the mathematical model, evaluated by using design variables and parameters.

The general abstract mathematical model is assembled as following:

Minimize:

$$f(X), [X]_n \tag{Eq.1}$$

Subject to:

$$[h(X)]_l = 0$$
$$[g(X)]_m = 0 \tag{Eq.2}$$
$$X^{low} \leq X \leq X^{up}$$

Minimize the objective function f, subject to l equality constraints, m inequality constraints, with the n design variables lying between prescribed lower and upper limits.

System Engineering Software Design

Experienced object-oriented developers (and other software developers) build up a repertoire of both general principles and idiomatic solutions that guide them in the creation of software. A design pattern is an expression of class combinations and accompanying algorithms that fulfill common design purposes. A design pattern expressed an idea rather than a fixed class combination. Accompanying algorithms express the pattern's basic operation. This research applies standard way for designing effecting Object-Oriented Analysis and Design. It can creates a clean mapping from the very beginning between the real world, in the form of requirements, and the design, in the forms of classes. The domain classes are keys in realizing this mapping. A user can integrate any number or any kind of chemical separation models or other utility model into the whole system model as long as these models satisfy defined interface and implemented simucode programs. The simucode programs create input and output.

A high-level architecture design deals with more on sufficiency and flexibility than on robustness and efficiency. Robustness and efficiency are usually better handled at lower levels of design. Converting the architecture into plain language, five use cases are identified:
- System initializes the systems engineering model.
- User integrates all the required models.
- User builds the study plans.
- User builds the solution views.
- User executes the study plans built.

AMUSE Simulator and UREX Process

The AMUSE (Argonne Model for Universal Solvent Extraction) code is a software package developed by Argonne National Laboratory for the analysis of a Generic UREX process. The UREX process, detailed in Figure 2, is a solvent extraction process capable of separating small quantities of transuranic elements (for example; Np, Am, Pu, and Cm) from aqueous nitrate and chloride solutions. These types of chemical streams are typically generated in reprocessing plant operations or in plutonium production and purification processes. To incorporate the AMUSE Code into the systems engineering model, AMUSESimulator program is introduced as a communication layer that allows the user to quickly and easily define the UREX process.

The framework of AMUSESimulator with systems engineering model and AMUSE macro are shown in Figure 3, all calculations related to uranium solvent-extraction process are made by the interaction with the MS Excel macros, defined within AMUSE codes. However, it is not required to run AMUSESimulator with System Engineering Program or TRPSEMPro together, AMUSESimulator can work with AMUSE Macro as a stand along program. First, each of the different steps in the UREX process is outlined on the screen that allows easy modification. After all the modifications have been made, AMUSESimulator will write all the modifications into Export File which is the input file for AMUSE Macro, and triggers the execution of AMUSE Macro. Finally, the execution of the AMUSE execution generates a report file with. To expedite the data usage, AMUSESimulator saves all Export and Report Files into database.
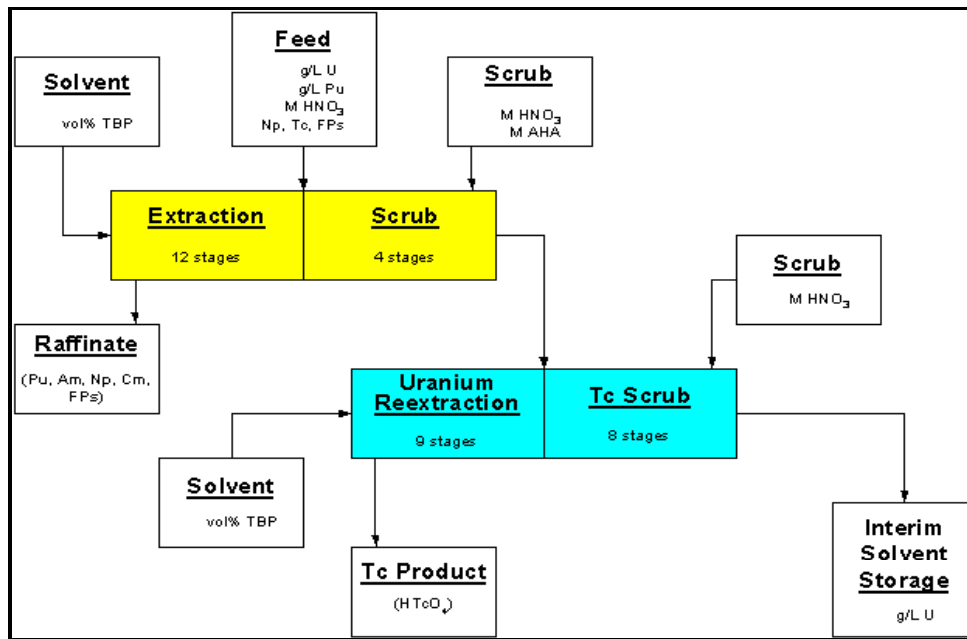
Fig. 2. Detailed description of UREX process, calculated by AMUSE macros.
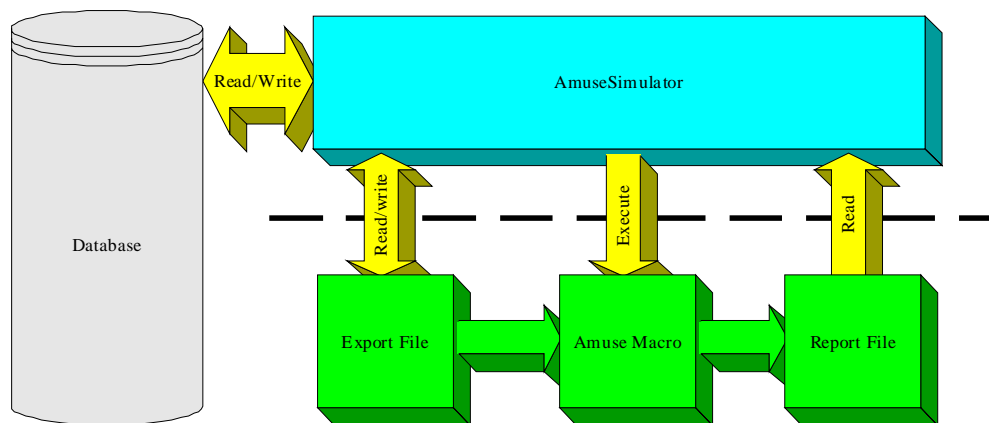

Fig. 3. The framework of AMUSESimulator

Functions for AMUSESimulator include drawing flowsheet to represent each object in UREX process, defining sections within property dialogs, defining stages within property dialogs, defining feed streams with concentration property dialog boxes, execute flowsheet that needs the creation of export file and finally viewing report and displaying information.

AMUSESimulator Interface Demonstration

As shown in Figure 4, the main graphical user interface (GUI) for AMUSESimulator includes Menu and Toolbar, Flowsheet contents (Tree View), Flowsheet contents (Drawing Blocks), Property list for flowsheet, section, stage, concentration and stream. The simulator requires user

to identify simulation scenarios - single-, multiple- and optimization runs. The results can be displayed in a separate chart format while optimization process can also be observed through the plot of Rosenbrock (Banana) Function shown in Figure 4.

A glovebox phase of UREX process shown in Figure 4 is a simplified scenario with limited parameters involved. All separated models from the flowsheet blocks in Figure 1 can be integrated into the system. At current stage the system cannot fully take advantage of the optimization process due to the lack of the chemical separation modules. Along with the development of the chemical separation process modules, the system will be able to demonstrate the complete systems engineering through defining constraints, study plan, and solution viewer, and executing the design run and finally conducting system analysis.
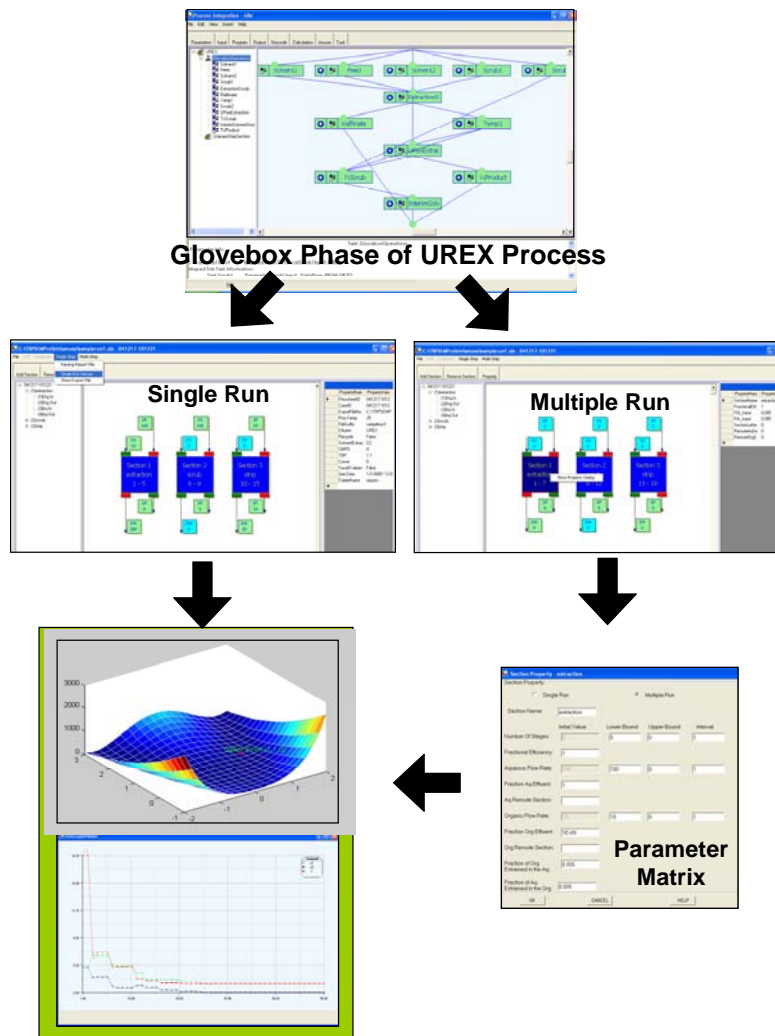

Glovebox Phase of UREX Process

Single Run

Multiple Run

Parameter Matrix

Fig. 4. A system engineering model interface and work flow demonstration.

CONCLUSIONS

Identifying suitable operation parameters during the separation process is complicate. To meet the target extraction rates among those processes, series trial-and-error attempts are inevitable. However, through the development of a general-purpose systems engineering model, the extraction parameters of the chemical separation can be more efficiently estimated. To design a more flexible and robust system engineering model, the research considers design concepts from requirements definition and conceptual design to system partitioning, and finally system validation.

The developed systems engineering model, Transmutation Research Program System Engineering Model Project (TRPSEMPro), includes four major modules: System Manager, Model Integration, Study Plan, and Solution Viewer. System Manager is used to supervise all case (problem) creation and functionality definition while Model Integration identifies chemical extraction processes and their execution sequence. Study Plan is the key to define modeling scenarios, such as optimization, design of experiments, single- and multiple-set parameter simulation. Solution Viewer provides a visual means to monitor the optimization process during and after model execution. The TRPSEMPro package can apply not only to chemical separation process, but also to a general system model.

Software engineering and Object Oriented Analysis and Design (OOA&D) play a critical role during our software development. Through the application of OOA&D, objects and concepts were defined from the problem domain and are quantitatively described by Unified Modeling Language (UML). The designed components were implemented by using MicrosoftTM.Net, the most up-to-date object-oriented programming language framework from Microsoft. Several up-to-date techniques, such as Microsoft.NET framework, MS SQL Server database, eXtensible Markup Language (XML), were applied for developing robust and flexible system.

Currently, only the UREX process module is available for implementation. Since chemical separation modules can be developed from various agencies with different development concepts and programming conventions, an intermediate bridge or interpreter is generally required. This research integrates the only available process, UREX with the TRPSEMPro system model through the AMUSESimulator interface that efficiently defines the UREX process – flowsheet, input streams, sections, and stages. Since the nature of the AMUSE code, the actual code validation and module simulation were carried out by the ANL while iterative code modification and interface improvement are done in the NCACM, UNLV.

ACKNOWLEDGMENTS

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