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Development of a Systems Engineering Model of the Chemical Separations Process

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ANNUAL REPORT

Development of a Systems Engineering Model of the Chemical Separations Process

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Technical Focus Area
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1. Introduction

The United States is embarking on a national program to develop accelerator transmutation of high-level radioactive waste (ATW) as part of the Advanced Accelerator Applications (AAA) project at its national laboratories. Through the AAA 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 (protons and/or neutrons). The research and development efforts will consider a coupled accelerator and sub-critical multiplying assembly, explore the transmutation of waste from used nuclear fuel, testing of advanced nuclear fuels, and the production of isotopes that may be required for national security and commercial applications.

The AAA program is 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. This process, as envisioned by Argonne National Laboratory (ANL) researchers, will be outlined later in this report.

Nearly all issues related to risks to future generations arising from long-term disposal of such spent nuclear fuel is attributable to ~1% of its content. This 1% is made up primarily of plutonium, neptunium, americium, and curium (the transuranic elements) and long-lived isotopes of iodine and technetium created as products from the fission process in power reactors. When transuranics are removed from discharged fuel destined for disposal, the toxic nature of the spent fuel drops below that of natural uranium ore (that was originally mined for nuclear fuel) within a period of several hundred years.

Removal of plutonium and other transuranics from material destined for geologic disposal also eliminates issues related to long-term (centuries) heat management within geologic environments. The removal of neptunium, technetium, and iodine render negligible the possibility of radioactive material penetration into the biosphere far in the future. Finally, removal of plutonium negates any incentive for future intrusion into repositories driven by overt or covert recovery of material for nuclear proliferation.

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.

Developing a systems engineering model of the overall process would be beneficial to analyzing complex interactions between proposed process changes. The model will evolve to incorporate all process steps and to improve process modules as more knowledge is gained. The improvements will be based on empirical data or from numerical models as appropriate.

An integral part of the overall chemical process is a UREX (Uranium Extraction) process. This portion of the process can and will be modeled by the software package AMUSE, as developed by researchers at Argonne National Laboratory. A brief description of this portion of the project is given later in this report.

2. Project Overview

The main research objectives for this project are listed below.

- Develop a framework and environment for a systems engineering analysis of the chemical separations system for the AAA program.
- Establish a baseline systems engineering model from which modifications and improvements can be made.
- Refine the existing AMUSE program that gives a detailed examination of the UREX process, a critical component of the overall separation scheme.

In order to meet these research objectives, two general activities were defined. These activities related to the Systems Engineering portion of the project and the AMUSE code. Each of these activities was broken down into individual tasks. These tasks are outlined and discussed next.

Activity 1: System Engineering Model

1. *Define Goals and Needs* – Discussions were held with ANL personnel to clearly define their long-term needs for a Systems Engineering Model of the fuel processing. These needs may include models relating to mass balances, system control, plant layout and design, and other features as needed.
2. *Define All Unit Operations* – Information was collected and discussions were held with ANL staff to clearly define all current and future unit operations.
3. *Selection of Development Environment* – Commercial software packages were analyzed to determine what – if any – software exists that will meet all of the needs defined in Task 1 of this activity. Potential advantages and limitations of different packages were compared. A commercially available software environment was to be used if at all possible to streamline model development.
4. *Develop Basic System Model* – Upon the selection of the proper development environment, the definition of those components or modules defined in Task 2 will start.
5. *Demonstrate Modeling Concept* – Perform system analyses/simulations using the basic model that has been developed.

Activity 2: Improvement/Automation/Modernization of AMUSE

1. *Review/Analyze Code Structure* – Obtained appropriate files from ANL and studied the layout and development history of the code. Analyzed the data flow through the package to

determine how the different process steps are included and how the calculations are performed.

2. *Examine Other Possible Implementations* – Once the structure of the AMUSE tool was reviewed, efforts were undertaken to determine if the code could be easily converted to a more general programming environment with graphic modules (i.e., Visual Basic, C/C++, newer version of Excel, etc.)
3. *Define Year 1 Software Tasks* – Establish a reasonable set of modifications that can be made to AMUSE by a graduate student over the remainder of the year. The selection of these tasks will be related to the importance of a particular component or process to the AAA Program.
4. *Develop Verification Plan* – All changes to the code will be verified numerically. A set of test problems or other plan will be developed to demonstrate the numerical accuracy of the actual software changes.
5. *Modify/Improve Software* – Make changes to the software as defined in Tasks 3. These changes will be made to benefit the AAA Program.

3. Progress - Systems Engineering Model

A brief overview of the work completed for the Systems Engineering Modeling portion of the project is discussed in following subsections.

3.1 Define Goals and Needs

We will apply general systems engineering techniques/tools to the complex processes of the AAA Chemical Separation Process. We will work on determining

- The development process for a tool that allows process changes to be modeled on a system level
- What impact does one change have on the overall process?
- Developing a mass balance for all process streams
- The impact changes in the input streams have on waste streams.
- Methods to optimize the system: cost, waste streams, etc.
- What detailed models of process components are needed.
- The impact of different assumptions on process performance

3.2 Define All Unit Operations

Figure 1 shows an overall process for dealing with the spent nuclear fuel. There are other potential modifications to the process that can be included as needed in the future. This proposed process was obtained from Argonne National Laboratory Researchers.

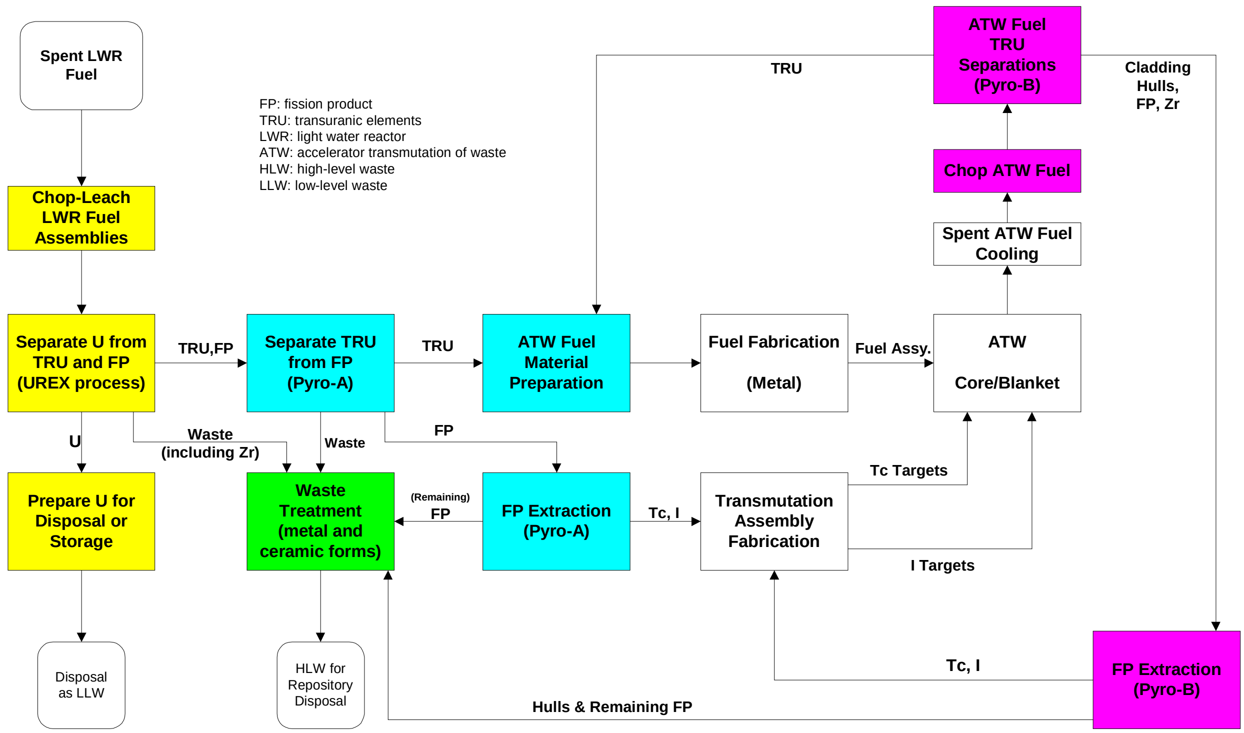

Figure 1 - Overall Chemical Separations System for AAA Program. This figure depicts the fuel cycle scheme in which the transuranic elements and long-lived fission products from spent LWR fuel are sent directly to an accelerator-driven subcritical reactor for transmutation.

3.3 Selection of Development Environment

There are a number of possible ways this complete system model could be implemented. These include

- Development of a new software product specifically for this process.
- Modify an existing software product to give the needed flexibility, or
- Use an existing software product.

A number of potential development environments were considered for the project. Typical environments included

- MATLAB™
- LBNL – SPARK (systems tool)
- ASPEN™ – process modeling tool
- Easy 5™ (Boeing)
- Visual Basic™ / Visual C/C++™

Each of the proposed approaches has its advantages and disadvantages. Developing a new software product from scratch requires a great amount of time, quality control, and verification.

The use of an existing software product saves development time, but may have less flexibility. The last approach leads to quicker model development and the user can focus on analyzing the process rather than on software development. This last approach was the method chosen.

The product iSight™ was selected because it has great flexibility and is designed to interface with a number of different software products. The types of software tools that must be interfaced with are very diverse. They include codes in FORTRAN, C++, Excel Spreadsheets, etc. iSight™ has the ability to interface directly with each of these products.

iSight™ is a generic software shell that improves productivity in the design process. In iSight, design problems are specified, and simulation codes from multiple disciplines are coupled in a description file. After a description file is created, you can use the iSight interface to set up, monitor and analyze a design run.

The iSight Graphical User Interface (GUI) is comprised of four main module types that address different aspects of specifying, formulation, monitoring, and analyzing a design problem. The main Capabilities and Features in iSight are the ability to couple simulation codes from multiple disciplines, easy to set up design problems, DOE (Design of Experiments) studies to explore design space, optimization techniques, the ability to combine the best features of existing optimization technologies, and it runs in distributed processing and Parallel Execution modes.

3.4 Develop Basic System Model

A system is any process that converts inputs to outputs. A system creates outputs based on inputs, over which it has no direct control, and the system's present state. The current system state and a sequence of inputs allow computation of the future states of the system.

The term "systems engineering" means different things to different people. Here are two common definitions :

Definition 1: John G.Truxal, former Dean of Engineering at Brooklyn Polytechnic Institute, says, "System Engineering includes two parts: modeling, in which each element of the system and the criterion for measuring performance are described; and optimization, in which adjustable elements are set at values that gives the best possible performance.

Definition 2: A division manager at Hughes Aircraft Company defined systems engineering as performing: (a) requirements definition, (b) conceptual design, (c) partitioning of a system into subsystems (guidance, propulsion, etc) for other engineering teams to create, and (d) system validation, i.e., ensuring the system works when the subsystems are put together to form the system. Particular attention must be paid to the interface between the subsystems.

One of the primary tasks of the systems engineer is to ensure the optimization of the design process. System engineering is defined as an intellectual, academic, and professional discipline principally concerned with ensuring that all requirements for a human/machine/software system are satisfied throughout the life cycle of the system. There are six categories of system requirements that the systems engineer must specify:

1. Input/Output and Functional Requirement
2. Technology Requirement
3. Input/Output Performance Requirement
4. Utilization of Resources Requirement
5. Trade-Off Requirement (between last two items)
6. System Test Requirement

In this project we undertake the important task of identifying and quantitatively modeling the AAA process. Frequently, a very valuable aid in the initial identification of the inputs and outputs and various subsystems of a given system is to graphically model the overall system, including explicit designation of all subsystems and internal inputs and outputs. The powerful influence of visual and special conception and recognition of the model in a graphic format can be very revealing and productive for both model analysis and synthesis. The visual definition of the process is in progress and we are actively defining inputs/outputs for each process module. This definition is the key to a proper mass balance.

Block diagrams, signal-flow graphs, and organizational diagrams, as graphical modeling tools will be developed in this project. These types of features can effectively be developed within iSight™. Then several major specific engineering system identification and modeling techniques will be examined. The basic single-input, single-output model has been widely used and justified as an excellent beginning model for many systems. For the present process, some process steps may allow a simple model to be used for the initial process evaluation.

The use of experimental methods for system modeling and verification will be studied; including the valuable aids provided by dimensional analysis and least squares methods. As experimental test data is obtained for any portion of the process, this information can be fed back into the systems engineering process to insure the models are accurately representing the real process.

A method called weighted input and output modeling provides a rational means for ranking and weighting inputs and outputs on the basis of their contribution to the system's behavior. Stochastic system modeling and heuristic system modeling with some of essential features of this important field will also be studied. Either or both of these techniques will be evaluated for use when we consider the overall "optimization" of the process.

The graphical representation of the systems engineering model, which includes its inputs and outputs and possible feedback, is very useful tool in the initial modeling and formulation stage of a system study. The act of graphically and schematically portraying the system is conducive to accurate identification and improved understanding of what inputs interact with the system components and how these interactions produce the outputs anticipated. It is in the graphical representation stage of modeling that the system investigator or apprentice could be as thorough and critical of all the known or anticipated system factors as possible. The investigator or apprentice could attempt to detail the system and individually "componentize" the system elements as much as possible.

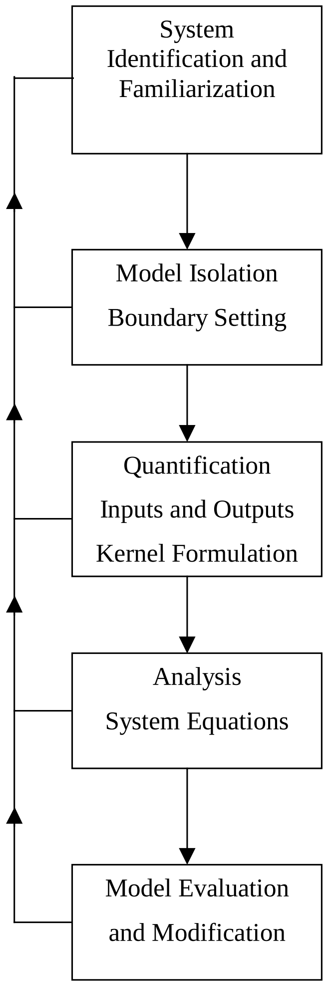

Figure 2 – Process for designing and analyzing a systems engineering model.

Schematically, the approach that is going to be used here is shown in Figure 2. The beginning of any system study is Block 1 in Figure 2, System Identification and Familiarization. Often, identifying the essential components of the system that collectively undergo the cause and effect action associated with the system is obvious, such as the illness (the output) that results when a person (the system) consumes toxic food or water (the input). However, the identification and isolation of other systems, such as a study of the causes of inflation where the general system is the world economic system, is undoubtedly complex, diverse, and presents a serious modeling challenge. For this project, clearly defining the process flow sheet is a critical first step (UREX, PYRO-A, PYRO-B, etc.). Figure 1 shows one presentation of the proposed process.

All of the present work centers on the three center blocks of Figure 2. The AMUSE code is being modified to allow it to be included as one set of the “system equations.” Each of the Process Blocks as shown in Figure 1 will have a set of equations or relationships to model the transport of mass through that process. These relationships may be relatively simple, or complex computer codes, like the AMUSE code.

3.5 Demonstrate Modeling Concept

The ultimate goal of the project is to develop an overall systems model that can be used to analyze proposed processes for handling spent nuclear fuels. The systems engineering process has been defined and will continued to be studied in order to develop an effective systems engineering model. This knowledge is then used for the defined process of interest (Figure 1). In our present work (see Figure 3), the AMUSE™ code is a detailed model of one major process step that feeds information/data back into the defined AAA process. All of this information is then used to develop an overall model within iSight™.

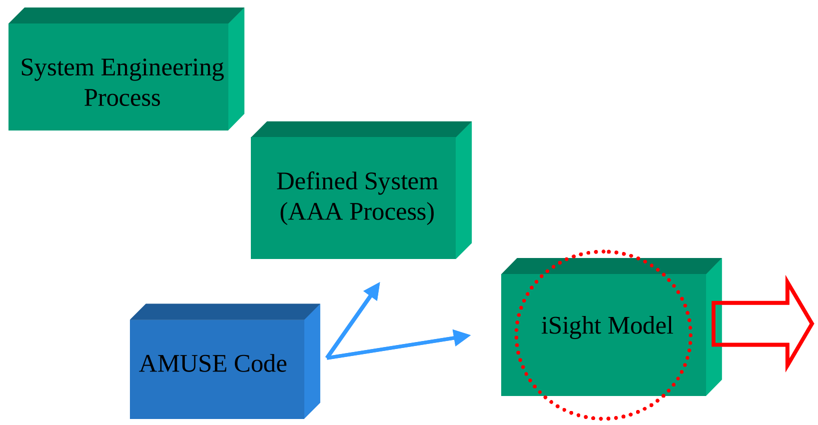

Figure 3 – Schematic presentation of how AMUSE code interacts with a detailed systems engineering model of the AAA process.

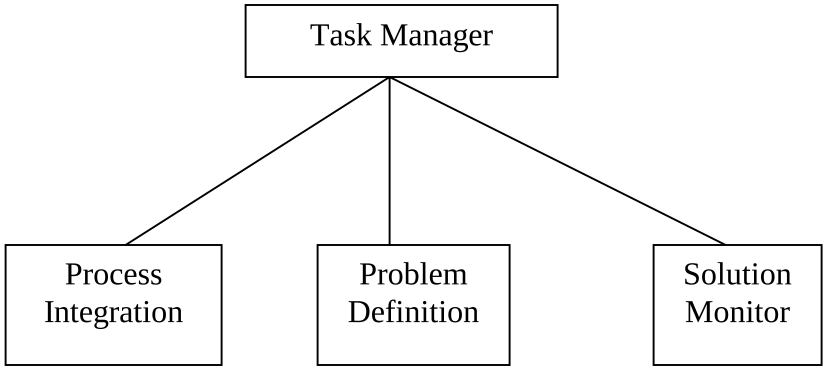

Figure 4 - iSIGHT modules.

The iSIGHT Graphical User Interface (GUI) is comprised of four main module types that address different aspects of specifying, formulating, monitoring, and analyzing a design problem. Figure 4 illustrates the four main iSIGHT modules.

The main iSIGHT interface is the Task Manager. From here a user can launch any of the iSIGHT interfaces. The Task Manager also allows user to ser up and run a design problem.

Process Integration is the iSIGHT module that enables user to couple simulation programs to iSIGHT and specify their execution sequence. Process Integration provides a GUI that acts as a front end for creating an iSIGHT description file written in iSIGHT MDOL language.

Problem Definition provides a convenient means to provide problem formulation information to specific design parameters, allowing user to control information in user's problem. Problem Definition also includes the design exploration techniques used by iSIGHT to reach an optimum during design exploration. The following techniques are available in iSIGHT: (a) optimization, (b) design of experiments, (c) quality engineering methods, (d) multi-criteria tradeoff analysis, (e) approximations, and (f) knowledge rules.

Solution Monitor is the part of iSIGHT that provides a visual means to monitor the optimization process as it moves through the design space. Solution Monitor provides several tables and graphs that can be used to view the runtime changes.

Figure 5 shows a simple representation of the UREX process as developed within the iSight™ software package. The individual arrows show data transfer within the system. This information could include chemical species, concentrations, reaction rates, etc.

4. Process – Modernization of AMUSE

The AMUSE (**A**rgonne **M**odel for **U**niversal **S**olvent **E**xtraction) code is a software package developed by Argonne National Laboratory for the analysis of a Generic TRUEX process. The TRUEX process 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.

UNLV's role is to develop a general user interface to aid researchers in analyzing different process scenarios. In addition, UNLV researchers will incorporate the AMUSE Code into the overall systems engineering model. This will be a key component to the overall analysis of the process.

4.1 Review/Analyze Code Structure

Researchers (students and staff) examined the software package from a user interface standpoint and from a software development standpoint. We will have to continually refer back to the original software to insure that proper reference to Excel cell locations are used for the development of the new interface.

The type of tasks undertaken included: setup and evaluation of sample problems, a training class presented by ANL research staff, review of existing Visual Basic interface, and the general evaluation of where data was stored within the Excel spreadsheets.

4.2 Examine Other Possible Implementations

Examination of the code showed that it was not possible to take the code and recast it in another environment. The software was developed within Excel spreadsheets, using the available macro language and subsets of Visual Basic. It would be an enormous task to rewrite the code because it depends heavily on numerical calculations. The verification and validation of a new package making similar calculations would be a daunting task.

4.3 Define Year 1 Software Tasks

During the year, there was the concern that the software would be classified as "Export Controlled Information." Upon notification of this concern from ANL, we stop direct work on directly interfacing with the AMUSE package. But, we were able to have the students continue on the development of a generic software interface that could later be linked to the existing AMUSE code.

Tasks for Year 1 included

- Train staff and students on the chemical process associated with AMUSE.
- Specify the number and type of process blocks needed for the UREX process.
- Develop a "drag-and-drop" type interface for defining the UREX process blocks.
- Develop a general plot interface to allow access to data within an Excel spreadsheet.

4.4 Develop Verification Plan

A simple verification plan was developed. The plan is to run sample problems on the existing AMUSE code and to then run the identical problem on the modified version of AMUSE. Detailed comparisons of process outputs will be examined to insure the proper transfer of data to AMUSE and the proper calculation of process parameters.

This approach is relatively simple, but it will entail a significant amount of analysis by the researchers to insure the results are accurate. Discussions will be held with ANL researchers to select critical variables that can be used to indicate errors within the code.

4.5 Modify/Improve Software

Initial efforts have centered on improving the user interface for the AMUSE code. A "drag and drop" type of interface is under development. The interface will allow the user to quickly and easily define the UREX process and define process inputs. More straightforward ways to examine different process designs will be useful for the engineering analyst.

Figure 5 shows the UREX main page design which contains the different chemical separation modules on the left-hand side of main page. User can drag and drop the various chemical process modules to the main page which is shown in Figure 6. Then user can make the line connection among those chemical process modules and indicate the mass flow directions among them by using arrows that are shown in Figures 7 and 8, respectively. Figure 9 below shows what a typical screen will look like for the analyst. Each of the different steps in the UREX process is outlined on the screen and allows easy modification by the user. The goal is to allow the user to input data directly into the process blocks, or to allow the user to define a file that contains chemical species, concentrations, etc. The user will have access to this data file, which allows them to directly examine the assumed process streams.

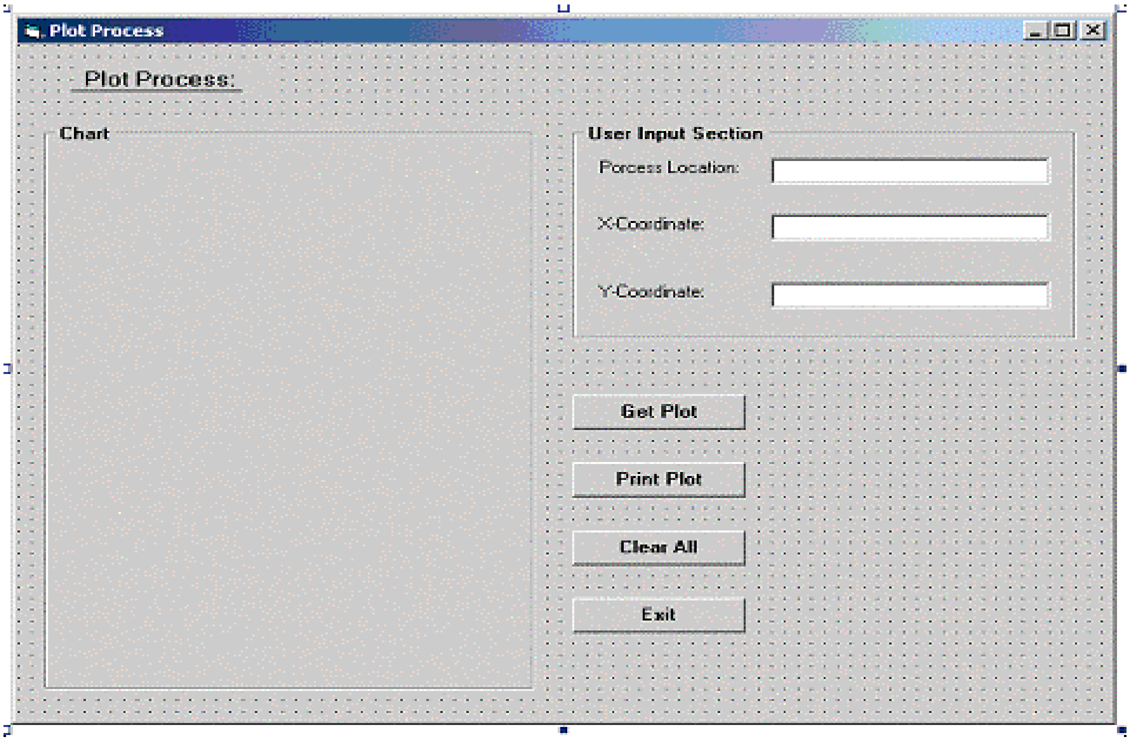

Figure 11 - General plot interface to view/postprocess the results of an AMUSE simulation.

The mass balance interface code has been designed and developed. The UREX Visual Basic interface design and implementation is still in progress. Figure 12 shows the window interface design for the mass balance calculations.

Two options are available for the user input in the mass balance interface design. Those are desired stages which is an integer input with feeder input which can use either by manually or from an existing input text file, and desired efficiency which a decimal is used as input with feeder. User can select the different type of the desired design stages and efficiencies as the input information. User can also have the flexibility of selecting the different type of chemical concentrations such as by volume percentage, molarity, etc. If desired stages is selected by user then total efficiency will be calculated and displayed according to the AMUSE code. The user will be able to view the chart plots of each stage efficiency by clicking the "Get Chart" button on the window interface. All simulated results and data output are based on the provided formulas from AMUSE code and ANL-East technical information. The link between AMUSE code and Window interface will be developed in the next quarter.

Using iSight software to develop and integrate AMUSE (UREX) – Uranium Strip Section for a Window application is shown in Figure 13. User can specify the upstream and downstream for the different operation tasks according to the chemical process designs. Each of dialog boxes will be linked to AMUSE Visual Basic interface. Figure 14 shows the data transfer correlation between systems engineering modeling using iSight software and AMUSE code from the Visual Basic interface.

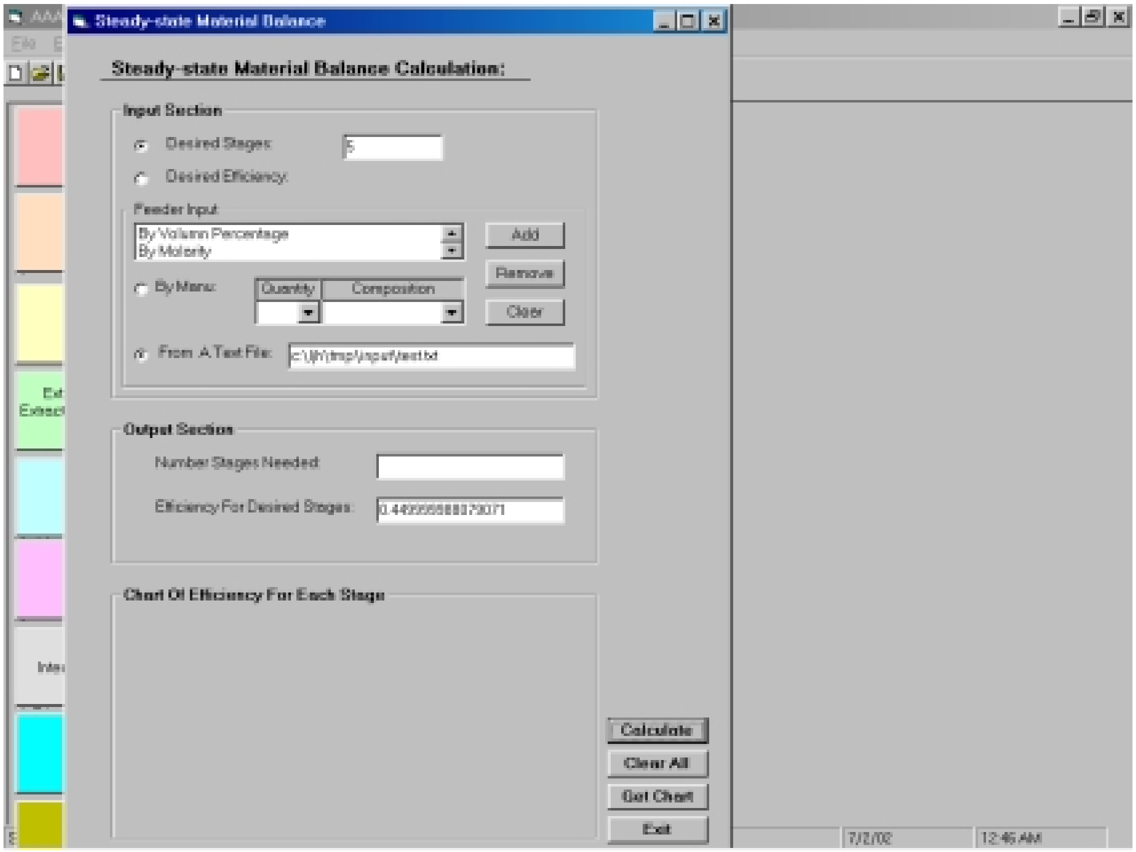

Figure 12 - Window interface design for the mass balance calculations.

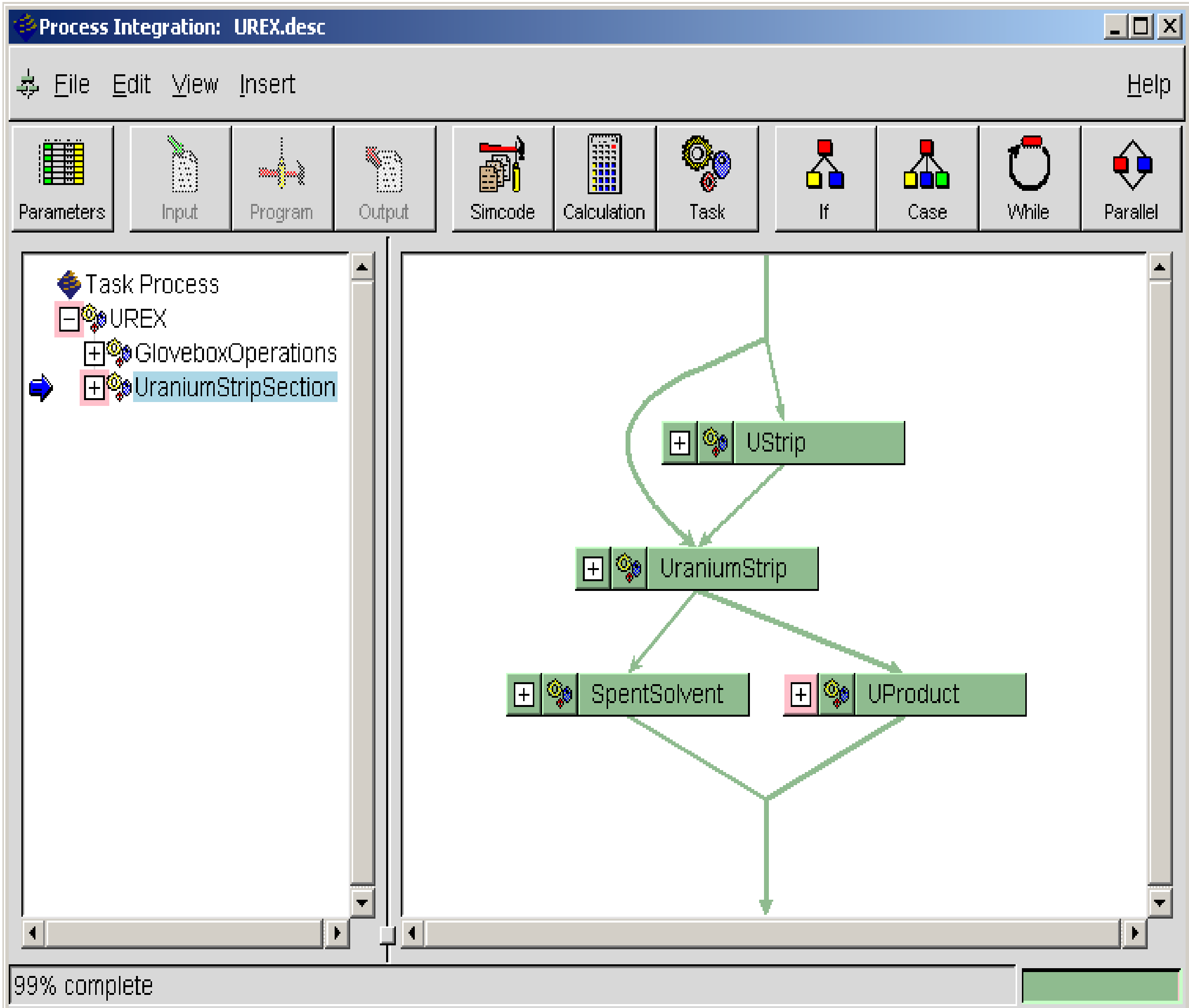

Figure 13 - Integration of AMUSE (UREX) – Uranium Strip Section.

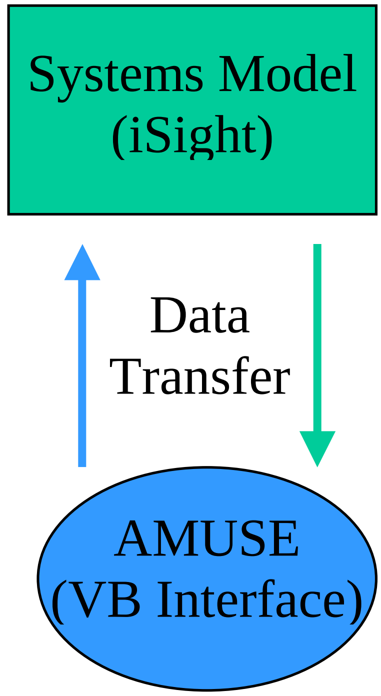

Figure 14 - The data transfer correlation between system engineering modeling and AMUSE.

5. Summary

A framework and environment for a systems engineering analysis of the chemical separations system has been developed in the phase I research work. A baseline system engineering model from which modifications and improvement can be made has also been studied. The long-term needs for a systems engineering model of the fuel processing included mass balances, system control, plant layout and design, and other features will be discussed with ANL-East engineers and scientists. Commercial software package of iSight™ was selected to perform the systems engineering analysis and simulation. A simple representation of the UREX process has been developed within the iSight™ software package.

A “drag and drop” type of graphical user interface (GUI) has been designed and developed. The interface will allow the user to quickly and easily define the UREX process and define process inputs. More straightforward ways to examine different process designs will be useful for the engineering analyst. AMUSE code has been studied and analyzed. Initial efforts have centered on improving the user interface for the AMUSE code. The input and output parameters are carefully being tracking and marking. The capability of graphs and tables output and displaying has been designed. The system engineering model will be coupled with the graphical interface, AMUSE code, MATLAB and iSIGHT in the phase II work. The mass balance interface code has been designed and developed. The UREX Visual Basic interface design and implementation is still in progress. Using iSight software to develop and integrate AMUSE (UREX) – Uranium

Strip Section for a Window application has been studied. A simple verification plan was developed. The plan is to run sample problems on the existing AMUSE code and to then run the identical problem on the modified version of AMUSE. Detailed comparisons of process outputs will be examined to insure the proper transfer of data to AMUSE and the proper calculation of process parameters. The final results from this developed project will provide engineers and scientist a friendly and useful Window GUI package that can simulate the chemical separation under the different input conditions of actinides and solvents and the required separation efficiencies of various equipment.

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