8-15-2002

Development of a Systems Engineering Model of the Chemical Separations Process: Quarterly Progress Report 5/16/02- 8/15/02

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

Randy Clarksean
University of Nevada, Las Vegas

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

Development of a Systems Engineering Model of the Chemical Separations Process

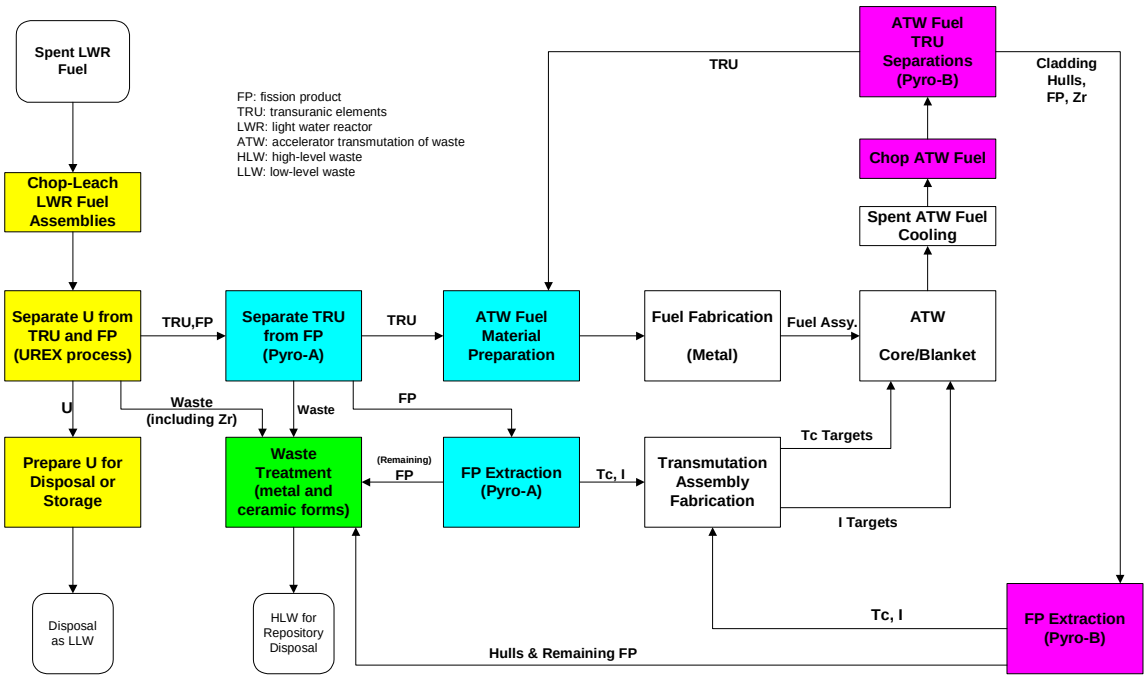
Quarterly Progress Report
5/16/02- 8/15/02

UNLV-AAA University Participation Program

Principle Investigator: Yitung Chen
Co-Principle Investigators: Randy Clarksean and Darrell Pepper

Purpose and Problem Statement

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. The following figure shows a block diagram of the current process as envisioned by Argonne National Laboratory (ANL) researchers.



Two activities are proposed in this Phase I task: the development of systems engineering model and the refinement of the Argonne code AMUSE (Argonne Model for Universal Solvent Extraction). The detailed systems engineering model is the start of an integrated approach to the analysis of the materials separations associated with the AAA Program. A second portion of the project is to streamline and improve an integral part of the overall systems model, which is the software package AMUSE. AMUSE analyzes the UREX

process and other related solvent extraction processes and defines many of the process streams that are integral to the systems engineering model.

Combining these two tasks is important in ensuring that calculations made in AMUSE are accurately transferred to the overall systems model. Additional modules will be developed to model pyrochemical process operations not treated by AMUSE. These modules will be refined as experiments are conducted and as more knowledge is gained in process steps.

Integrating all aspects of the proposed separations processes will allow for detailed process analyses, trade-off studies or the evaluation of proposed process steps, complete material balances that include all potential waste streams, the impact of changes in feed streams, studies detailing the importance of process control and instrumentation, and the ultimate optimization of the process.

Personnel

Principle Investigator:

- Dr. Yitung Chen (Mechanical Engineering)

Co-Principle Investigators:

- Dr. Randy Clarksean (Mechanical Engineering)
- Dr. Darrell Pepper (Mechanical Engineering)

Graduate Students:

- Mr. Lijian (Rex) Sun, Ph.D. Graduate Student, (Mechanical Engineering)
- Ms. Jianhong Li, M.S. Graduate Student, (Computer Science)

National Laboratory Collaborators:

- Dr. James Laidler, Senior Scientist, Chemical Technology Division, ANL-East
- Dr. George Vandergrift, Senior Scientist, Chemical Technology Division, ANL-East
- Ms. Jacqueline Copple, Information Systems Group, ANL-East

Management Progress

Budget Issues:

- The first year of research expenditures are under good control and well managemner.

Student Issues:

- Ms. Haritha Royyuru, a graduate student of Mechanical Engineering, has been admitted into the M.S. program at UNLV. She will replace Ms. Jianhong Li from the fall semester 2002.

Management Problems

Ms. Jianhong Li delivered her baby daughter on June 10. She was on the maternity leave for six weeks. Ms. Li has also accepted the Teaching Assistant assignment and support from the Computer Science Department in the fall semester 2002.

Technical Progress

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.

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. In our present work (see Figure 1), 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™.

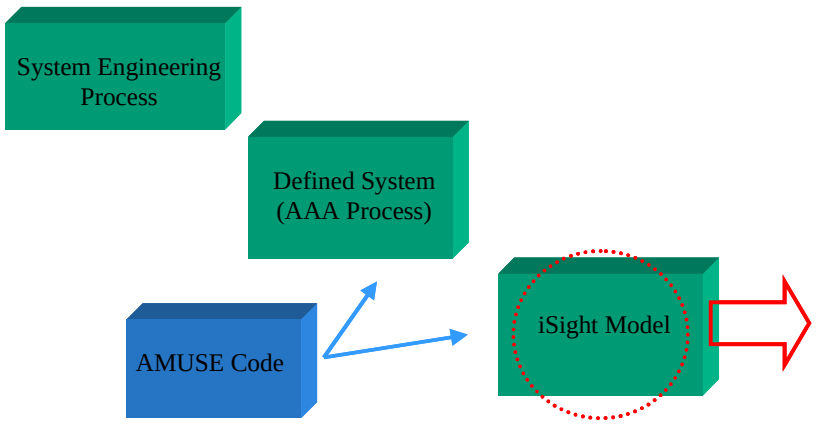


Figure 1 – Schematic presentation of how AMUSE code interacts with a detailed systems engineering model of the AAA process.