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Development of a Systems Engineering Model of the Chemical Separations Process: Quarterly Progress Report 2/16/02- 5/15/02

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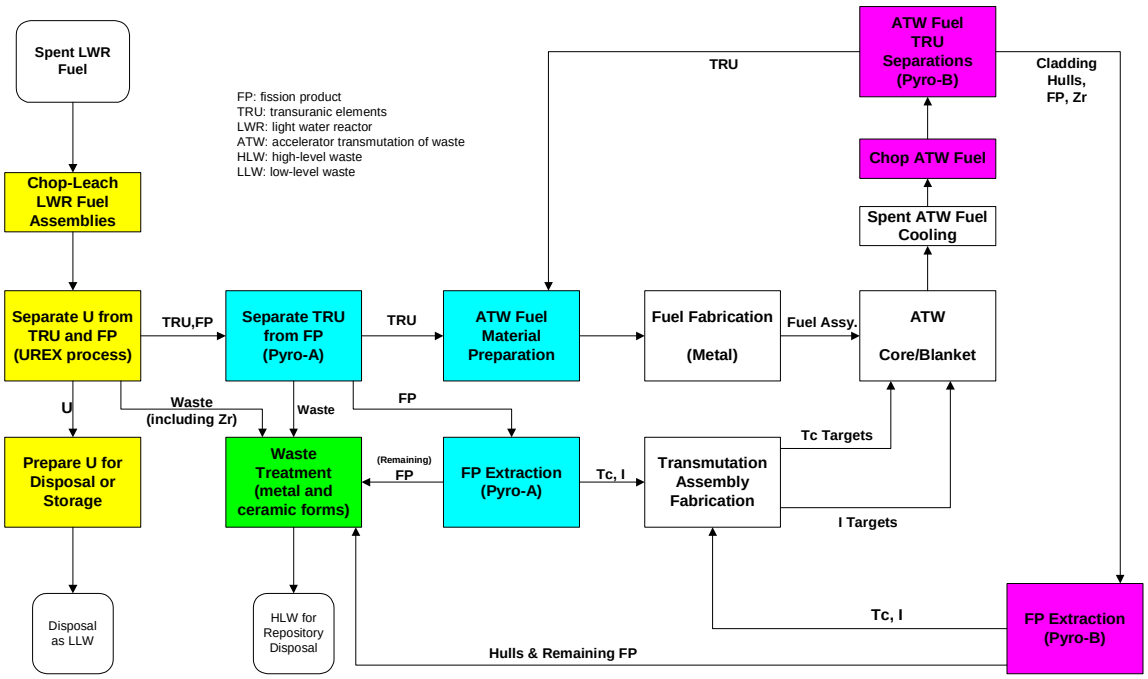
UNLV-AAA University Participation Program

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)

Students:

- Mr. Lijian (Rex) Sun, Ph.D. Graduate Student, (Mechanical Engineering)
- Ms. Jianhong Li, M.S. Graduate Student, (Computer Science)
- Ms. Yulien Chen, Undergraduate Student, (Management Information System)

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 9-month budget was set up when the project started in September 2001. The budget account closing date is April 20, 2001 and the last quarter of budget didn't set up in time which has caused a problem to prepare the student and professional contracts in April and May.
- Undergraduate student wage is overspent. The budget will be slightly adjusted to balance off the overspent.

Management Problems

The secretary at the Mechanical Engineering Department was hesitated to prepare students and professional contracts because of the budget closing date issue. Also, students and research faculty couldn't get their paychecks in time in May due to the budget closing date problem.

Ms. Jianhong Li will deliver her first baby in the end of May or the first week of June. Her progress in the research work was slow down due to her pregnancy. One undergraduate student from the Department of Management Information System (MIS) was hired to help Jianhong to work on the AMUSE GUI design.

Technical Progress

The mass balance interface code has been designed and developed. The UREX Visual Basic interface design and implementation is still in progress. Figure 1 shows the window interface design for the mass balance calculations.

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.

One of our primary tasks of the systems engineering modeling is to ensure the optimization of the AMUSE UREX process. System engineering modeling will be designed and developed 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 engineering modeling has been considered and sepcified:

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

Using iSight software to develop and integrate AMUSE (UREX) – Uranium Strip Section for a Window application is shown in Figure 2. 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 3 shows the data transfer correlation between systems engineering modeling using iSight software and AMUSE code from the Visual Basic interface. Figure 4 shows the integration of AMUSE (UREX)– Glovebox Operations using iSight software. User can specify the different functions for each dialog box. For example, user can select the solvent type and specify what kind of chemical property of solvent is and any physical correlations of this chemical solvent. Then it will be linked to the upstream and downstream according to the chemical process design information.

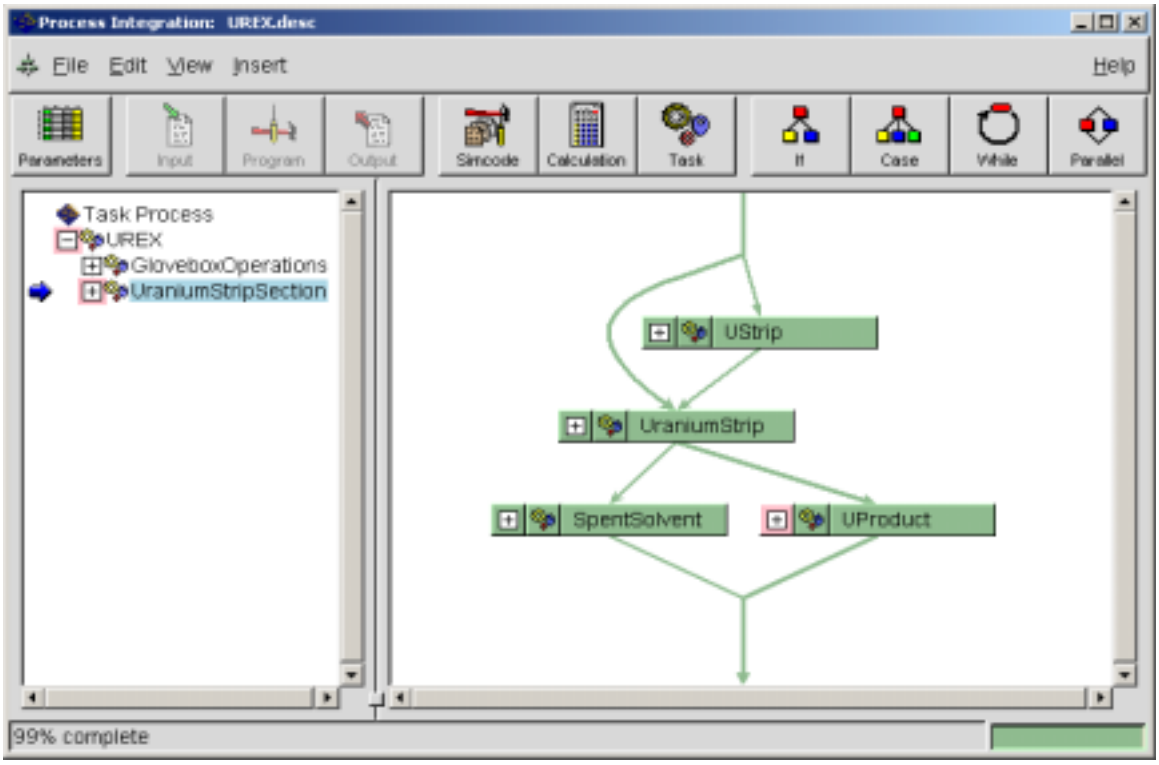


Figure 2. Integration of AMUSE (UREX) – Uranium Strip Section

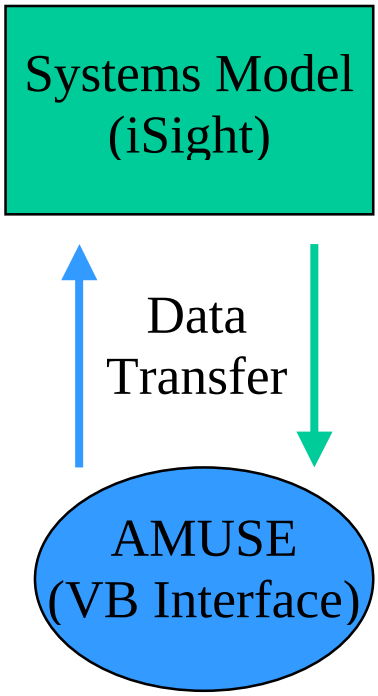


Figure 3. The data transfer correlation between system engineering modeling and AMUSE

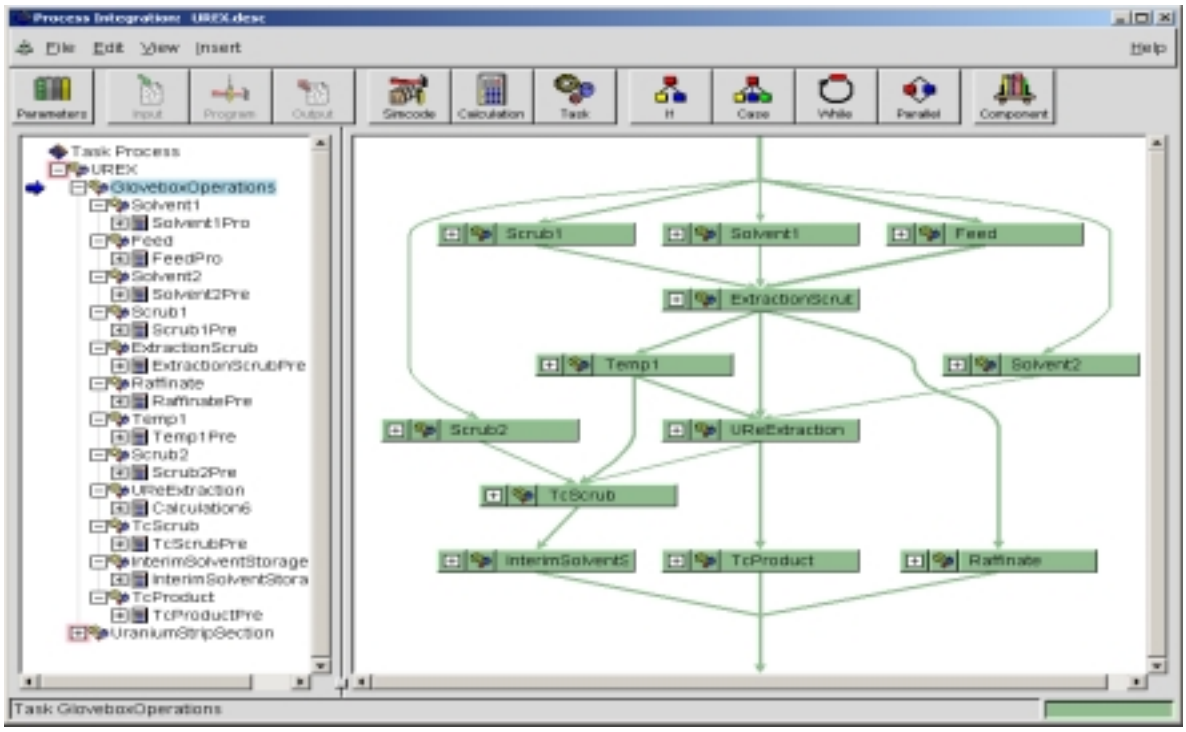


Figure 4. Integration of AMUSE (UREX) – Glovebox Operations