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Development of a Systems Engineering Model of the Chemical Separations Process

Quarterly Progress Report
8/16/01- 11/15/01

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 a 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, M.S. Graduate Student, (Mechanical Engineering)
- Mr. Sridhar Munaga, M.S. Graduate Student, (Computer Science)

Notes:
1. Mr. Sridhar Munaga will be leaving the project at the end of November of 2001.
2. Mr. Qingguang Lu or Ms. Jianhong Li, M.S. Graduate Student of Computer Science, will replace Mr. Munaga to continue working on the interface design associated with AMUSE code development

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:
- Annual user license of commercial system engineering software iSight™ will be purchased. The academic price is currently under negotiation.
- One computer system has been ordered and other one will be ordered for one undergraduate student.
• Salary expenditures need to be adjusted because the secretary of mechanical department has not revised the correct student’s name according to the proper account number

Management Problems

The first year budget of the phase I research task is from 08/20/01 to 05/20/02. The academic fiscal budget year is from the first day of July of the current year to the end of June in the next year. So Students and faculty can’t have their contracts from 05/21/02 to 6/30/02. The other three months research funding from 05/21/02 to 8/19/02 need to be allocated as soon as possible.

One high-end personal computer has been ordered since the fall semester began, but at this moment we haven’t received the computer yet. This serious delay has caused a lot of research problem for us. We have to find a temporary old personal computer (i.e. Pentium II 300 MHz, 32 MB RAM) to let student to do the research work. And the student has been complaining about its performance and not enough memory.

We are looking for one undergraduate student to work with us on this project. Many undergraduates already had their part-time jobs in or out of UNLV campus. Some of them will be available from the spring semester 2002. We will keep contacting with qualified student and recruit him/her in the beginning of spring semester 2002.

Technical Progress

The project kick-off meeting was held on September 26, 2001 and the AMUSE code training was held on October 9, 2001. The AMUSE-models for TRUEX, SREX, UREX and PUREX solvent extraction have been discussed during the kick-off meeting and AMUSE code training. The interface of AMUSE has been designed using Visual Basic software. The draft of the interface is shown in Figure 1. The drag-and-drop techniques were employed on the interface designing.

A number of different software products are being evaluated for use in the systems engineering modeling project. These products include iSight™, MATLAB™, LBNL SPARK (systems tool), ASPEN process modeling tool, Easy 5 (Boeing), Visual Basic/Visual C/C++ and others.

The criteria for selecting one of these products included the

• Ability to interact with a wide range of existing simulation tools written in a number of different languages and forms (Fortran, C/C++, Visual Basic, Excel Spreadsheets, etc.).
• Ability for the user to seek out and determine all input values and assumptions for each simulation package.
• Potential for integration over a disperse network system.
- Need for a “drag-and-drop” approach to adding additional components to the process.
- Simple process to transfer data between components.
- Ability to optimize individual processes or the complete system

Figure 1. UREX demonstration flowsheet for glovebox operations and uranium strip section.

At present, the most likely candidate software product is iSight™. The evaluations continue and will conclude by mid-December. A WebX conference for iSight will be held from 9-10:30 a.m. on December 14.

Once the software product has been selected, a student will be trained on the product and the complete process will be defined within the software environment over the next several months.

Attendance at the ANL Transmuter Fuel Development Workshop made it clear that the product must have the ability to analyze a wide range of processes quickly and easily. In addition, it is clear that developing a systems engineering model of the complete process will be very valuable in assessing many of the proposed concepts.

AMUSE code is currently being studied and analyzed. The input and output parameters are carefully being tracking and marking. The capability of graphs and tables output and
displaying is currently under designing. The system engineering model will be coupled with the graphical interface, AMUSE code, MATLAB and iSight.