11-11-2002

Development of a Systems Engineering Model of the Chemical Separations Process: Quarterly Progress Report 8/16/02- 11/15/02

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

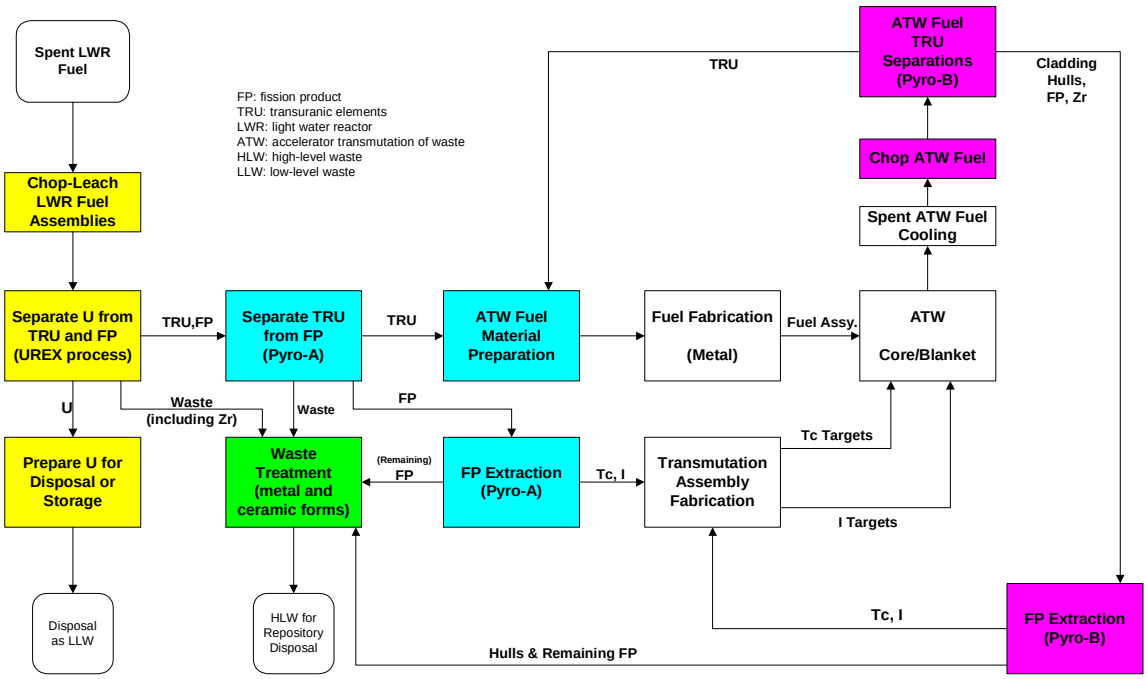
Quarterly Progress Report
8/16/02- 11/15/02

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 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)

Graduate Students:

- Mr. Lijian (Rex) Sun, M.S. Graduate Student, (Mechanical Engineering)
- Ms. Haritha Royyura, M.S. Graduate Student, (Mechanical Engineering)

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:

- 9 months of the second year funding has been allocated to the current research account.

Student Issues:

- Ms. Haritha Royyura who is a M.S. graduate student of Mechanical Engineering Department has joined the research team from the fall semester 2002.

- We will keep looking for one undergraduate or graduate student to work with us on part time on the system engineering model flow chart design and GUI development.

Management Problems

No management problem issues at this time.

Technical Progress

Ms. Haritha Royyuru has been extensively reviewed and studied the developed Graphical User Interface (GUI). She has also studied the AMUSE code and tried to develop the links between AMUSE code and our developed GUI. She is also learning the Visual Basic language. We have encountered some running error messages when we tried to run the AMUSE code. Dr. Vandegrift and his staff are aware about this problem. They will send us the new version of AMUSE code. A few examples of how to simulate UREX and PUREX processes from the AMUSE code are absolutely needed. The systems engineering modeling is currently under studied and it will be connected to those backbone calculations in order to find the optimized designs and solutions. Ms. Haritha Royyuru is working on the GUI development of AMUSE code. The core structures of SASPE and SASSE are studied. The "D" value of actinides from the solvent extraction for the aqueous phase and organic phase are calculated by SASPE. The mass balance is calculated SASSE. Bases and consequences of AMUSE calculations are being studied.

Mr. Lijian Sun has developed the structure of systems engineering modeling. Later, he will implement it coupled with AMUSE when the GUI is successfully developed. Work was also undertaken to evaluate other potential software products that could be used for the systems engineering model. The existing software is expensive, making it difficult to install enough licenses to aid the students in model development.

Dr. Vandegrift and his staff visited us the week of October 21 to provide more details for the development of the AMUSE code and the systems engineering model. The discussions helped us determine how we can link our developed Windows GUI to the AMUSE code. The functions, theoretical correlations, and empirical correlations associated with each process data were discussed during the visit in order to find the possible way to link to backbone of our developed GUI. They also gave us a presentation on the latest developments of the chemical separation process for the nuclear spent fuels.

Many useful suggestions are provided by Dr. Vandegrift and his staff during the meeting. A number of technical questions were also answered. They were pleased to see the progress of the research. We will focus on UREX and PUREX processes first, based on the recommendations of Dr. Vandegrift and his staff suggestions.

<u>Technical Progress in the Development of Systems Engineering Model:</u>

1.Written the code to extract data from VB-Interface to export file and then link to the Excel Macros.
2.Modified the code in the Excel Macros to get the output.
3.Written the code to open and save the files in the interface.

VB-Code:

Code is written to transfer the data given by the user in the interface to the export file. Export file is a Data Carrier which connects the VB-Interface to the AMUSE. The data given by the user in the front-end need to be transferred to the export file which then links the data to the AMUSE for further calculations. The data like number of sections in the process, recycle organic, Concentrations of TBP and CMPO etc are stored in the export file.

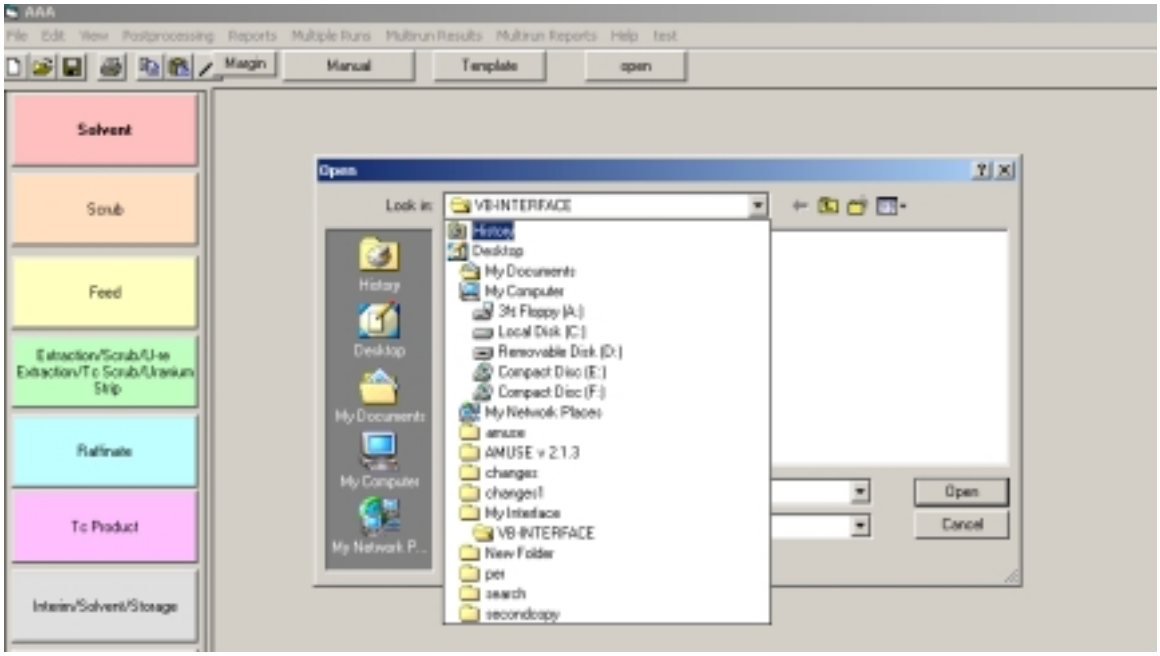
To run AMUSE, this data need to be transferred to the AMUSE macros. A code is written to initiate the AMUSE macros from the GUI and link the export file generated by the VB-Interface to the macros.

Modification Of AMUSE Macros:

AMUSE macros are written in a way to suit their front end. Some of the code from the Macros which refer to the AMUSE front end is been removed and replaced with the VB-Interface. The code is changed in such a way that the Macros directly refer to the VB front-end for calculations. This makes the VB-Interface independent of AMUSE interface. At this point our interface depends on AMUSE just for calculating the required values.

Open & Save Options:

Some of the files opened in the VB-Interface need to be saved for further usage in the future. With this idea Open and Save options were implemented in the interface. The user can open a file from the existing location and can save the file in the desired location. Code is written to Open and Save the files in desired locations.



Future Work:

The following work is determined for future implementation:

1. Designing the report format for SASSE, SASPE and SPACE for both single and multiple runs.
2. Run all the macros from the VB-Interface. Now we are getting some errors in the calculations which will be removed by changing the code.
3. Implement the Edit commands for Process blocks.
4. Create a format for saving the files.
5. Maintain a database to store the calculations that will be useful in retrieving the data back to the front-end.