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## Development of a Systems Engineering Model of the Chemical Separations Process: Quarterly Progress Report 11/16/02- 2/15/03

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# Development of a Systems Engineering Model of the Chemical Separations Process

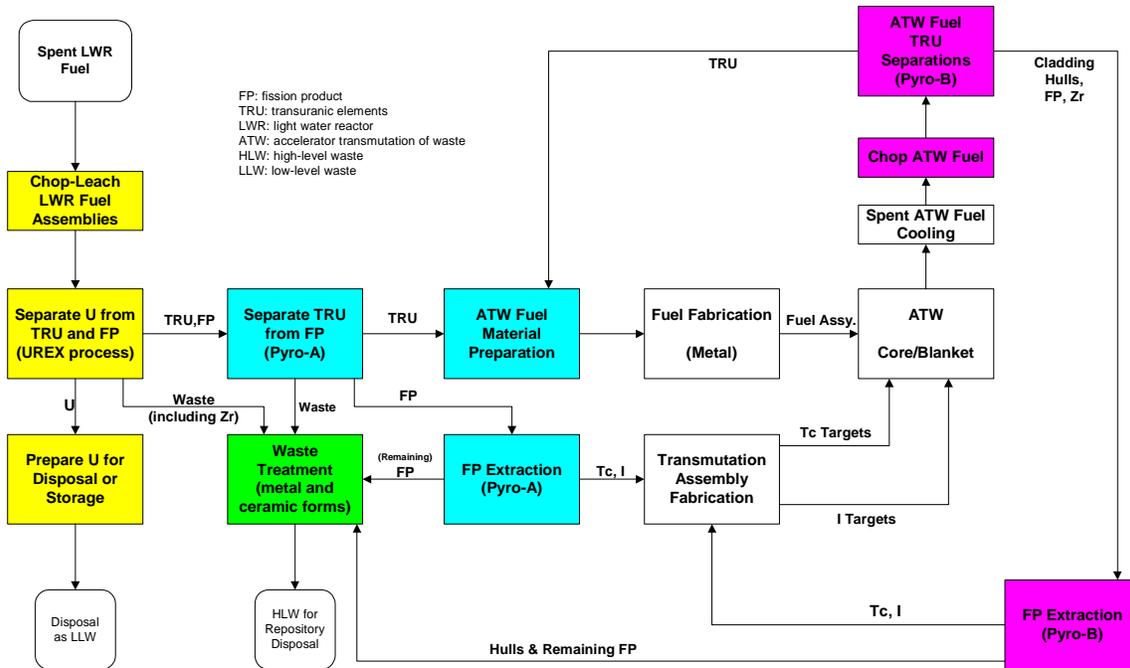
## Quarterly Progress Report 11/16/02- 2/15/03

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 TRP 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)
- Ms. Sushma Gujjula, M.S. Graduate Student, (Electrical and Computer 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:

- The Letter of Appointment contract for Dr. Randy Clarksean has been prepared through April 30, 2003. Another contract will be prepared for Dr. Clarksean from May to August 2003 after the rest of research funding is allocated.

## **Management Problems**

Ms. Sushma Gujjula who is a M.S. graduate student of Electrical and Computer Engineering Department was hired on part time to develop the system engineering model flow chart and GUI design from the spring semester 2003.

## **Technical Progress**

Ms. Haritha Royyuru has written the code to extract data from VB-Interface to export file and then link to the Excel Macros. 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. She has also modified the code in the Excel Macros to get the output. 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. She has successfully to write the code to open and save the files in the interface. 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.

Mr. Lijian Sun continues to work on the overall systems engineering model for the fuels reprocessing. MATLAB software has been evaluated. It can integrate mathematical computing, visualization, and a powerful language to provide a flexible environment for technical computing. The open architecture makes it easy to use MATLAB and its companion products to explore data, create algorithms, and create custom tools that provide early insights and competitive advantages. The Optimization Toolbox extends the MATLAB environment to provide tools for general and large-scale optimization. Additional tools are provided for linear programming, quadratic programming, nonlinear least-squares, and nonlinear equations. The interactive MATLAB environment allows optimization problems to be easily refined and adapted, providing users with valuable feedback and useful insight into a problem's "best" solution. So the MATLAB with Optimization Toolbox will be used to develop the system engineering model. It will couple with AMUSE code (EXCEL and VB script) and VB interface (VB 6.0). DOE (Design of Experiments) will be studied and explored design space. Combining the best features of existing optimization technologies will also be studied. It will also couple with Microsoft SQL Server Database. The solution monitor will also be developed from MATLAB.

Ms. Royyuru will continue to develop and improve post-processing environment and prepare the function links. The following work will be implemented. (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. Mr. Lijian Sun will continue to apply the general systems engineering techniques/tools on chemical separation Process. He will develop a tool that allows process changes to be modeled on a system level. He will investigate what impact of one change has on overall process. Mass balance for all process streams will be studied. Changes of input on waste streams will also be examined. The ability to optimize system such as cost, waste streams, etc. will also be scrutinized. The performance of detailed models of process components such as reactors, electrorefining, chopping, separation, etc. will also be examined.

The abstract of conference paper titled as "Development of Systems Engineering Model for UREX Process" for the 2003 American Nuclear Society Accelerator Applications Division AccApp'03, San Diego, June 1-5, 2003 was submitted on January 22, 2003.

The abstract of conference paper titled as "Development of Systems Engineering Model for Uranium Extraction (UREX) Process" for the 2003 ASME-International Mechanical Engineering Congress and R&D Expo. Washington, D.C., USA, November 16 - 21, 2003 was submitted on January 24, 2003.

Able to connect to AMUSE from the VB-Interface:

The export file created from our interface is used by the AMUSE to calculate the results. The AMUSE macros were not changed, they were just called in our interface for calculations. Export file was created long before and thought that the errors were due to macros. Spent so much time in understanding the macros and changing them to observe the results. The errors were due to 2 spelling mistakes in the export file i.e diluent and efficiency. There was one error with FILENAME.XLS. Even-though the file was present in the same directory as all the AMUSE files it showed this error. This is because the directory from which the macros were called (VB-Interface) is not the same as the AMUSE directory. This error was removed by copying all the files in the AMUSE directory to the VB-Interface where all the forms were stored. Hence in order for the AMUSE to run correctly all the files in the VB-Interface and all the AMUSE files should be there under the same directory.

Previously the user have to change the path of the macros to call them in the interface whenever the directory is changed or the program is copied to a different system. The program is modified now so that it detects the systems path and sets that to the path for calling the macros.

Problem with multi-run option:

AMUSE is designed in such a way that for each run it needs to create a new export file. It becomes a problem to open and close a number of excel files in multi run option, as the output files will be too many because 7 output files were created for each run. Need to do something for storing the output in one file so that all the results can be taken from that file.

#### Difference between Aqueous and Organic feed:

Two types of input option is present in the AMUSE Interface, one is for Aqueous feed and other for Organic feed. We don't know which type of feed we are giving in our interface. By default Aqueous feed option is given in the AMUSE interface. If both types of input need to be given for a process, then we should have one option to provide for Organic feed. For this reason we need to know which type of feed we are giving in our interface so that we can design for that.

#### Process temperature and Fractional Efficiency:

In AMUSE interface we have an option to change the process temperature and Fractional Efficiency for each stage. We can include this option in our interface once we have a clear idea of the input that is going in our interface. We need to have the sample inputs for all the different possible conditions for programming accordingly.

#### Stage Sampling:

If more than one stage is specified in the AMUSE interface then in the stage-sampling section an extra box is provided for input. Need to know the type of input that should be given here.

#### List Of parameters used for Multi run:

- 1.TBP Concentration
- 2.Process Temperature for whole process
- 3.Aqueous Flow rate
- 4.Organic Flow rate
- 5.Fraction of Organic Effluent
- 6.Fraction of Aqueous Effluent
- 7.Fraction of Aqueous entrained in the Organic
- 8.Fraction of organic entrained in the Aqueous
- 9.Aqueous reroute section
- 10.Organic reroute section
- 11.Concentration Of individual Components
- 12.Fractional efficiency

#### File System Objects:

For saving and opening the files we have to use File System Objects (FSO). All the information regarding the process blocks and the connectors like their position, name, content etc need to be stored in a file. Using FSO files can be saved in two formats text file and binary file. Text file option is preferred as the user can change the data in the text file and run the code. If it is stored in binary format then it becomes difficult to change content. Text file is easier to debug if any error occurs. Studying the FSO to work with it.

#### Multi run Interface:

Multi run interface is created in which a list of variables, which change the end result, is included. All the input is validated with maximum and minimum values. When the parameters are changed a click on RUN button runs Amuse and a click on EXIT button takes the user to the main form.