Development of a Systems Engineering Model of the Chemical Separations Process

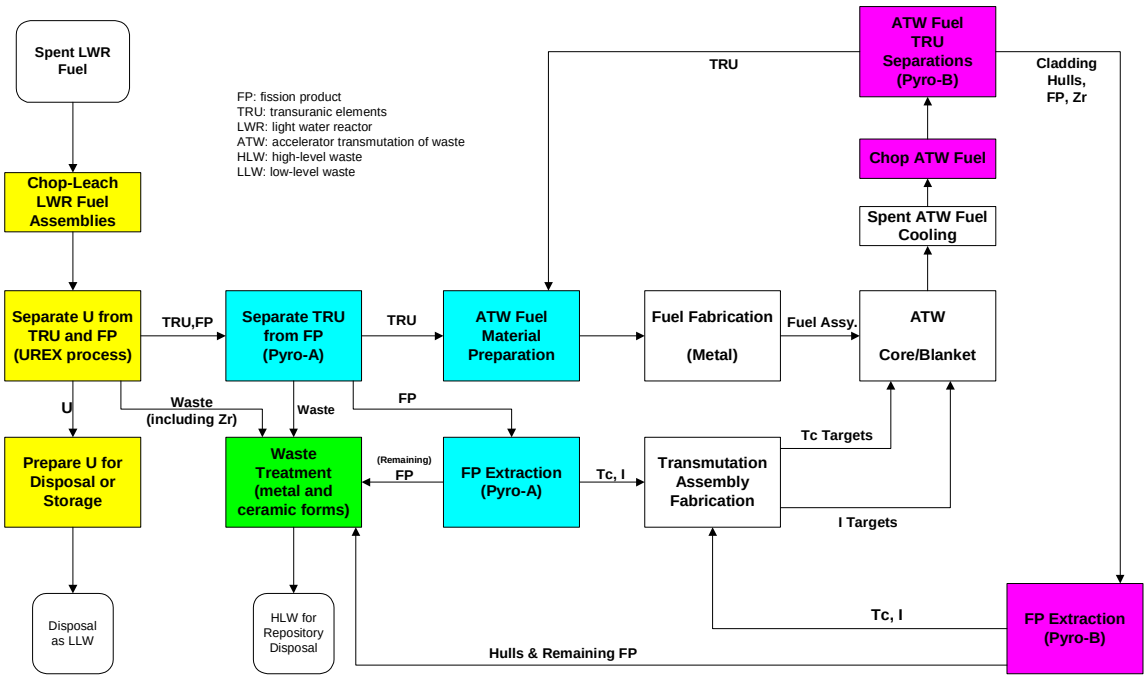
Quarterly Progress Report
11/16/01- 2/15/02

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)

Students:

- Mr. Lijian (Rex) Sun, M.S. 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:

- Annual user license of commercial system engineering software iSight^{TM} has been purchased. The academic price was granted.
- Salary expenditures have been adjusted according to the proper account number and student names

Management Problems

The Program Director of AAA-UPP at UNLV, Dr. Anthony Hechanova, has indicated that the funding for this research project was already allocated to our research account. The students' and professional stuffs' contracts will be prepared from 05/01/02 to 06/30/02 and 07/01/02 to 08/31/02.

One high-end personal computer has been received in the middle of December 2001. This serious delay has caused a lot of research schedule timeline problems for us.

We are still looking for one undergraduate student to work with us on this project in summer.

Technical Progress

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. Graphical User Interface of login prompt is shown in Figure 1.

A WebX conference for iSIGHT has be held from 9-11:20 a.m. on December 14. Work continues on two fronts for the systems engineering modeling work. The efforts center around a complete process model in the iSIGHT software and in the development of a general interface for the AMUSE code. Efforts are currently underway to determine if AMUSE is Export Controlled Information (ECI). If it is considered to be export controlled, changes in the way this information is dealt with will have to be made. At present, the students have been made aware of the change in status of the software and we have abided by all of the requirements provided to us by ANL.

The iSIGHT software has been procured, installed, and the students are presently learning how to use the software. While this training effort is ongoing, work is also being started to define the complete process according to published reports. iSIGHT was chosen because of the flexibility it offers in interfacing with numerous types of software packages and languages. The present efforts are preparing students to quickly and efficiently develop a system model later this year. Sample problems and test cases are be setup within the package to verify

iSIGHT is a generic software shell that improves productivity in the design process. In iSIGHT, design problems are specified, and simulation codes from multiple disciplines are coupled, in a description file. After a description file is created, user can then use the iSIGHT interface to set up, monitor, and analyze a design run.

The iSIGHT Graphical User Interface (GUI) is comprised of four main module types that address different aspects of specifying, formulating, monitoring, and analyzing a design problem. Figure 8 illustrates the four main iSIGHT modules.

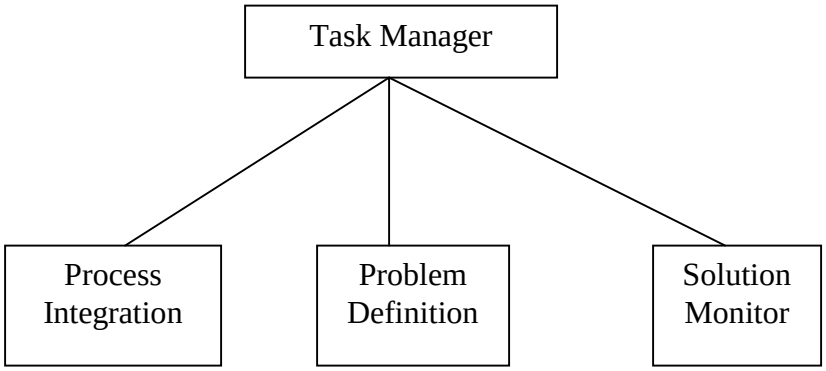


Figure 8. iSIGHT modules

The main iSIGHT interface is the Task Manager. From here a user can launch any of the iSIGHT interfaces. The Task Manager also allows user to ser up and run a design problem.

Process Integration is the iSIGHT module that enables user to couple simulation programs to iSIGHT and specify their execution sequence. Process Integration provides a

GUI that acts as a front end for creating an iSIGHT description file written in iSIGHT MDOL language.

Problem Definition provides a convenient means to provide problem formulation information to specific design parameters, allowing user to control information in user's problem. Problem Definition also includes the design exploration techniques used by iSIGHT to reach an optimum during design exploration. The following techniques are available in iSIGHT: (a) optimization, (b) design of experiments, (c) quality engineering methods, (d) multi-criteria tradeoff analysis, (e) approximations, and (f) knowledge rules.

Solution Monitor is the part of iSIGHT that provides a visual means to monitor the optimization process as it moves through the design space. Solution Monitor provides several tables and graphs that can be used to view the runtime changes.

An example of the data flow is shown in Figure 9. The different executable program files can be linked to the main and/or sub-main routines which is shown in Figure 10. The output graphs and tables are generated in the end of simulation of processes. These are shown in Figures 11 and 12.

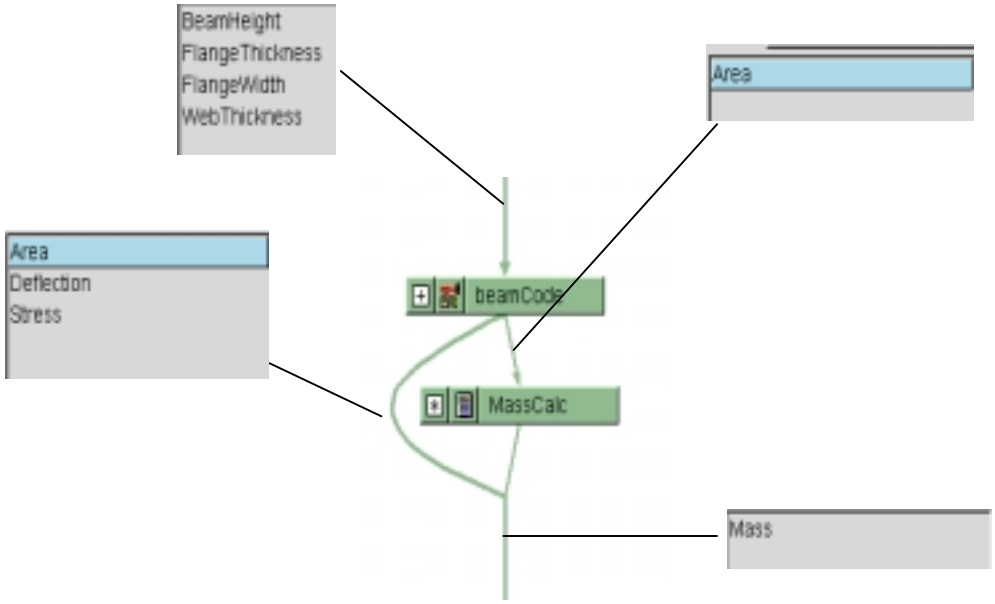


Figure 9. Example of data flow

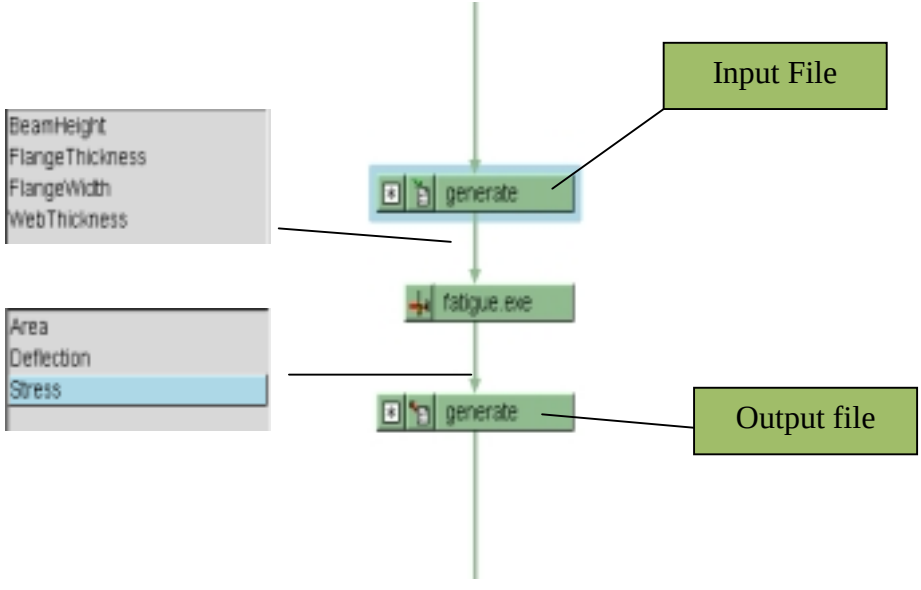


Figure 10. Link to different type of executable program files (.exe)