8-15-2003

Development of a Systems Engineering Model of the Chemical Separations Process: Quarterly Progress Report 5/16/03- 8/15/03

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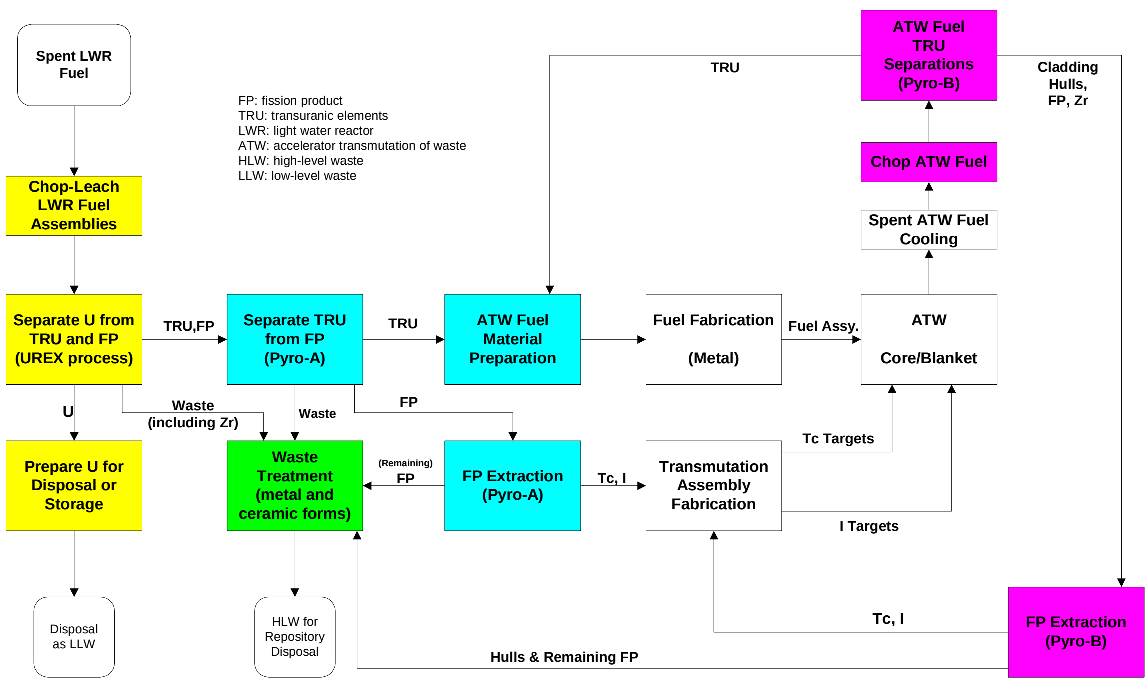
UNLV-AAA University Participation Program

Principle Investigator: Yitung Chen
Co-Principle Investigators: Hsuan-Tsung (Sean) Hsieh, 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. Hsuan-Tsung (Sean) Hsieh (Mechanical Engineering)
- 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:

- N/A

Student Issues:

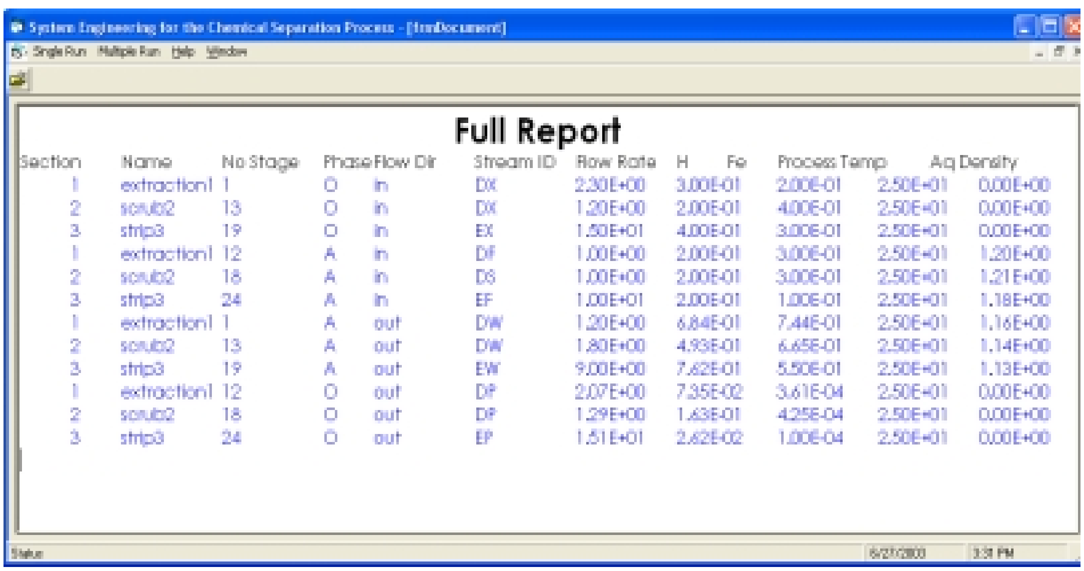
- N/A

Management Problems

No management problem issues at this time.

Technical Progress

Efforts have started on the storage of all results in a MS-Access database to speedup and streamline the analysis of multiple runs (parametric studies for design purposes). An Object Oriented Programming (OOP) approach has been developed and implemented for the final three sections of the new modeling approach (First, Intermediate, and Last sections). Discussions were held with ANL researchers to clarify data transfer and data update issues for the AMUSE code. This will clarify the data flow within AMUSE. A number of AMUSE analyses were conducted to demonstrate the ability of the code to store the data, plot the data, and to obtain feedback from ANL on how to improve the interface. The AMUSE code can now be called from within MATLAB as part of the Systems Engineering Modeling effort. Preliminary results and interface are shown in Figure 1.



Full Report

Section	Name	No Stage	Phase	Flow Dir	Stream ID	Flow Rate	H	Fe	Process Temp	Aq Density
1	extraction1	1	O	in	DX	2.30E+00	3.00E-01	2.00E-01	2.50E+01	0.00E+00
2	scrub2	13	O	in	DX	1.20E+00	2.00E-01	4.00E-01	2.50E+01	0.00E+00
3	strip3	19	O	in	EX	1.50E+01	4.00E-01	3.00E-01	2.50E+01	0.00E+00
1	extraction1	12	A	in	DF	1.00E+00	2.00E-01	3.00E-01	2.50E+01	1.20E+00
2	scrub2	18	A	in	DS	1.00E+00	2.00E-01	3.00E-01	2.50E+01	1.21E+00
3	strip3	24	A	in	EF	1.00E+01	2.00E-01	1.00E-01	2.50E+01	1.18E+00
1	extraction1	1	A	out	DW	1.20E+00	6.84E-01	7.44E-01	2.50E+01	1.16E+00
2	scrub2	13	A	out	DW	1.80E+00	4.93E-01	6.65E-01	2.50E+01	1.14E+00
3	strip3	19	A	out	EW	9.00E+00	7.62E-01	5.50E-01	2.50E+01	1.13E+00
1	extraction1	12	O	out	DP	2.07E+00	7.35E-02	3.61E-04	2.50E+01	0.00E+00
2	scrub2	18	O	out	DP	1.29E+00	1.63E-01	4.25E-04	2.50E+01	0.00E+00
3	strip3	24	O	out	EP	1.51E+01	2.62E-02	1.00E-04	2.50E+01	0.00E+00

Figure 1. Preliminary results and interface integrated with AMUSE code and MATLAM.

Input files and results files can be successfully generated for individual runs and for multiple runs through MATLAB calls. Refinements will be made to this approach to allow for more runs and to allow for optimization. We have successfully implemented the OOP which remains three sections i.e. First, Intermediate, and last sections. Move command is also implemented to all the above three sections. The database has been created and tested using ACCESS of Microsoft. SQL server has been used to implement the database design. Tables were modified completely so that redundancy is reduced. Four tables can take all the data from the VB interface. Tables have been designed for output so that reports can be generated from the developed interface by NCACM instead of AMUSE. Each table has filename as primary key so that foreign key relationship can be established. It enables user to easily handle the data for a particular flow sheet which the structure of database design is shown in Figure 2.

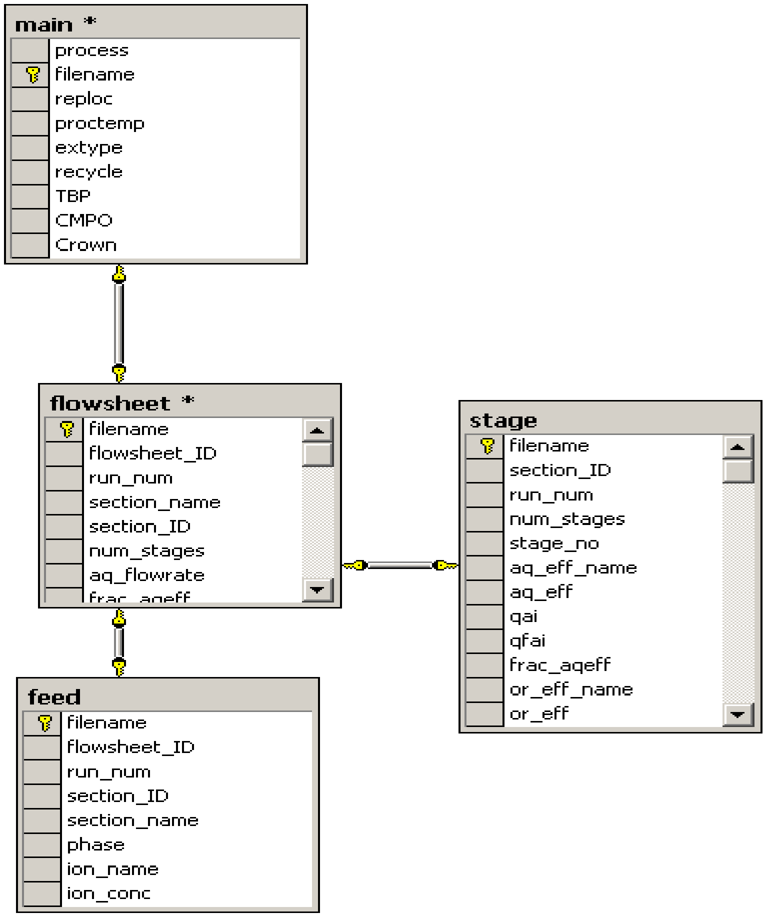


Figure 2. The structure of database design for a particular flow sheet

ANL-East need to provide us the following information to use ADO connection functionality to connect to database from VB and create the export files.

- Confirm the working flow for the new interface design.
- Need to know how the values in stage sampling form gets updated whenever a stream is added or deleted.
- What type of data should be there in either effluent in the main object?
- Data that comes in the output streams?
- Validations for all the input including section, stage sampling, stage specific input, feed cards, and stream values.
- AMUSE is not working when we add section 19 & 20. No change in the output even if we add 'n' number of sections. The result is same as a single section with data of last section.

Several runs were made and charts for different inputs versus outputs were created. Based on these charts we have got some relationship between input and output which can be used for optimization process in the system engineering modeling. A few examples of charts are shown in Figures 3, 4 and 5.

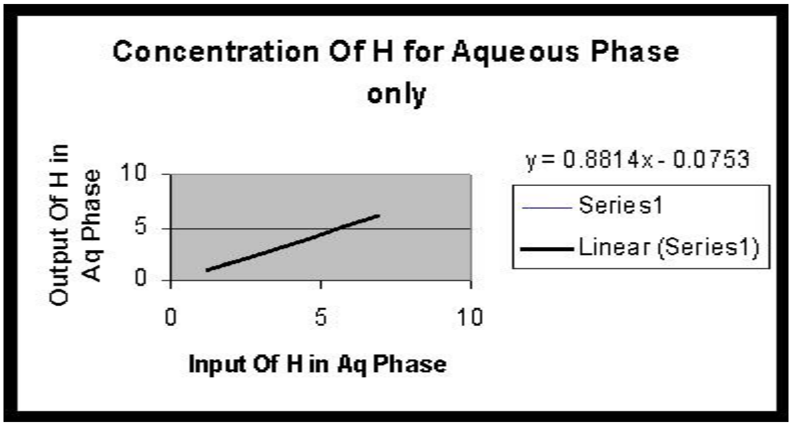


Figure 3. Concentration of H for only aqueous phase in the system engineering modeling

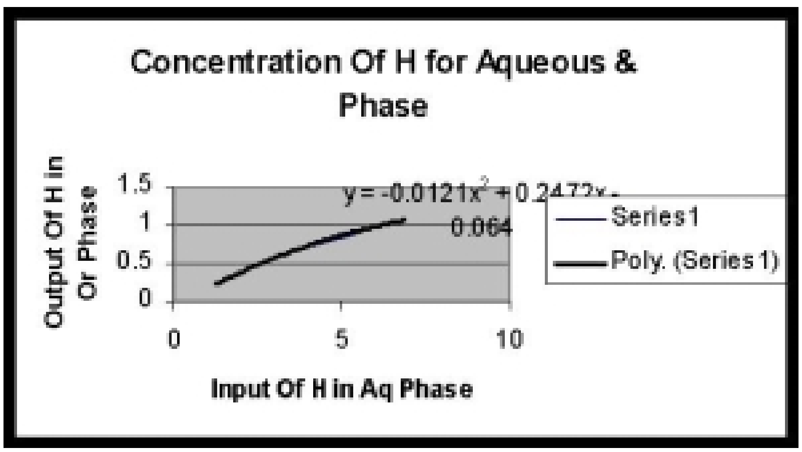


Figure 4. Concentration of H for aqueous and phase in the system engineering modeling

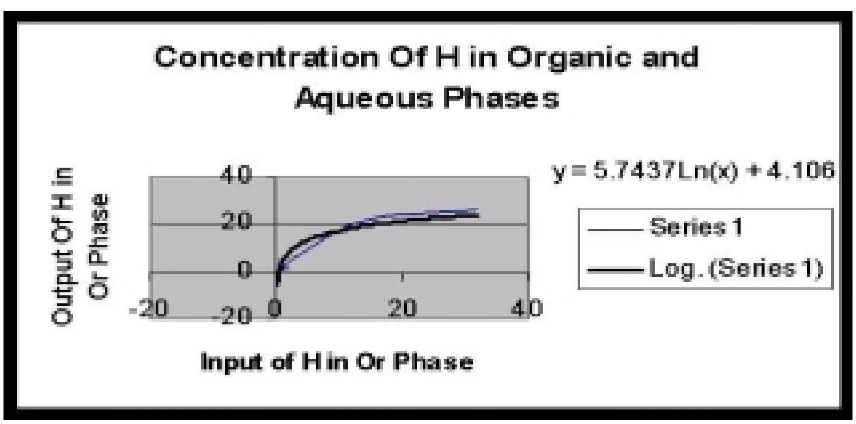


Figure 5. Concentration of H in organic and aqueous phases in the system engineering modeling

FLOWSHEET-SIMULATOR has been developed which has the following features:

- Create a new FLOWSHEET from scratch
- Open a FLOWSHEET from export file
- Open a FLOWSHEET from SQL server database
- Edit the FLOWSHEET by simply visually dragging and dropping
- Save result to database
- Save result to export file
- Call AMUSE code to run

The great advantages for the FLOWSHEET-SIMULATOR development are that it is developed using OOP technologies and can hide all the information about connection with AMUSE and data flow with database, export file and report file. FLOWSHEET-SIMULATOR provides the entire friendly interface for user to implement all the functions. A FLOWSHEET-SIMULATOR screen is shown in Figure 6. System Engineering Model Flow Chart has been developed as shown in Figure 7.

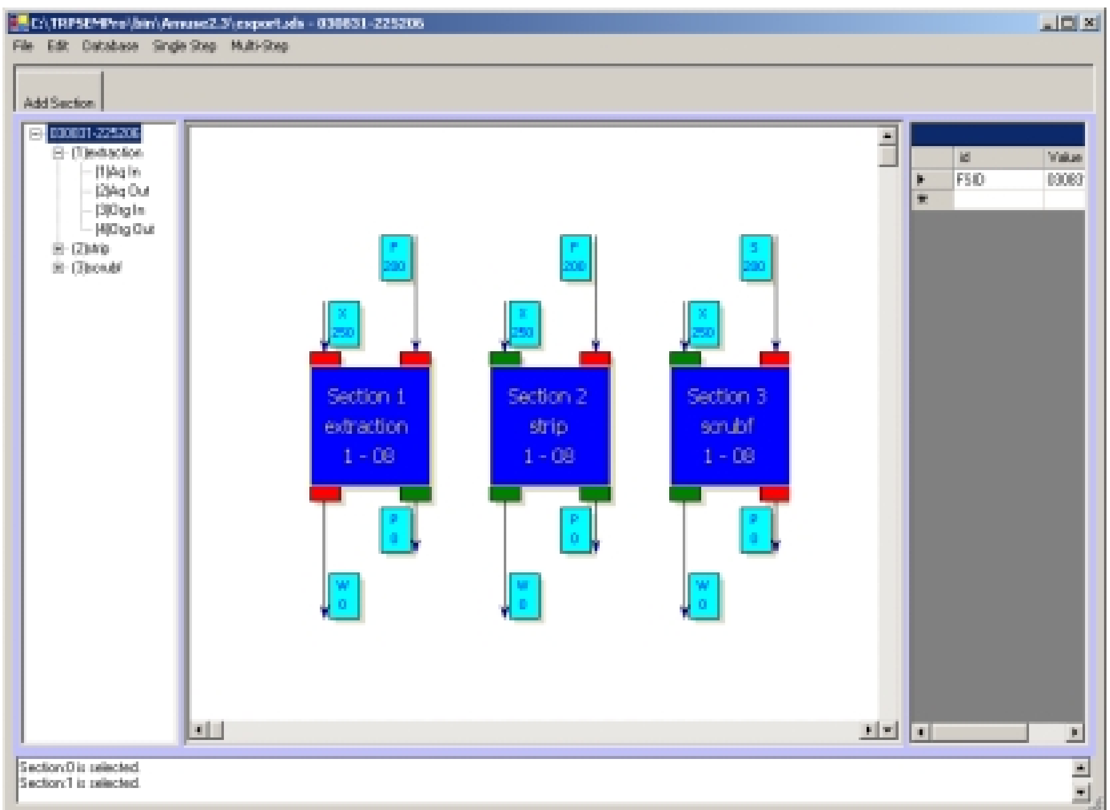


Figure 6. A FLOWSHEET-SIMULATOR screen

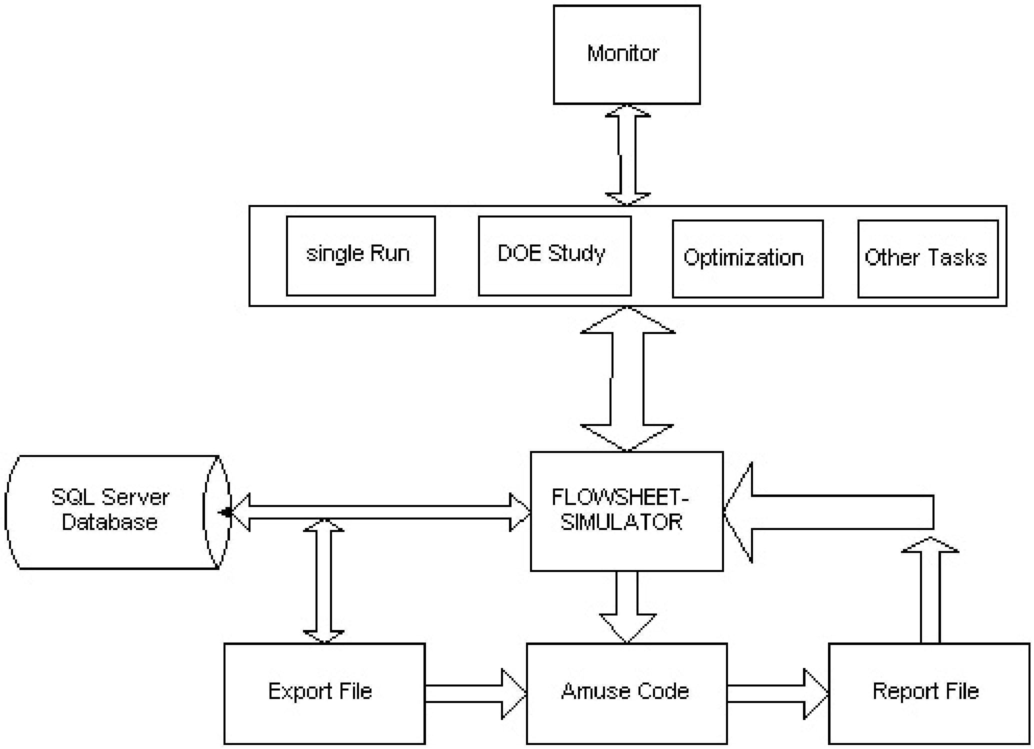


Figure 7. System Engineering Model Flow Chart

Task-Integration module has been continuously developing and revising.

- Create a new task from scratch
- User can dynamically add simulation module, simulation code, and chemical separation module such as AMUSE code to the main task
- User can dynamically define the dataflow among all the tasks
- Save the simulation results to the developed database
- Save the simulation results as XML file

Main Window of Task-Integration is shown in Figure 8. Parameter-Define dialog boxes in Task-Integration module is shown in Figure 9. Parameter-Map dialog boxes in Task-Integration module is shown in Figure 10.

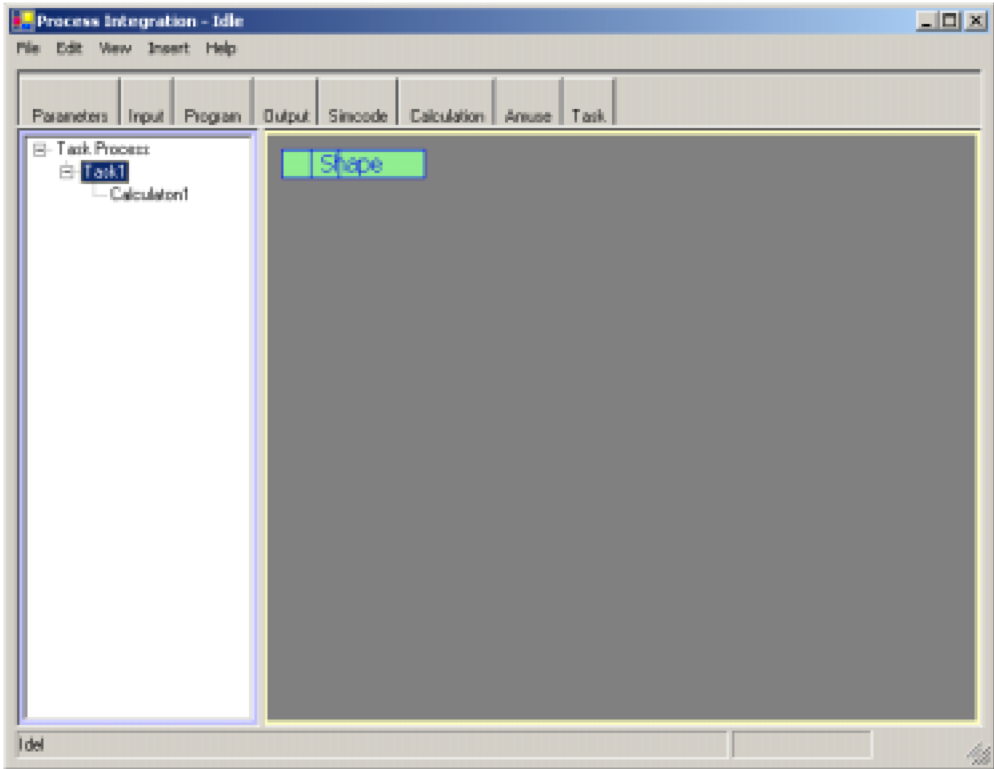


Figure 8. Main Window of Task-Integration

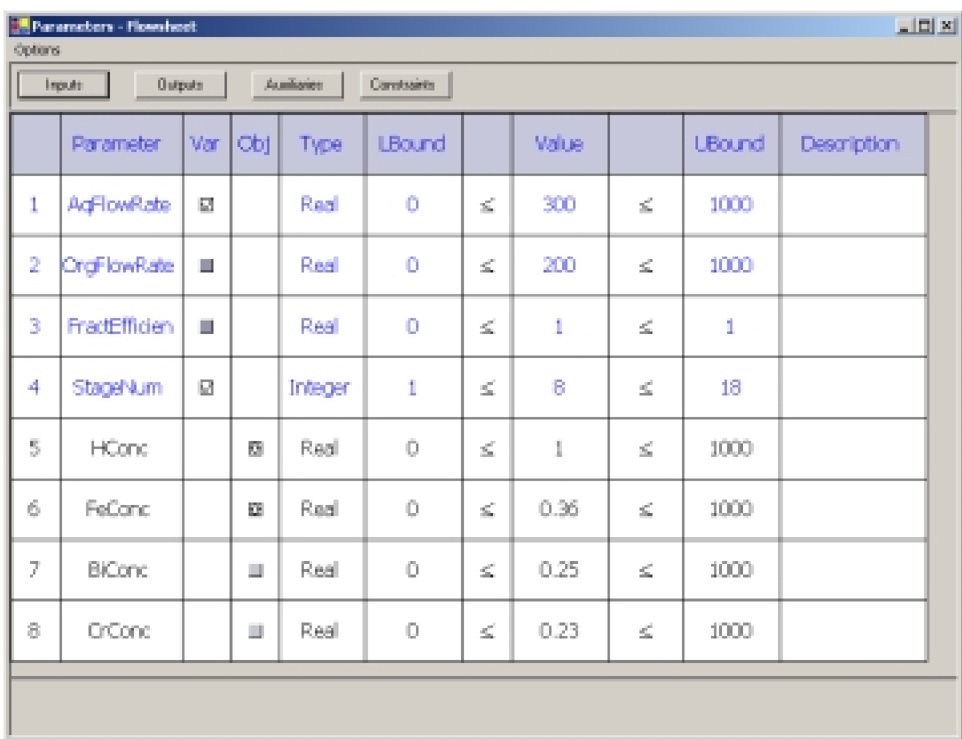


Figure 9. Parameter-Define dialog boxes in Task-Integration module

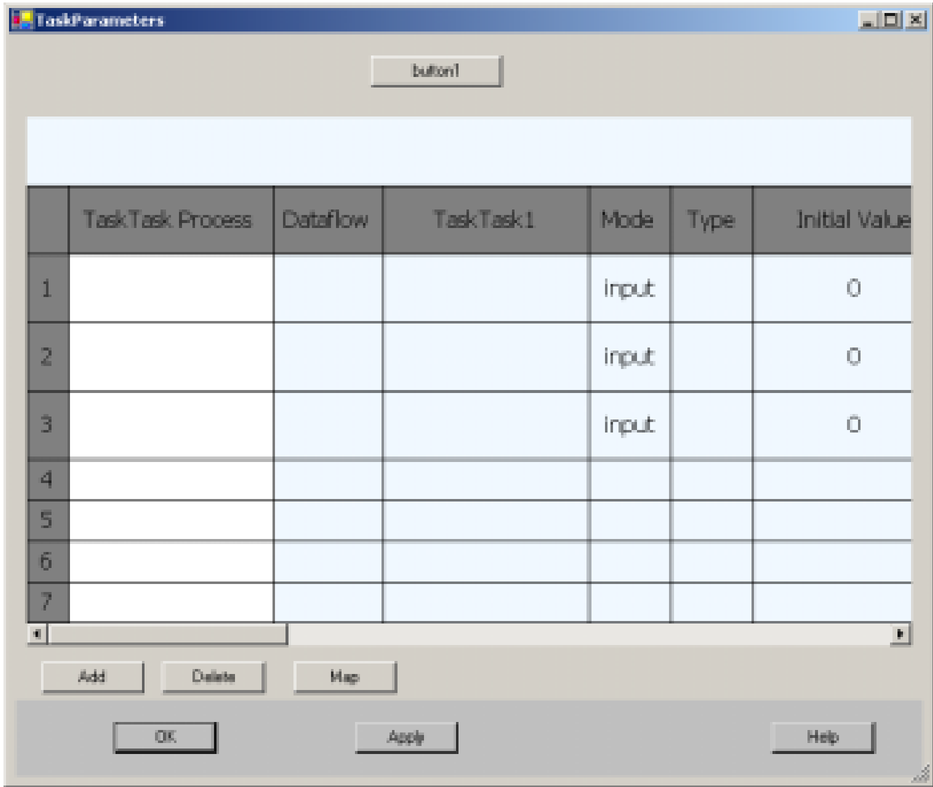


Figure 10. Parameter-Map dialog boxes in Task-Integration module

We can use the above Task-Integration module to build the whole flowsheet to simulate the chemical separation process. User can then apply the different system study tools to study the system engineering modeling and analysis from the Task-Manager module. The Task-Manager module has been designed. Currently, we are in the coding phase.

A successful meeting was held June 30 and July 1 with Argonne National Laboratory (ANL) researchers to discuss project details. We had good communication and feedback from our collaborators and they are very supportive to this project.

The poster of “Development of Systems Model for UREX Process” has been presented to the AFCI semi-annual meeting in Santa Fe, NM, August 25-28, 2003.

The paper of “Development of Systems Model for UREX Process,” IMECE2003-42043, has been peer reviewed and accepted by 2003 International Mechanical Engineering Congress and Exposition Conference which will be held in Washington, D. C., November 16-21, 2003.