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Purpose and Problem Statement

The AFCI 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)
- 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:**
- N/A

**Student Issues:**
- N/A
Management Problems

No management problem issues at this time.

Technical Progress

A successful meeting was held March 6th and 7th with Argonne National Laboratory (ANL) researchers to discuss project details and where they communicated good feedback and support for the project. Five specific objects are being implemented for the graphical user interface as a result of the meetings with ANL researchers: Flow sheet, Section, Streams, Stages and Concentrations. Work continues on the development of flow sheet objects that allows the user to select flow sheet name, reports location, type of process and other required input (see Figure 1 below).

![Figure 1. Representative example of flow sheet](image)

A Separations area called “Tools” is being developed to allow the user to develop process blocks within the software environment to build a specific process flow sheet, which includes the ability to generate process streams, sections, stages and input data for each of them. Development of an overall process model continues using MATLAB with SIMULINK that will eventually allow the top five most influential factors to the process
to be automatically selected those factors will be used for the design variables for the optimization. The interface has been changed to implement the Object Oriented Programming (OOP) approach. With this approach our interface will be able to do all operations as done in AMUSE. Based on the following constraints we have developed three user controls to define the flow sheet.

- All the sections should have a section name and number of stages.
- First section should have both aqueous and organic streams.
- Aqueous feed is mandatory to all sections.
- Stage Sampling and Stage Specific Input can be given to any section.
- Last section should have organic stream.
- First section should have aqueous effluent as output
- Last Section should have Organic Effluent as output.

They are first, last and intermediate sections. The color pattern is used to differentiate the type of input. Red color is used to indicate a mandatory input and green color is used for optional input. Figure 2 shows the three types of sections.

![Diagram of three different types of sections](image)

**Figure 2. Three different types of sections.**

The flowsheet object is integration of different objects. We have section, stage, aqueous and Organic streams and Aqueous and Organic Feeds as objects. Events are written for each object to give input. For this a number of forms are created which takes input. Figure 3 shows the flowsheet object integrated with different objects.
Figure 3. Flowsheet object integrated with different objects or sections.

The main form will have flowsheet object and Tools to create the flow sheet and to give input. Connectors are removed because by default the streams go from one block to the consecutive block. The drag and drop mechanism is now implemented only for last section which is shown in Figure 4.

Figure 4. The drag and drop mechanism on the flowsheet.
The user now clicks on each object to give input. For example,

![Image](image.png)

**Figure 5.** Input dialogue box for each object.

The following developments are being implemented.

- Implement the OOPS to remaining two tools.
- Create an export file based on the new format.
- Link Amuse with the new export file.
- Implement the move and resizing for the tools.
- Implement the delete command to the tools.

Dr. George Vandergrift from ANL-East will provide us the constraints for the system optimization modeling. In the meantime, we have practiced by using graphical optimization method in MATLAB to solve the structural mechanical problem. We need to select appropriate optimization scheme and apply it to AMUSE code. Since this is multi-objective function optimization, we need to consider more than one design objective. We are developing and building all chemical separation flow sheet structure for the system engineering modeling which include not only UREX, AMUSE code related, but also other blocks. We can plug in those functions provided by ANL-East to each block in the future. SIMULINK will also be used to develop the system engineering modeling. Mr. Sun is learning how to implement functions in each block and how to call AMUSE code and our developed VB code within MATLAB and SIMULINK. The main form will have flow sheet object and Tools to create the flow sheet and to give input. The drag n drop mechanism is now implemented only for last section. A label for each section to raise the events for mouse moments is created. User is allowed to raise events from any of the objects but in the user control all the objects raise events for taking input.
from the user. Now the section can be moved anywhere within the screen by clicking and moving the label we see above. The events are raised from the user control which then links with the code in the VB project. Hence three functions are defined in the user control which calls the same functions in the VB project. These functions are global to the user control and local to the project. Some changes were also made to the feed cards. The input for streams has changed. The GUI of aqueous input stream is created which is shown in Figure 6. The GUI of organic input stream is also created which is shown in Figure 7.

![Aqueous Streams GUI](image)

**Figure 6.** The GUI of aqueous input stream.

![Organic Streams GUI](image)

**Figure 7.** The GUI of organic input stream.

Six tables were created by using MS Access as database to store the input. They are:
1. Aqstream
2. Orgstream
3. Section
4. Select
5. Conc
6. Exp
Table 1. Aqueous stream database for storing input values

<table>
<thead>
<tr>
<th>stname</th>
<th>aqflorate</th>
<th>FAQE</th>
<th>AQrerooute</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

Table 2. Organic stream database for storing input values

<table>
<thead>
<tr>
<th>oName</th>
<th>orflorate</th>
<th>FOE</th>
<th>ORrerooute</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

Table 3. Section database for storing input values

<table>
<thead>
<tr>
<th>sName</th>
<th>typeabc</th>
<th>numstages</th>
<th>stageff</th>
<th>FAE0</th>
<th>FOEA</th>
<th>fraceff</th>
<th>temp</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

Table 4. Select functions database for storing input values

<table>
<thead>
<tr>
<th>process</th>
<th>sheetname</th>
<th>location</th>
<th>proctemp</th>
<th>etype</th>
<th>recycle</th>
<th>TBP</th>
<th>CMPO</th>
<th>crown</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
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</tbody>
</table>

Table 5. Experiment database for storing input values

<table>
<thead>
<tr>
<th>run SPACE</th>
<th>run SASSE</th>
<th>file suffix</th>
<th>folder name</th>
<th>sections</th>
<th>useable sect</th>
<th>absolute feed</th>
<th>year</th>
<th>recycle</th>
</tr>
</thead>
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<td></td>
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</tbody>
</table>
We have successfully used and developed the Active X technique from Visual Basic program to run the instance of MATLAB and execute MATLAB function and export the result back to the main GUI which is shown in Figure 8.

![Figure 8. MATLAB associated with Active X and Visual Basic development.](image)

We have successfully developed MATLAB command and Figure 9 is shown generated by MATLAB in VB form by using DDE technique from VB. Then user can call

```
a=magic(5):A=inv(a), [x,y]=meshgrid(3:0.1:3:2:0.1:2),z=(x:

A =
-0.0049 0.0512 -0.0354 0.0012 0.0034
0.0431 -0.0373 -0.0046 0.0137 0.0015
-0.0303 0.0031 0.0031 0.0031 0.0364
0.0047 -0.0065 0.0108 0.0435 -0.0370
0.0028 0.0050 0.0415 -0.0450 0.0111
```
MATLAB function and export the result back to main GUI by using Active X technique from VB.Net.

We have also successfully developed to open Excel application program, add workbook, and change active worksheet by using ActiveX automation technique from MATLAB program. Following figure demonstrates what user can get after running the code which the specific program of MATLAB has been developed and used.

Figure 9. MATLAB in Visual Basic form using DDE technique.
Figure 10. Open Excel application program, add workbook, and change active worksheet by using ActiveX automation technique from MATLAB program.

The complete flow sheet for the chemical separation process within SIMULINK and MATLAB is under studied. The development of connecting each model to individual appropriate function, like AMUSE code, will be accomplished by the end of summer. The Nonlinear Programming Optimization method is being studied. Mr. Lijian Sun has also been studying the numerical techniques for solving unconstrained and constrained optimization problem. He will also study the Discrete Optimization method which can be used to the systems engineering modeling of chemical separation process.


Dr. George Vandegrift and his staff from ANL-East will visit us in June to provide the system engineering modeling constraints and update the latest flowsheet designs.