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Development of a Systems Engineering Model of the Chemical Separations Process: Quarterly Progress Report 2/16/03- 5/15/03

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Development of a Systems Engineering Model of the Chemical Separations Process

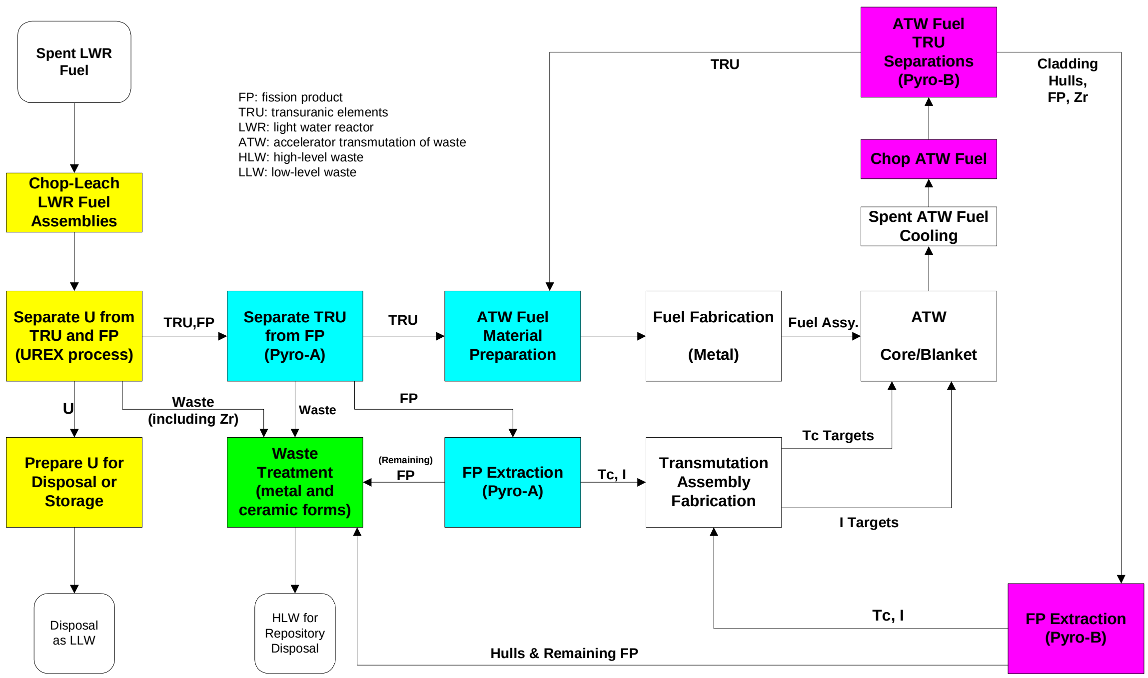
Quarterly Progress Report
2/16/03- 5/15/03

UNLV Transmutation Research Program

Principal Investigator: Yitung Chen
Co-Principal Investigators: Randy Clarksean and Darrell Pepper

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).

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.

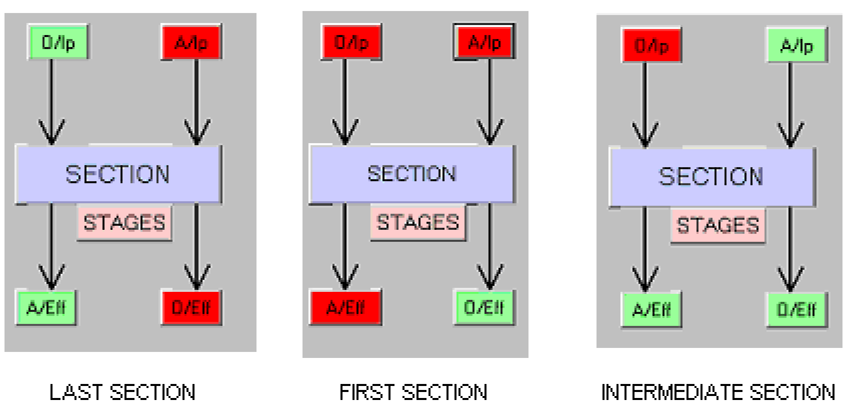


Figure 2. Three different types of sections.

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.

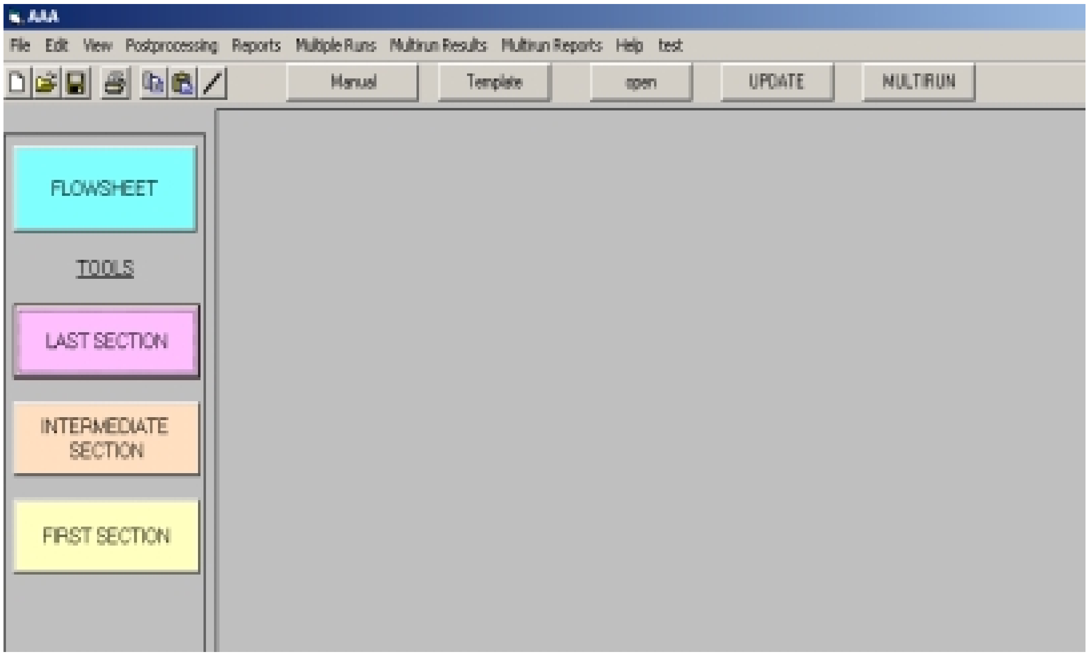


Figure 3. Flowsheet object integrated with different objects or sections.

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.

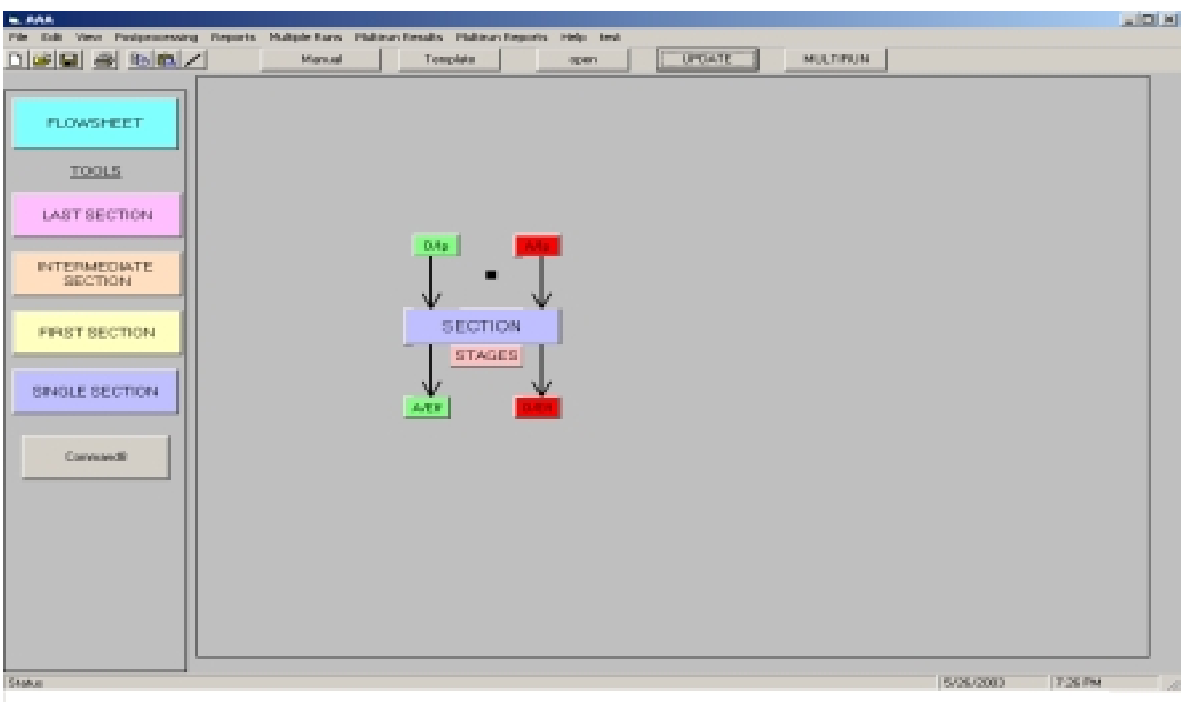


Figure 4. The drag and drop mechanism on the flowsheet.

- 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.

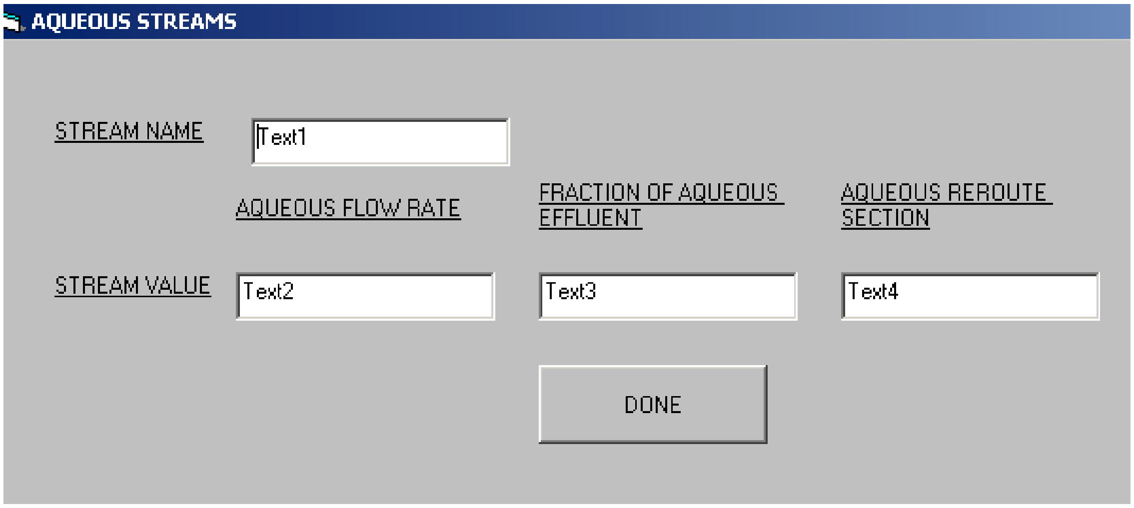


Figure 6. The GUI of aqueous input stram.

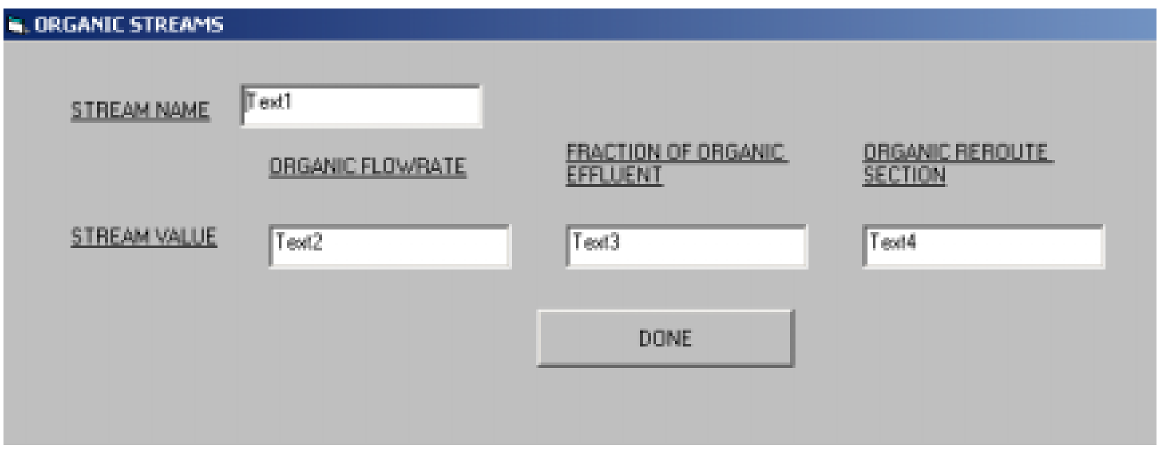


Figure 7. The GUI of organic input stram.

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

aqstream : Table

stname	aqflorate	FAQE	AQreroute
	0	0	

Table 2. Organic stream database for storing input values

orstream : Table

ostname	orflorate	FOE	ORreroute
	0	0	

Table 3. Section database for storing input values

section : Table

secname	typeofsec	numstages	stageff	FAEO	FOEA	fraceff	temp
		0	0	0	0	0	0

Table 4. Select functions database for storing input values

select : Table

process	sheetname	location	proctemp	extype	recycle	TBP	CMPO	crown
			0			0	0	0

Table 5. Experiment database for storing input values

exp : Table

run_SPACE	run_SASSE	file_suffix	folder_name	sections	useable_sectic	absolute_feed	year	Recycle
				0	0	0	0	

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.

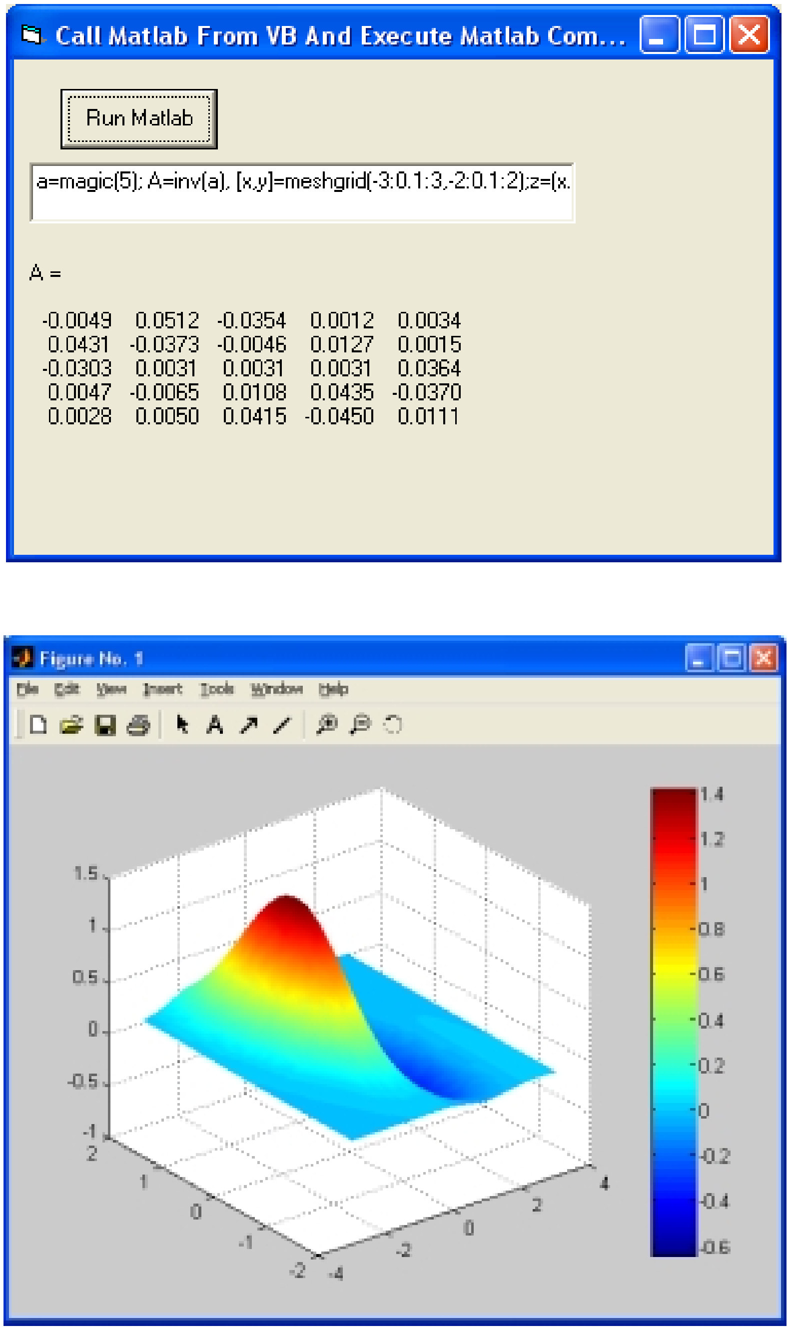


Figure 8. MATLAB associated with Active X and Visual Basic development.

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

MATLAB function and export the result back to main GUI by using Active X technique from VB.Net.

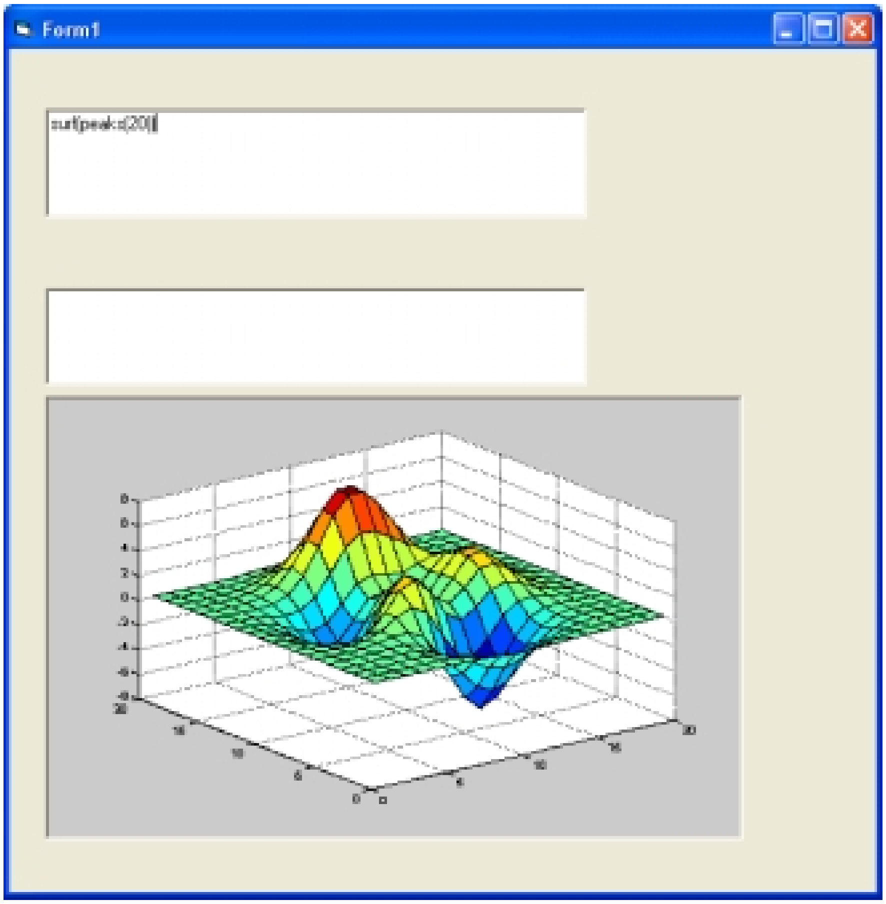


Figure 9. MATLAB in Visual Basic form using DDE technique.

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.

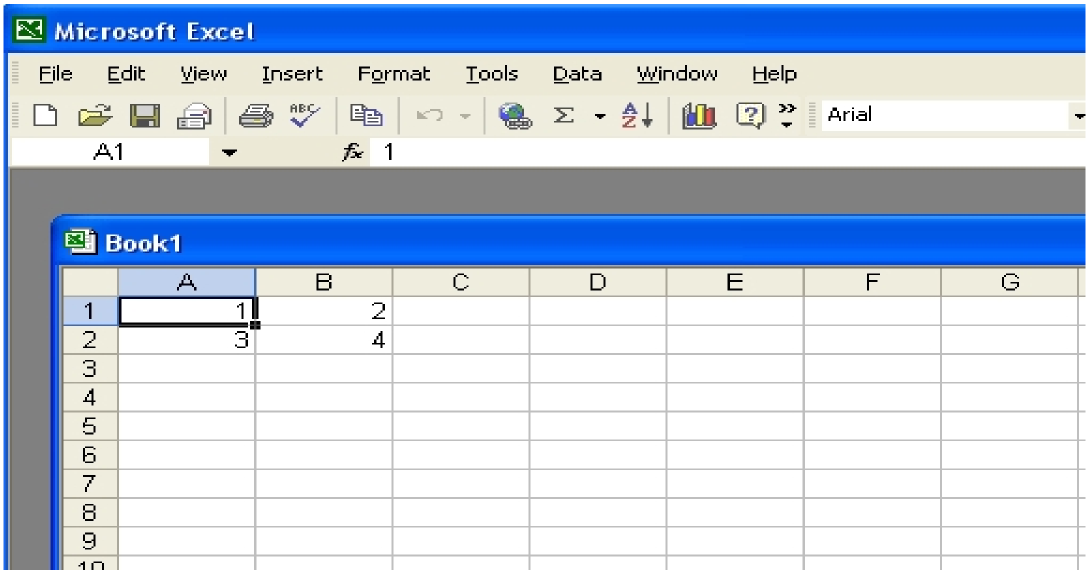


Figure 10. Open Excel application program, add workbook, and change active worksheet by using ActiveX automation technique from MATLAB program

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.

Ms. Haritha Royyuru and Mr. Lijian Sun have presented “Development of a Optimization Systems Engineering Model for Spent Fuel Extraction Process” to the American Nuclear Society (ANS) Student Conference in Berkley, CA, April 2-5, 2003.

Ms. Haritha Royyuru and Mr. Lijian Sun will attend the Sixth of the International Meeting on Nuclear Applications of Accelerator Technology (AccApp’03) to present “Development of a Optimization Systems Engineering Model for Spent Fuel Extraction Process” to the American Nuclear Society (ANS) Conference, San Diego, California, June 1-5, 2003.

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.