5-31-2002

Development of a Systems Engineering Model of the Chemical Separations Process

Yitung Chen
University of Nevada, Las Vegas, yitung.chen@unlv.edu

Darrell Pepper
University of Nevada Las Vegas, pepperu@nye.nscee.edu

Randy Clarksean
University of Nevada, Las Vegas

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Proposal

Development of a Systems Engineering Model of the Chemical Separations Process

Submitted to

Advanced Accelerator Applications Program
Technical Focus Area
Chemical Separations Development Research
ATTN: Dr. Anthony Hechanova
Harry Reid Center
University of Nevada Las Vegas

Submitted by

Dr. Yitung Chen, Principal Investigator, uuchen@nye.nscee.edu
Dr. Darrell W. Pepper, Co-Principal Investigator, pepperu@nye.nscee.edu
Dr. Randy Clarksean, Co-Principal Investigator, rclark@lakesplus.com
Department of Mechanical Engineering
University of Nevada Las Vegas
4505 Maryland Parkway, Box 454027
Las Vegas, NV 89154-4027
Phone: (702) 895-1202
Fax: (702) 895-3936

Collaborators

Dr. James J. Laidler, Senior Scientist
Dr. George F. Vandergrift, III, Senior Scientist
Chemical Technology Division
Argonne National Laboratory, Argonne, IL

Proposed Budget

$ 141,567

Project Dates: 9/1/02 – 8/31/03

May 31, 2002

Abstract

Two activities are proposed: 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 will be the start of an integrated approach to the analysis of the materials separations associated with the AAA Program. A second portion of the project will 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.

Proposed Work

Two graduate student research projects are proposed. Both of these projects are inter-related and support the overall goal of developing a systems engineering model of the chemical separations portion of the AAA program. These students will work under the direction of the researcher associated with this project.

The first activity is the development of a systems engineering model. The activities for this project include defining project goals and needs, defining all unit operations (process and waste streams), selection of a development environment (commercial software packages/environments to be evaluated), develop a basic system model, and to demonstrate the utility of the modeling concept.

The second activity is the improvement and streamlining of AMUSE (Argonne Model for Universal Solvent Extraction). Project tasks include the review/analysis of the code structure, the examination of other possible implementations, definition of first year software activities, development of a verification plan, and the modification/improvement of the software.

If successfully funded for this project, an effort will be made to incorporate the analysis of the separations process into undergraduate student design projects. AMUSE would be incorporated into a design class to allow students to learn more about nuclear technology and the transmutation program itself.

1. Progress in Year 1

Work progressed as scheduled in year one of this research project. Activities related to the modification of the AMUSE code and the development of a systems engineering model were carried out.

The majority of the work related to the AMUSE code centered on the development of a new interface in Visual Basic. Work related to the code itself was delayed because the code and its documentation were initially considered to be Export Controlled Information. Staff at ANL pursued this issue and determined that the current state of the code allowed it to not be considered Export Controlled Information. The work within the code itself is in progress as this proposal is written.

During this time of uncertainty relating to the code, efforts were concentrated on developing an interface in Visual Basic. A "screen-shot" of the interface is shown in Figure 1.

Each of the different steps in the UREX process is outlined on the screen and allows easy modification by the user. A streamlined plotting process is also being developed. This will allow the user of the code to select which portion of the process and to then plot any of the variables related to that process step. All of the output will be presented in the Visual Basic interface and the use of the Excel spreadsheet will be transparent to the user. The graphical images of real instruments can be added to replace the dialogue boxes styles later.

The second portion of the AMUSE modification is to allow the model to be used within the systems engineering model itself. The systems engineering model will send data to the AMUSE code (for example: flow stream inputs from chopping operations) and will require data back out of the AMUSE code to send on to any of the next process steps. Conceptually this is shown in Figure 2.

All of the process steps will have the type of interaction shown in Figure 2 with the systems engineering code. Each process model, no matter how simple or complex will require input from the systems engineering model and it will send output back to the systems engineering model for other process streams.

Systems Model

Data Transfer

AMUSE (VB Interface)
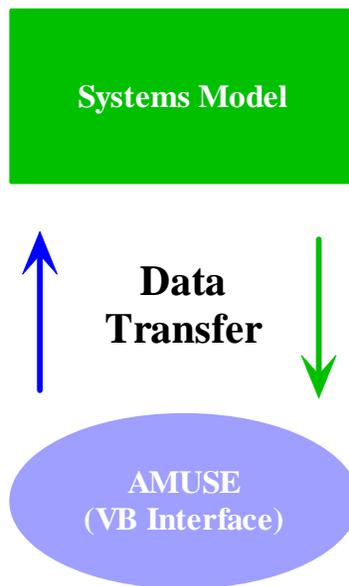
Figure 2 - Interaction between the systems engineering model and AMUSE code.

Development on the general systems engineering model has also progressed. A review process was carried out to select the type of software development environment that would work best for the project. Options for the development environment included source code development of a unique environment, modification of existing software packages, or the use of an "off-the-shelf" product. The product iSight™ was ultimately selected for the project.

iSight™ has a number of features that make it uniquely suited for the project. It allows the user to:
- Couple simulation code from multiple disciplines or development environments (C, C++, Fortran, Excel spreadsheets, etc.,)
- Easily set up design problems through a graphical interface.
- Perform DOE (Design of Experiments) - study and explore design space for a given problem
- Perform optimization studies
    - Combines the best features of existing optimization technologies
    - Allows the user to use a single technique or a combination of techniques

- Distributed Processing and Parallel Execution

The parallel computing features will be particularly important in the future when the complete process model has been defined within iSight. There will be numerous analysis codes to analyze each process step, hence the need for multiple computers to analyze the complete system.
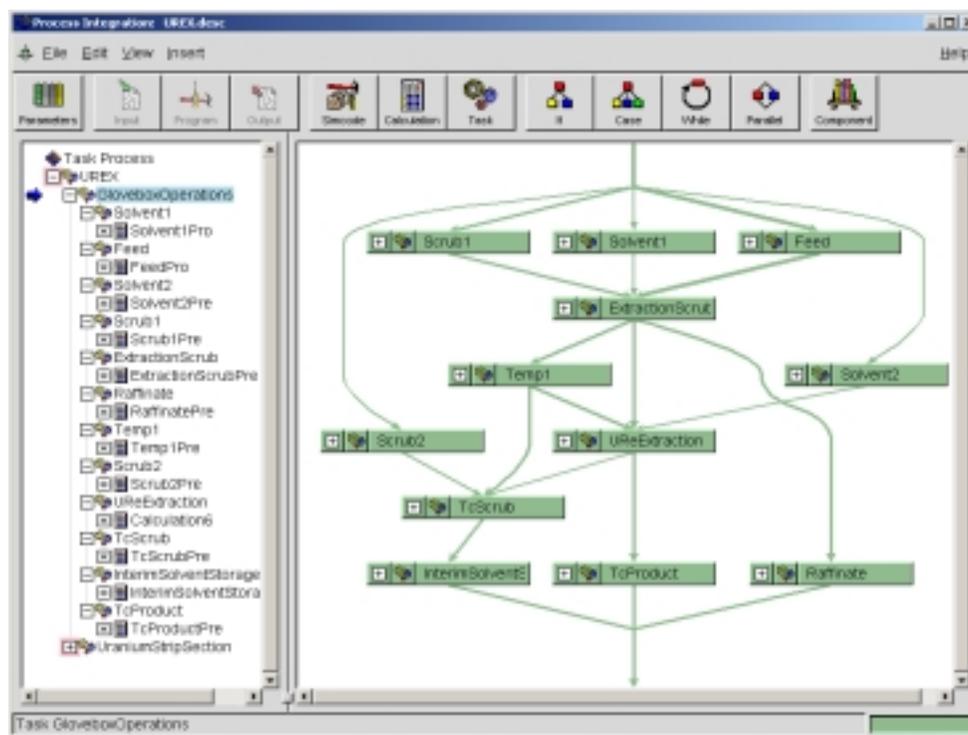
Figure 3 - Typical screenshot of the Systems Engineering model from within iSight™.

At present, efforts are being made to make simple, preliminary definitions to each of the process blocks for one of the proposed AAA Chemical Separations Process.

2. Background and Rationale

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. Figure 4 shows a block diagram of the current process as envisioned by Argonne National Laboratory (ANL) researchers. This is the same process as presented in year one and initially will be the model used for the systems engineering model. The modeling environment has the flexibility to allow the modeling of any process changes.

Nearly all issues related to risks to future generations arising from long-term disposal of such spent nuclear fuel is attributable to ~1% of its content. This 1% is made up primarily of plutonium, neptunium, americium, and curium (the transuranic elements) and long-lived isotopes of iodine and technetium created as products from the fission process in power reactors. When transuranics are removed from discharged fuel destined for disposal, the toxic nature of the spent

fuel drops below that of natural uranium ore (that was originally mined for nuclear fuel) within a period of several hundred years.
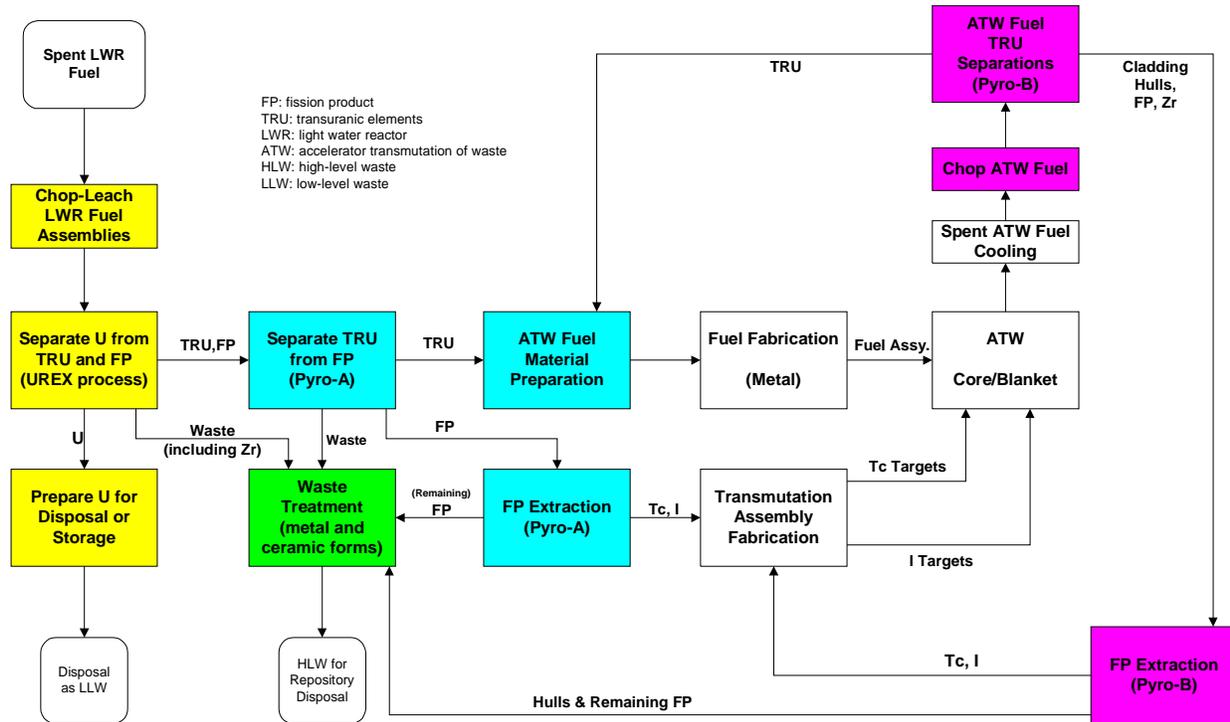
Figure 4 – Overall Chemical Separations System for AAA Program. This figure depicts the fuel cycle scheme in which the transuranic elements and long-lived fission products from spent LWR fuel are sent directly to an accelerator-driven subcritical reactor for transmutation. Other schemes under consideration involve intermediate critical reactor steps; this would result in major changes in the design, development and analysis of separations systems. Systems engineering would enhance the ability to respond with such changes.

Removal of plutonium and other transuranics from material destined for geologic disposal also eliminates issues related to long-term (centuries) heat management within geologic environments. The removal of neptunium, technetium, and iodine render negligible the possibility of radioactive material penetration into the biosphere far in the future. Finally, removal of plutonium negates any incentive for future intrusion into repositories driven by overt or covert recovery of material for nuclear proliferation.

The complete process considers existing LWR spent fuel, separation processes, fuel fabrication, transmutation, disposal as a low-level waste (LLW), and the reprocessing of fuel after transmutation. This is an involved process that can be varied in a number of ways. Any proposed change to the process can have impacts on the fuel design, amount of waste generated by the process, number of cycles through the reactor, etc. In a nuclear growth scenario, the introduction of advanced thermal reactor designs will almost certainly result in changes in separations system requirements that must be met with optimized systems.

The development process is considered a multi-year task. Year 1 has laid the groundwork for the systems engineering model. This groundwork was discussed in Section 1 of this proposal. The second year's effort will continue to develop details of the process model and to modify the AMUSE code to streamline it's use and to make sure it interfaces nicely with iSight.

Developing a systems engineering model of the overall process would be beneficial to analyzing complex interactions between proposed process changes. All of this work will be conducted in conjunction with researchers at the national laboratories to insure its usefulness.

The beginning of any system study is the recognition of the rational system that is responsible for the inputs or outputs of interest. Often, identifying the essential components of the system that collectively undergo the cause and effect action associated with the system is obvious, such as the illness (the output) that results when a person (the system) consumes toxic food or water (the input). However, the identification and isolation of other systems, such as a study of the causes of inflation where the general system is the world economic system, is undoubtedly complex, diverse, and presents a serious modeling challenge. For this project, clearly defining the process flow sheet is a critical first step (UREX, PYRO-A, PYRO-B, etc.).   This work has been completed with the assistance of our National Laboratory Partners, as shown in Figure 1.

When the essential task of identifying and defining those input and output variables that will be employed for a given system model is completed, the system investigator or apprentice then must quantitatively formulate each kernel component for a given input and output. When the essential variables (inputs and outputs) have been identified for the given model, the next step is the quantification and formulation of the system kernel. The system investigator or apprentice, in formulating the system kernel, must seek to quantify each kernel component by determining those system variables and parameters that contribute to that system kernel component. Obviously, successful kernel formulation requires sound knowledge of the particular system and broad experience in system synthesis and analysis such as chemical separation process in UREX etc. Clearly, the integration of the AMUSE tool into the overall process is critical.

Table 1 provides a typical scheme for conducting a system study. The particular nature of each study phase and the efforts expended is, admittedly, system specific, but the study sequence is typical and will be used in developing a systems model for the chemical separations program.

A set of dashed ellipses in Table 1 indicates the stage of the project for year two. The work will continue to focus on defining the necessary data transfer between process models (mass balance of important constituents) and the definition of models or relationships for each of the process blocks. These process models may be individual software packages, or they may be simple assumptions relating to assumed mass balances.

Table 1. Evolution of a Typical System Study

- Background information on actual system
- Observation and experimental data
- Determine system characteristics
  - -Continuous or discrete
  - -Determinant or stochastic
  - -Number and ranking of inputs and outputs

System Identification and Familiarization

- Separation of system model and environment
- Distinguish between inputs and outputs
- Assessment of intrinsic and extrinsic feedback

Model Isolation Boundary Setting

- Measurement scheme for inputs and outputs
- Formulation of each kernel component
- Identification and evaluation of system parameters
- Use linear kernels if appropriate

Quantification Inputs and Outputs Kernel Formulation

Year 2

- Simplification and reduction
- Linearization and parameter minimization
- Analytical solution(s)
- Computer solution(s)

Analysis System Equations

- Evaluation of analysis
- Comparison with actual system
- Modification and iteration on steps as necessary

Model Evaluation and Modification
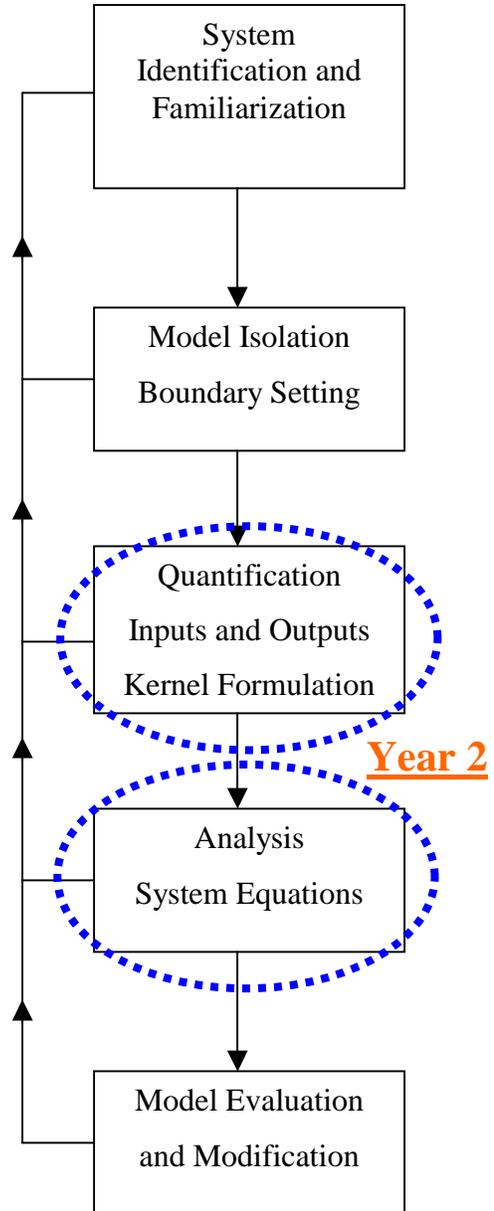
3. Research Objectives

The follow objectives remain the same from year one of the project. Meeting these objectives will lead to a concrete and useful systems engineering model.

- Develop a framework and environment for a systems engineering analysis of the chemical separations system for the AAA program.
- Establish a baseline systems engineering model from which modifications and improvements can be made.
- Refine the existing AMUSE program that gives a detailed examination of the UREX process, a critical component of the overall separation scheme.

4. Technical Impact

A comprehensive systems engineering model of AAA chemical separations processes can greatly facilitate the evaluation of overall systems options. This capability will be become increasingly important as it becomes necessary to down-select reactor types, fuel types, and multi-recycle modes. Systems analysis will make it possible to present decision-makers with concise evaluations of system options and their characteristic features.

In year two, as the level of sophistication of the systems engineering model is increased, it will conceivably be possible to make relative comparisons of process options with regard to waste generation, proliferation resistance, throughput capabilities, facility requirements, and cost. With confidence in the models, the decision-making process can be given greater objectivity and technical credibility.

5. Research Approach

The two proposed research activities have been broken down into several tasks. These tasks are outlined below.

Activity 1: System Engineering Model

1. *Define Process Models* – Discussions will be held with ANL personnel to clearly define which components of the process are most important to the overall process. Each step of the process will need a "model" to define how it is an integral part of the overall process. This will include the important task of defining the inputs/outputs from each model and how it is passed to the other process steps.
    - Specify input streams associated with typical spent fuel.
    - Determine all inputs and outputs for each process block.
    - Select key components to monitor throughout process.
    - Document key individuals or organizations for each process block.
2. *Demonstrate Modeling Concept* – Perform system analyses/simulations using the basic model that has been developed. Determine deficiencies and troubleshoot any possible errors that are found in the model.

Activity 2: Improvement/Automation/Modernization of AMUSE

1. *Review/Analyze Code Structure* – This work will continue from year one to insure that all input data is properly stored within the existing AMUSE environment. Obtain the appropriate files from ANL and study the layout and development history of the code. Analyze the data flow through the package to determine how the different process steps are included and how the calculations are performed.
2. *Develop Verification Plan* – All changes to the code will be verified numerically. A set of test problems or other plan will be developed to demonstrate the numerical accuracy of the actual software changes. This task will continue in year two as this work was moved back in year one because the AMUSE code was considered Export Controlled Information.
3. *Modify/Improve Software* – Make changes to the software that allows it to be used as a part of the overall systems engineering model and that allows it to be used as a stand-alone process model. Determine what modifications would be necessary to allow the optimization of the process.
4. *Systems Analyses* – Use the software to analyze a variety of proposed configurations (input from Argonne National Laboratory Collaborators).

Efforts will be made to bring this research directly into the undergraduate program at UNLV. During year one of this task, this was not feasible because of development process. The Mechanical Engineering Department will be approached to consider incorporating portions of this work in a Senior Design Project. The students would have the opportunity to work with the AMUSE code to study a number of different design options and evaluate the impact of process changes on the waste streams. These students would then present their work to the research staff at ANL. In the course of this work they will have an excellent opportunity to learn the issues associated with spent nuclear fuel and nuclear energy in the United States and the world.

Dr. Chen's efforts have centered on developing a framework and environment for a systems engineering analysis of the chemical separations system. He also establishes a baseline systems engineering model from which modifications and improvements can be made. Dr. Clarksean's work has been crucial in developing Visual Basic interface and the use of the Excel spreadsheet that properly represents the AMUSE. He refines the existing AMUSE program that gives a detailed examination of the UREX process, a critical component of the overall separation scheme

In addition, Drs. Chen and Clarksean will develop and implement the measurement scheme for inputs and outputs, formulation of each kernel component, identification and evaluation of system parameters, use linear kernels if appropriate, simplification and reduction, linearization and parameter minimization, analytical solution(s), and computer solution(s) in phase II project.

6.   Capabilities at UNLV and DOE Labs

Dr. Yitung Chen is Research Associate Professor of the Department of Mechanical Engineering and Interim Director of the Nevada Center for Advanced Computational Methods (NCACM) at the University of Nevada, Las Vegas, and would serve as Principal Investigator. He received his B.S. degree in Chemical Engineering in 1983, and his M.S. and Ph.D. degrees in Mechanical Engineering in 1988 and 1991, respectively, from the University of Utah. He also has a minor degree in Nuclear Engineering. He was a consultant for several engineering companies from 1991 to 1993. Dr. Chen is an expert in experimental and computational aspects of momentum, heat, and mass transfer. His research interests include chemical kinetics modeling, high level radioactive waste repository design, design and analysis for melt casting metallic fuel pins incorporating volatile actinides, niobium cavity design, atmospheric sciences, magnetohydrodynamics modeling, ground water transport, energy conservation, and biomedical engineering. He also has a strong background in organic chemistry, biochemistry, polymer chemistry, and physical chemistry. His research experience includes being PI and co-PI on many projects involving the study of flow and heat transfer and species transport in unsaturated porous media and fuel fabrication funded by DOE, the burning of rocket motors under the Joint Demilitarization Technology (JDT) program funded by DOD, and atmospheric modeling funded by the NOAA Cooperative Institute for Atmospheric Sciences and Terrestrial Applications. He was also co-PI on an EPA project dealing with environmental monitoring for public access and a groundwater modeling project funded by DOE.

Dr. Pepper is Interim Dean of College of Engineering at the University of Nevada, Las Vegas. Dr. Pepper would serve as Co-Principal Investigator. He has been actively involved in the generation, development, and use of hybrid, multi-dimensional algorithms for environmental transport and CFD applications for many years, and has developed atmospheric models for the NRC, NOAA, and DOE (OHER; NVOO). His previous work experiences at the Savannah River Site (E. I. Du Pont de Nemours), the Marquardt Company, and Advanced Projects Research, Inc., have resulted in numerous publications and presentations. Dr. Pepper organized and directed the first modeling workshop for the DOE-OHER on mesoscale atmospheric transport modeling. He served on a NRC project to assess consequences of natural phenomena on various reactor sites and fuel fabrication facilities located within the U.S., and has developed 3-D dispersion models for the NRC and DOD. Dr. Pepper is the co-author of three textbooks on the finite element method, co-editor of two books on environmental modeling, and directs the AIAA Home Study Courses and ASME short courses on finite elements. He is a Fellow of ASME and Associate Fellow of AIAA.

Dr. Randy Clarksean's experience in system modeling, programming, and system optimization provides him with an ideal background to guide the development of this comprehensive System Model. Dr. Clarksean would serve as Co-Principal Investigator. He has taught programming classes, performed system optimization studies, and is knowledgeable of the issues associated with spent fuel processing from his work at Argonne National Laboratory. Dr. Clarksean completed his Ph.D. at the University of Utah in 1990, with an emphasis on computational methods in the thermal and fluid sciences. In 1990, he started work for Argonne National Laboratory at their Idaho facilities. He worked on a number of different process and safety projects while with Argonne National Laboratory. Since 1995, Dr. Clarksean has worked on a

number of projects independently. These projects have involved materials processing, spent nuclear fuel storage, system optimization, electronics cooling, phase change, and other general heat and mass transfer processing. Funding for these projects have come from the D.O.E., D.O.D., private industry, international research organizations, and the State of California. He is an expert in the analysis of engineering systems and has numerous publications in heat transfer and fluid mechanics.

Researchers in the Chemical Technology Division of Argonne National Laboratory have been involved in the development of chemical separations technologies for the nuclear industry since formation of the division in 1948. Argonne is leading the development of chemical processing technology for the AAA program and, along with the Savannah River Technology Center and the Oak Ridge National Laboratory, is actively involved in the conception and experimental confirmation of advanced separations processes for a variety of spent fuel types. Two senior scientists with Argonne's Chemical Technology Division, Drs. Laidler and Vandegrift, will provide support to this project. Dr. Laidler is currently responsible for all U.S. work on the development of chemical separations technology for the AAA program, and Dr. Vandegrift has over two decades of experience in the development of solvent extraction processes for chemical separations. Dr. Vandegrift is the developer of the GTM code that was recently renamed AMUSE.

7. Project Timeline with Milestones and Deliverables

The proposed schedule for all tasks and significant meetings is shown on the following page.

Tasks:	Qtr 1			Qtr 2			Qtr 3			Qtr 4		
	Sept	Oct	Nov	Dec	Jan	Feb	March	April	May	June	July	Aug
Systems Engineering Model												
1. Define Process Models												
2. Demonstrate Modeling Concept												
3. Reporting Requirements				●		●			●			●
Scheduled Meetings	◇ 1				◇ 2							◇ 3
A.M.U.S.E.												
1. Review/Analyze Code Structure												
2. Develop Verification Plan												
3. Modify/Improve Software												
4. Systems Analysis												
5. Reporting Requirements				●		●			●			●
Scheduled Meetings	◇ 1				◇ 2							◇ 3
Notes:	In addition to the proposed formal meetings, researchers and ANL staff will correspond as needed to insure program goals are being met.											
Trip 1	Meet with ANL - Obtain Assistance in Defining Process Steps.											
Trip 2	Meet with ANL - Review Progress in A.M.U.S.E. modifications and discuss Systems Engineering Model.											
Trip 3	Meet with ANL - Discuss progress made during the year.											

Figure 4 - Proposed Timeline for Research Tasks.

Work is assumed to commence on September 1, 2002. Additional travel may be necessary for interactions relating to other specific tasks.