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Development of a Systems Engineering Model of the Chemical Separations Process

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Project Title:

Development of a Systems Engineering Model of the Chemical Separations Process

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Investigators (UNLV): Two Graduate Students to be determined

Collaborator (DOE): Dr. James J. Laidler, Senior Scientist
Dr. George F. Vandergrift, III, Senior Scientist
Chemical Technology Division
Argonne National Laboratory, Argonne, IL

AAA Research Area: **Separations**

First Year Request: $ 150,463 (out years comparable)

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 national 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 to ensure 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 researchers 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. 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.

An effort will be made to incorporate the analysis of the separations process into undergraduate student design projects if the small amount of additional funding can be obtained from other sources. AMUSE would be incorporated into a design class to allow students to learn more about nuclear technology and the transmutation program itself.

1. 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 1 shows a block diagram of the current process as envisioned by Argonne National Laboratory (ANL) researchers.

Nearly all issues related to risks to future generations arising from long-term disposal of such spent 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.
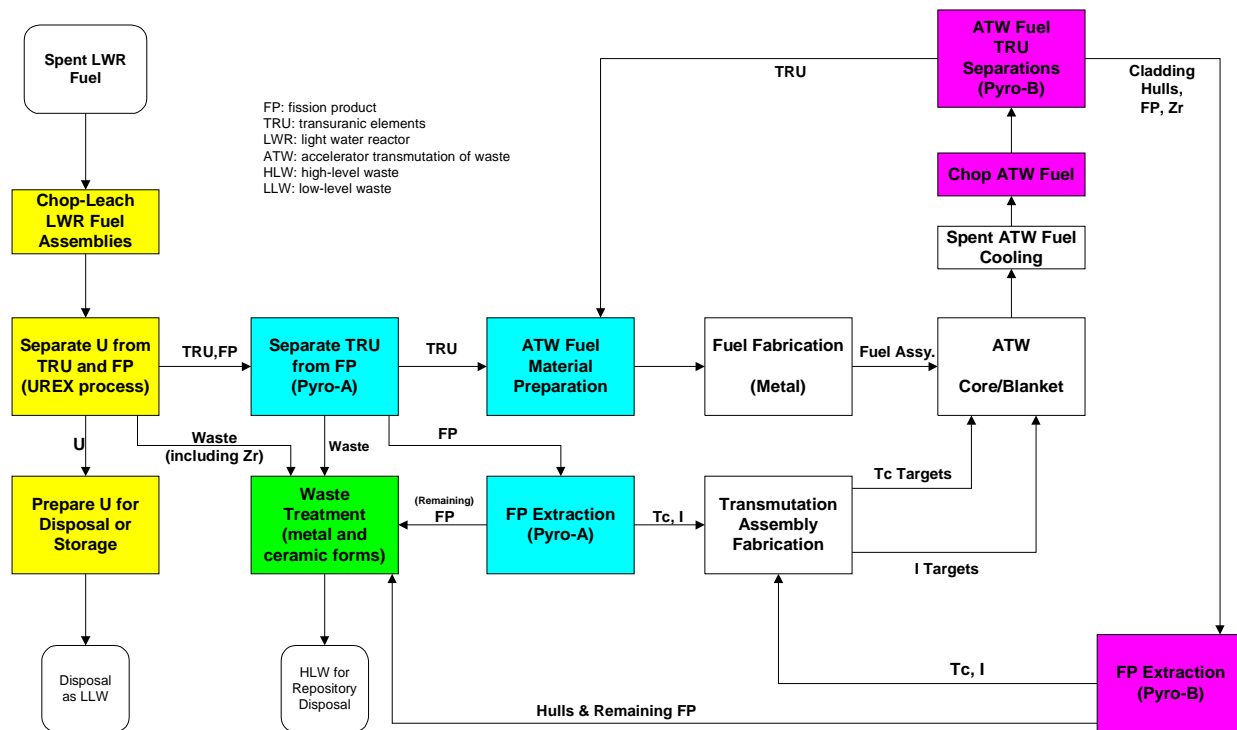
Spent LWR Fuel

FP: fission product
TRU: transuranic elements
LWR: light water reactor
ATW: accelerator transmutation of waste
HLW: high-level waste
LLW: low-level waste

Chop-Leach LWR Fuel Assemblies

Separate U from TRU and FP (UREX process) → TRU,FP → **Separate TRU from FP (Pyro-A)** → TRU → **ATW Fuel Material Preparation** → **Fuel Fabrication (Metal)** → Fuel Assy. → **ATW Core/Blanket**

U

Waste (including Zr)   Waste   FP

Prepare U for Disposal or Storage

Waste Treatment (metal and ceramic forms) ← (Remaining) FP ← **FP Extraction (Pyro-A)** → Tc, I → **Transmutation Assembly Fabrication**

Tc Targets

I Targets

Disposal as LLW

HLW for Repository Disposal

Hulls & Remaining FP

Tc, I

ATW Fuel TRU Separations (Pyro-B) ← TRU

Cladding Hulls, FP, Zr

Chop ATW Fuel

Spent ATW Fuel Cooling

FP Extraction (Pyro-B)

Figure 1 – Overall Chemical Separations System for AAA Program.

Figure 1 depicts the fuel cycle scheme in which the transuranic elements and long-lived fission products from spent light water reactor (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 to 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 will lay the groundwork for the systems engineering model. This groundwork will include improvements to AMUSE (see discussions below) and the ability of AMUSE and other software or models to directly be incorporated into the overall model. Subsequent years will continue the basic model development, add other solvent extraction processes as appropriate, incorporate empirical test data to improve the models, and consider in greater detail critical parts of the process. All of this work will be conducted in conjunction with researchers at the national laboratories to insure its usefulness.

Developing a systems engineering model of the overall process would be beneficial to analyzing complex interactions between proposed process changes. The model will evolve over a three-year period to incorporate all process steps and to improve process modules as more knowledge is gained. The improvements will be based on empirical data or from numerical models as appropriate. A brief background on the Systems Engineering approach is given below.

Background – Systems Engineering Models

In this project we undertake the important task of identifying and quantitatively modeling engineering systems. Frequently, a very valuable aid in the initial identification of the inputs and outputs and various subsystems of a given system is to graphically model the overall system, including explicit designation of all subsystems and internal inputs and outputs. The powerful influence of visual and special conception and recognition of the model in a graphic format can be very revealing and productive for both model analysis and synthesis.

Block diagrams, signal-flow graphs, and organizational diagrams, as graphical modeling tools will be developed in this project. Then several major specific engineering system identification and modeling techniques will be examined. The basic single-input, single-output model has been widely used and justified as an excellent beginning model for many systems. The use of experimental methods for system modeling and verification will be studied; including the valuable aids provided by dimensional analysis and least squares methods. A method called weighted input and output modeling provides a rational means for ranking and weighting inputs and outputs on the basis of their contribution to the system's behavior. Stochastic system modeling and heuristic system modeling with some of essential features of this important field will also be studied.

The graphical representation of the systems engineering model, which includes its inputs and outputs and possible feedback, is very useful tool in the initial modeling and formulation stage of a system study. The act of graphically and schematically portraying the system is conducive to accurate identification and improved understanding of what inputs interact with the system components and how these interactions produce the outputs anticipated. It is in the graphical representation stage of modeling that the system investigator or apprentice could be as thorough and critical of all the known or anticipated system factors as possible. The investigator or apprentice could attempt to detail the system and individually "componentize" the system elements as much as possible.

A major strength and advantage of graphical representation lies in the pictorial, panoramic overview of the total system offered to the investigator or apprentice. Once the investigator or apprentice is satisfied with graphical representation of the model, the methodologies offered by block diagramming and signal-flow graphs provide a rational, systematic mechanism for reducing the system to the basic generalized canonical system.

Graphical representation methods are very useful for both qualitative and quantitative system modeling and analysis. The graphical representation methods that will be considered are: (1) block diagramming, (2) signal-flow graphs, and (3) organizational charting. Each method is useful in developing accurate and complete system engineering models.

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.).

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 the 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.

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

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

- 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)
- Computer solution(s)

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

System Identification and Familiarization

Model Isolation
Boundary Setting

Quantification
Inputs and Outputs
Kernel Formulation

Analysis
System Equations

Model Evaluation
and Modification
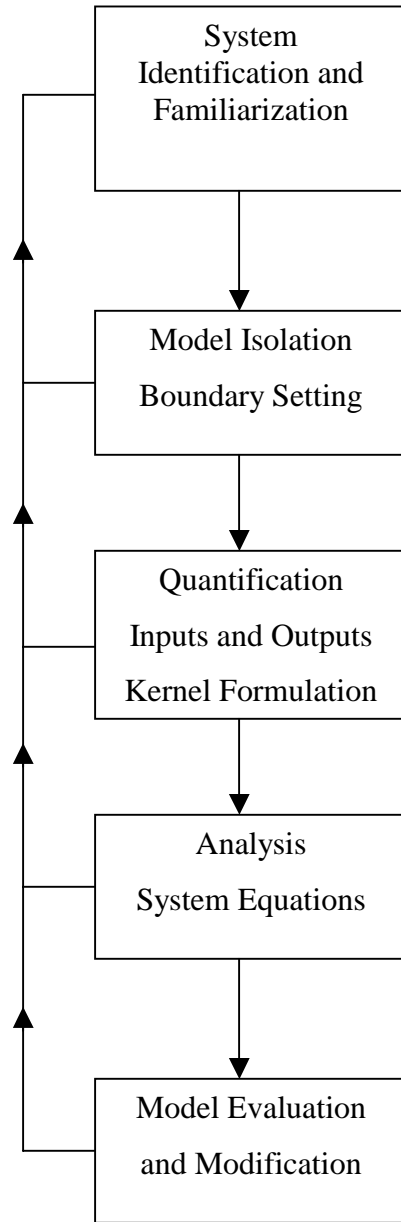
2. Research Objectives

- 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.

If this proposal is funded, additional efforts will be undertaken to develop an option in the UNLV Mechanical Engineering senior design course sequence to allow undergraduate students to study variations in the separations program. The introduction of the separation process of chemical engineering, which is a 400/600 level course, may also be taught to enhance graduate and undergraduate students abilities and knowledge. Approval would be sought from the Mechanical Engineering Department for this innovative program to educate students on the complex issues associated with Nuclear Engineering and the AAA program goals.

3. 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. 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.

4. Research Approach

The proposed research would be conducted in three phases. Each of the phases would be carried out over a one-year period. Phase I (discussed in this proposal) would include the study and analysis of development of a systems engineering model of the chemical separations process. Phase II of the program would lead to case studies and designs at ANL and UNLV to demonstrate the basic or advanced engineering system model. Additional analysis work would be conducted during this time to validate the engineering systems model efforts and to support the testing program associated with UREX, PYRO-A, PYRO-B, etc. Detailed modeling work would continue from Year 1 to refine the existing models and to make detailed comparisons to the experimental test results. These detailed modeling results would also be used to assist in the system design. Two master's degree students will work on the design and analysis of the proposed development of a systems engineering model of the chemical separations process. Students would develop the systems engineering model, work with ANL engineers and scientists to acquire the proposed design, procure background information on actual system, determine system characteristics, study the separation of system model and environment, formulate of each kernel component, evaluate the analysis, and make comparison with actual system with the

assistance of ANL scientists. Phase III would be a joint effort between UNLV and ANL to demonstrate the acceptable use of the systems engineering model in the chemical separations process in a simulated environment. The Phase III work would also include the modification and iteration on the engineering systems model. Students will be assigned to ANL-East to work in conjunction with scientists and engineers there to design and develop the systems of model in the chemical separation process.

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

Activity 1: System Engineering Model

1. *Define Goals and Needs* – Discussions will be held with ANL personnel to clearly define their long-term needs for a Systems Engineering Model of the fuel processing. Based on these needs, goals and milestones will be developed for each year of the project. Preliminary meetings have been held and if this research is funded more in-depth discussions will be held to clearly focus the efforts where most needed. These may include mass balances, system control, plant layout and design, and other features as needed.
2. *Define All Unit Operations* – Reports will be collected and discussions held with ANL staff to clearly define all current and future unit operations. By including all potential future operations, plans for a complete model can be developed that allows for changes or additions as the process is analyzed and developed.
3. *Selection of Development Environment* – Commercial software packages will be analyzed to determine what – if any – software exists that will meet all of the needs defined in Task 1 of this activity. Potential advantages and limitations of different packages will be compared. A commercially available software environment will be used if at all possible to streamline model development.
4. *Develop Basic System Model* – Upon the selection of the proper development environment, the definition of those components or modules defined in Task 2 will start.
5. *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* – 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. *Examine Other Possible Implementations* – Once the structure of the AMUSE tool has been analyzed, efforts will be undertaken to determine if the code can be easily converted to a more general programming environment with graphic modules (e.g., Visual Basic, C/C++, newer version of Excel, etc.)
3. *Define Year 1 Software Tasks* – Establish a reasonable set of modifications that can be made to AMUSE by a graduate student over the remainder of the year. The selection of

these tasks will be related to the importance of a particular component or process to the AAA Program.

4. *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.

5. *Modify/Improve Software* – Make changes to the software as defined in Item 3. These changes will be made to benefit the AAA Program.

Efforts will be made to bring this research directly into the undergraduate program at UNLV. The Mechanical Engineering Department will be approached to consider incorporating portions of this work in the Senior Design Projects. 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 fuel and nuclear energy in the United States and the world.

5. Capabilities at UNLV and DOE Labs

Dr. Yi-tung Chen is a Research Associate Professor of the Department of Mechanical Engineering and Assistant 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.

Dr. Pepper is Professor and Chairman of the Department of Mechanical Engineering, and Director of the Nevada Center for Advanced Computational Methods (NCACM) 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. 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 fuel storage, system optimization, electronics cooling, phase change, and other general heat and mass transfer processing. Funding for these projects have come from the DOE, DOD, 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.

Extensive computing facilities exist for the system modeling efforts at UNLV. Computing facilities range from workstations to super computers. These facilities will be available for the analysis and design of the proposed concepts. A wide range of computational tools exists on these systems.

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. Drs. Laidler and Vandegrift do not require funding from UNLV to participate in this project.

6. Project Timeline with Milestones and Deliverables

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

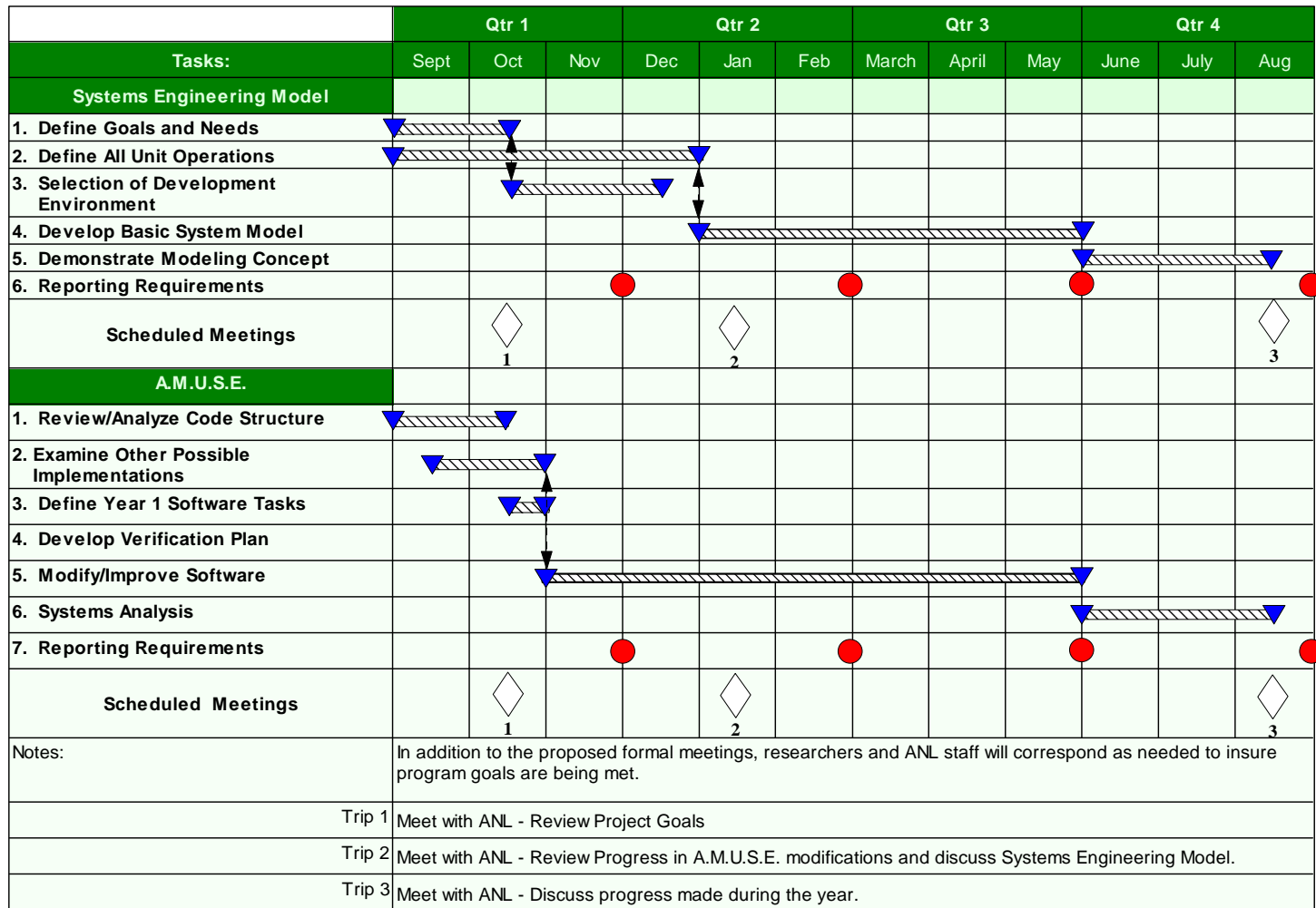|	Qtr 1			Qtr 2			Qtr 3			Qtr 4		
Tasks:	Sept	Oct	Nov	Dec	Jan	Feb	March	April	May	June	July	Aug
Systems Engineering Model												
1. Define Goals and Needs												
2. Define All Unit Operations												
3. Selection of Development Environment												
4. Develop Basic System Model												
5. Demonstrate Modeling Concept												
6. Reporting Requirements												
Scheduled Meetings		1			2							3
A.M.U.S.E.												
1. Review/Analyze Code Structure												
2. Examine Other Possible Implementations												
3. Define Year 1 Software Tasks												
4. Develop Verification Plan												
5. Modify/Improve Software												
6. Systems Analysis												
7. 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 - Review Project Goals											
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 1 - Proposed Timeline for Research Tasks.

Work is assumed to commence on September 1, 2001. Additional travel may be necessary for interactions relating to other specific tasks.

From: "Laidler, James J." <laidler@cmt.anl.gov>
To: Yi-Tung Chen <uuchen@clark.nscee.edu>
Cc: "Vandegrift, George F., III" <vandegrift@cmt.anl.gov>

Subject: Endorsement of proposal

Dear Professor Chen,

I have reviewed your draft proposal, "Development of a Systems Engineering Model of the Chemical Separations Process," by yourself, Darrell Pepper and Randy Clarksean. I find the proposal to be technically sound and fully consistent with the objectives of the AAA Program. I believe that the development of a comprehensive systems engineering model can contribute greatly to the development of AAA separations processes and to the ultimate success of the AAA Program. I am particularly pleased with the idea of using the model to expose undergraduates to the important issues facing nuclear power in this country and abroad.

We at Argonne look forward to collaborating with you on this important project.

Jim

Dr. James J. Laidler
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Chemical Technology Division
Argonne National Laboratory
Argonne, IL 60439-4837