

**Design and Analysis of a Process for Melt Casting Metallic Fuel Pins Incorporating
Volatile Actinides
(Year III Renewal)**

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Abstract

UNLV has developed and will continue to develop process models for the analysis of melt casting processes. This work will continue to be performed under the guidance of Argonne National Laboratory (ANL) engineers to insure that their knowledge and experience benefits the project. The research to be conducted during year three will center on performing detailed analyses on a conceptual design of an inductively heated skull-crucible casting furnace. Processing conditions will be analyzed, basic models utilized, and detailed heat and mass transfer models will be developed to analyze the most promising processes. The goal of this third year is to complete the preliminary design analyses for the proposed skull-crucible casting furnace, which will be developed and tested in subsequent funding years.

Accomplishments – Year 2

Efforts continued to develop more detailed heat and mass transfer models that could be used successfully in the analysis of an advanced casting furnace design. A combined conduction heating and heat transfer model was developed and tested. The mass transfer model was developed further as well.

Proposed Work – Year 3

UNLV is uniquely qualified to perform this work because of resident expertise in the analysis of engineering systems. Research efforts will focus on the validation of a coupled induction heating and heat transfer model for the proposed casting furnace design. Simple casting tests will be performed at Argonne National Laboratory-West. A series of analyses will also be performed to specify the design of a casting furnace based on this new technology.

1. Progress in Year 2

1.1 Parametric Model for Fuel Rod Casting

Work continued on improving a model for the casting of fuel pins. Work this year considered the flow of the melt into the mold and the analysis of the heat transfer into the mold during solidification (after flow has stopped).

Figure 1 shows the results from an energy balance model, which indicates that the thermal mass (sensible heat storage) would typically be greater than needed to solidify the melt within the mold.

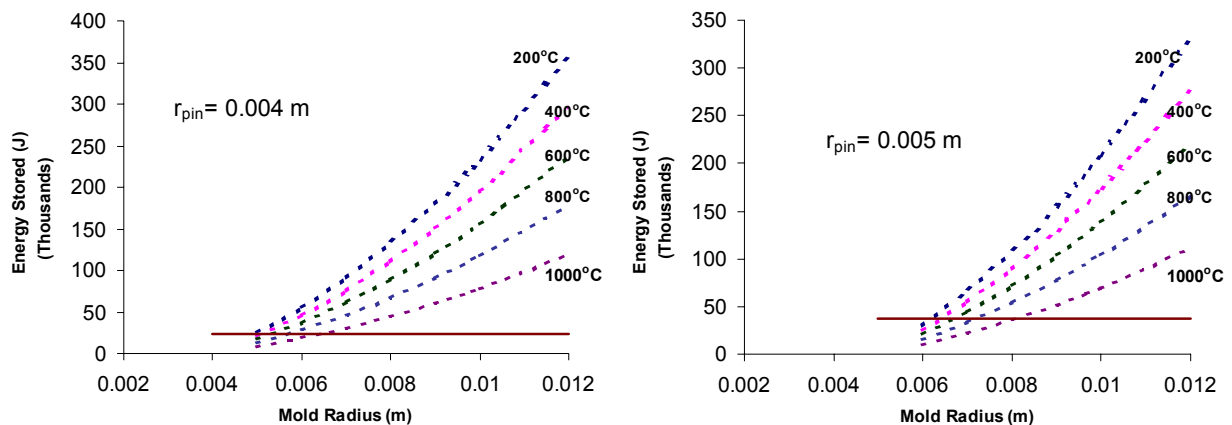


Figure 1 - Impact of mold preheat and fuel pin diameter on ability of mold to solidify all material in melt for 0.5 m fuel pin (properties for quartz glass are shown above, stainless steel and copper will also be evaluated).

1.2 Development of Mass Transfer Model

A model to analyze the transport of americium from the melt to the vapor phase above the crucible has been developed. The model considers mass transport in the melt, vaporization at the surface, and transport through the vapor phase. The greatest problem with the model is the uncertainty of the thermodynamic properties of the proposed ternary alloy. The details of the model and the specific quantities needed for the physical properties will be discussed.

The overall mass transfer coefficient is given by the equation:

$$\beta_{Am} = \frac{1}{\beta_m + \beta_v + \beta_g}$$

where

| | | |
|--------------|---|---|
| β_{Am} | = | overall mass transfer coefficient. |
| β_m | = | mass transfer coefficient in molten phase. |
| β_v | = | mass transfer coefficient across liquid to vapor (interface). |
| β_g | = | mass transfer coefficient for gas phase. |

Each of these mass transfer coefficients are evaluated from a thermodynamic point of view within the model. For example, β_v is sensitive to the vapor pressure of the americium in the gas phase and the equilibrium partial pressure of americium at a given temperature. In equation form this becomes:

$$\beta_m = K_L \varepsilon (P_e - P_g) \sqrt{\frac{M_i}{T_{ms}}} / C_{ms}$$

The equilibrium partial pressure P_e depends on the mole fraction, x_i , activity coefficient γ_i , and the equilibrium partial pressure of the pure substance, P_i^o , as shown below.

$$P_e = x_i \gamma_i P_i^o$$

Thermodynamic approximations are used to estimate γ_i to allow estimates for the thermodynamic properties. Parametric studies are underway to evaluate the impact of different properties or situations on the transport of americium from the melt.

1.3 Integration of Multiple Physics into Numerical Model

Work continues on the development of a detailed casting furnace model. Once completed, this model will be used to aid in the design of a new casting furnace. The design concept for this furnace will be detailed in the third year research efforts.

The model initially considers the effects of induction heating and heat transfer. The process for determining the induction heating field was discussed previously. The heat generation from induction heating is based on the calculation of two scalar fields S and C as shown below.

$$Q(r, z) = \frac{\sigma \omega^2}{2r^2} [S^2 + C^2]$$

The process for the overall calculations is outlined below:

- Define the geometry and mesh.
- Calculate the scalar fields S and C.

- Import these scalar fields into the heat transfer analysis to calculate the induction heating field.
- Perform the overall heat transfer analysis.
- Update the induction heating field as necessary.

This work is in progress and will be presented as part of the final report.

1.4 Review and Selection of Surrogate Materials

A preliminary analysis of potential surrogate materials has been completed. Manganese appears to be an acceptable surrogate material. Discussions will be held with Argonne National Laboratory staff members to insure there are no health and safety issues that prevent it from being used in future tests.

2. Research Objectives – Year 3

There are four research objectives for year 3 of this project. These objectives are to:

1. Continue to refine and assess americium transport issues through the use of a combined heat and mass transfer model of a representative furnace geometry.
2. Validate the model through comparisons to experimental tests. The model will be modified as necessary to make corrections to the modeling assumptions, or the model itself.
3. Perform a series of engineering analyses with the models to aid in the design of the next generation casting furnace. The outcome of these analyses will be design specifications for the preliminary design of a casting furnace.

By the completion of the research activities for year 2, a detailed model will exist for induction heating and heat transfer. Mass transfer will be incorporated into this model during year 3 along with fluid flow. Integrating as many of these physical phenomena as possible will aid in the assessment of what process parameters could be modified to decrease americium transport from liquid phase to vapor phase in the crucible.

In addition, the model will be validated by comparisons to other data in the literature and to experiments to be conducted by Argonne National Laboratory. Discussions with ANL researchers will be conducted to determine the type of tests that could easily be conducted in their existing skull crucible furnace. These discussions will also consider the type of data that can be easily collected for comparisons to the model.

A detailed model will be used for the preliminary design of an inductively heated skull-crucible casting furnace. This work will be carried out with the guidance and support of ANL-West staff. The ANL-West staff has experience with skull crucible furnaces.

3. Technical Impact

The AFCI program requires a non-fertile actinide form to serve as the “fuel” for the transmuted blanket. The currently proposed candidates for this fuel form still include a metallic alloy fuel, a cermet fuel, and a nitride fuel. Each of these candidates has been proposed based on known performance of the fertile fuel (i.e., uranium) analogue.

Of primary concern to the AFCI program is the requirement for fabrication of the selected fuel form in a remote, hot cell environment. The third year of funding for this activity will continue to develop a preliminary furnace design that can be built and tested with surrogate materials. The key to assessing the viability of metal fuels is in the ability to demonstrate fabrication in the presence of a volatile constituent.

The groundwork laid in years one and two of this project have developed a set of modeling tools to assist in the design of a realistic fabrication technique. The primary technical hurdle to overcome in the fabrication of a metallic alloy fuel is that of efficiently including the highly volatile actinide elements (i.e., americium).

As stated before, previous attempts at incorporating americium into metallic alloy fuels conducted at ANL on 1992 using standard injection casting processes resulted in the volatilization and loss of up to a half of the initial americium charge introduced into the melt. This magnitude of loss due to volatilization is unacceptable. More recent tests at ANL using arc melting have shown little or no americium loss occurs for short melt times. These recent tests prove the viability of using rapid melting technology such as induction skull melting for eliminating americium loss. Our goal is to assist in implementation of technology that will eventually be applicable to transmutation fuel fabrication on a production scale. This will be done by making an assessment of critical equipment and process variables required to build a successful system. In doing this, we will train students in the use of complex physics models related to the nuclear industry.

4. Research Approach

The proposed research is broken down into four specific tasks. These tasks are outlined below.

1. *Design of Skull Crucible Experiments:* UNLV researchers will work with ANL staff to design a set of basic experiments to aid in the validation of the models being developed here. Other simplified experiments will be considered as well.
2. *Refinement of Multi-physics Heat and Mass Transfer Model:* Work will continue in this area during year three. The model will be refined to be more realistic and to consider as many phenomena as possible. Comparisons to experiments or other results in the literature will be made whenever possible.
3. *Engineering Analyses for Preliminary Design of Furnace.* This effort will be carried out in conjunction with ANL-West staff. System throughput, processing rates, material handling, and other issues as necessary will be taken into consideration as the next generation casting furnace is developed.

4. *Reporting Requirements:* Monthly and quarterly progress reports will be completed and filed with the UNLV program office. Researchers will publish the results of this project at the appropriate technical conferences and journals. A final report will be compiled and submitted one month prior to project completion for review as well.

Dr. Clarksean's work has been crucial in developing an accurate model that properly represents the physics of the problem. His efforts have centered on working with the software developers at FLUENT in resolving and developing proper modeling techniques for the VOF method used within FIDAP for the accurate modeling of the flow. Properly modeling the flow, has led to more accurate heat transfer models.

In addition, Drs. Clarksean and Chen have developed and implemented an induction-heating model within FIDAP. This is a critical component in the complete analysis of the proposed casting furnace. To complete this work it was necessary to derive the governing equations in their proper form, develop a procedure that allows solution of the equations in rectangular coordinates, but at the same time allows for the results to be implemented into a cylindrical coordinate model. Proceeding in this fashion allows one code to be used for the calculation of the induction heating, fluid flow, and heat transfer.

Drs. Chen and Clarksean have been working to develop a detailed model of the mass transfer from the melt. This model is the critical component of the complete modeling process. The transport of americium from the melt to the surrounding areas is an important aspect of the project. Developing this model in a fashion that allows the mass transfer to be included along with all of the other important physics is difficult.

The complete model requires the solution of several sets of coupled equations. The equations include:

- Navier-Stokes equations for the flow of an incompressible fluid (two momentum and one continuity equation). These equations will eventually be coupled to the energy and induction heating equations (body force term).
- Mass transfer equation for the transport of americium.
- Heat transfer equation for heating and cooling of the melt material.
- A set of coupled second order partial differential equations for the real and imaginary parts of the induction heating equations (highly nonlinear and strongly coupled – stiff).
- Plus the setting of a number of important physical boundary conditions.

The solution of these equations is difficult numerically and very computationally intensive. Drs. Clarksean and Chen both have the knowledge and experience needed to attempt the solution of this complex problem. Limited research has been done on these complex materials processing problems. Drs. Chen and Clarksean will not only supervise and help graduate and undergraduate students to work on this research, but also serve as research engineers on this project to develop a preliminary furnace design for metallic fuel pins. Drs. Chen and Clarksean will also help graduate students to work on the experimental design associated with ANL-West facilities and staff in the third year.

5. Capabilities at UNLV and DOE Labs

Dr. Yitung Chen is Associate Research 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, 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 projects involving the study of flow and heat transfer and species transport in unsaturated porous media funded by DOE, the burning of rocket motors under the Joint Demilitarization Technology (JDT) program funded by DOD, Radiography Stockpile Stewardship Program funded by DOE, ATLAS project funded by DOE, JASPER project funded by DOE, high-level radioactive waste material repository design funded by DOE, high performance computing project funded by NSF, and atmospheric modeling funded by the NOAA Cooperative Institute for Atmospheric Sciences and Terrestrial Applications. He is also co-PI on an EPA project dealing with environmental monitoring for public access funded by EPA and a groundwater modeling project funded by DOE.

Dr. Darrell Pepper is Interim Dean of the College of 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 process modeling and the fuel casting process currently employed at ANL will provide a solid base from which to devise and evaluate new casting furnace concepts under the unique conditions that exist with volatile actinides. He is familiar with current casting furnace operations at ANL and has developed first order models of the system previously. Dr. Clarksean would serve as Co-Principal Investigator. 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, 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.

ANL-W has extensive experience in injection casting of uranium and plutonium alloys, having fabricated literally hundreds of thousands of metallic alloy fuel pins for irradiation in EBR-II using this process. Currently, two injection casting furnaces are in operation at ANL-W, and previous experimentation attempting to incorporate americium into U-Pu alloys has been conducted. This past experience has led investigators at ANL-W to hypothesize over the period of almost 10 years as to what process modifications or furnace design changes might improve the chances for successful melt casting of actinide alloys. The cooperation between the laboratories will provide a good working relationship to develop a solid approach to developing the next generation casting furnace for the AFCI program.

Extensive computing facilities exist for the 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.

6. Project Timeline with Milestones and Deliverables

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

