Appendix E
FCT Document Cover Sheet

Name/Title of Deliverable/Milestone	End of Year Report on S&T Engineering Analysis Accomplishments
Work Package Title and Number	ST Storage and Transportation Engineering Analysis – ORNL FT-13OR081001
Work Package WBS Number	1.02.08.10
Responsible Work Package Manager	John M. Scaglione John M. Scaglione (jvx) Digitally signed by John M. Scaglione (jvx) DN: c=US, o=U.S. Government, ou=Department of Energy, ou=Oak Ridge National Laboratory, cn=John M. Scaglione (jvx) Date: 2013.09.30 17:05:38 -04'00'
	(Name/Signature)
Date Submitted 9/30/2013	

Quality Rigor Level for Deliverable/Milestone	☐ QRL-3	☐ QRL-2	☐ QRL-1 ☐ Nuclear Data	☒ N/A*

This deliverable was prepared in accordance with Oak Ridge National Laboratory
(Participant/National Laboratory Name)

QA program which meets the requirements of
☒ DOE Order 414.1 ☐ NQA-1-2000

This Deliverable was subjected to:

☐ Technical Review

☐ Peer Review

Technical Review (TR)

Review Documentation Provided

☐ Signed TR Report or,
☐ Signed TR Concurrence Sheet or,
☐ Signature of TR Reviewer(s) below

Name and Signature of Reviewers

Peer Review (PR)

Review Documentation Provided

☐ Signed PR Report or,
☐ Signed PR Concurrence Sheet or,
☐ Signature of PR Reviewer(s) below

*Note: In some cases there may be a milestone where an item is being fabricated, maintenance is being performed on a facility, or a document is being issued through a formal document control process where it specifically calls out a formal review of the document. In these cases, documentation (e.g., inspection report, maintenance request, work planning package documentation or the documented review of the issued document through the document control process) of the completion of the activity along with the Document Cover Sheet is sufficient to demonstrate achieving the milestone. QRL for such milestones may be also be marked N/A in the work package provided the work package clearly specifies the requirement to use the Document Cover Sheet and provide supporting documentation.

LETTER REPORT

Reactor and Nuclear Systems Division

Project Title:	Storage and Transportation Engineering Analysis
Subject of Document:	Engineering Analysis Year End Status Report
Type of Document:	Letter Report
Authors:	J. M. Scaglione, B. Hanson, V. Tikare, M. Glazoff, J. Hales
Date Published:	September 30, 2013
Responsible Individual:	J. M. Scaglione, ORNL Work Package Manager

Prepared for the
Used Fuel Disposition Campaign
Fuel Cycle Research and Development (FCR&D) Program
Office of Nuclear Energy
DEPARTMENT OF ENERGY

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DEPARTMENT OF ENERGY
under contract DE-AC05-00OR22725

1. INTRODUCTION AND BACKGROUND

This letter report provides a summary of work performed supporting the Department of Energy-Office of Nuclear Energy (DOE-NE) Fuel Cycle Technologies Used Fuel Disposition Campaign (UFDC) under work breakdown structure element 1.02.08.10—Storage and Transportation (S&T) Engineering Analysis. In particular, this report fulfills the M4 milestone M4FT-13OR0810015, "End of Year Report on S&T Engineering Analysis Accomplishments." This report summarizes the FY 2013 S&T Engineering Analysis multi-laboratory efforts, including analyses of selected applications and plans for FY 2014.

The S&T Engineering Analysis control account was established in FY 2012 to apply and develop analysis capabilities to address the technical issues and data gaps associated with extended storage (ES) of UNF and transport of UNF following ES periods. The objectives of the S&T Engineering Analysis Control Account are to conduct analyses, integrate experimental data, and develop the technical basis for extended long term storage and subsequent transportation of used fuel. The analyses serve to augment and direct the experimental work as well as evaluate engineering design solutions that can be implemented to mitigate the amount and extent of experimental data needed. The scope of this work package includes the broad technical areas and associated regulatory requirements for ensuring the safety of UNF storage and transport, including used fuel characterization, materials, structural, thermal, radiation shielding/characterization, containment/confinement and nuclear criticality safety. FY13 activities under this WP include modeling to simulate hydride formation, distribution, and movement in Zircaloy cladding under thermal loadings during transfer and drying procedures. Also included are analyses to assess: actual loads that are imparted onto fuel assemblies/rods during normal conditions of transportation; realistic thermal profiles of used fuel and used fuel storage canisters to address in-situ storage system performance to better understand corrosion and stress corrosion cracking phenomenology; and development and application of uncertainty quantification methods to support understanding of specific parameter uncertainties and margins of safety.

2. FY 2013 ACTIVITIES AND STATUS

In the second year (FY 2013) of this multi-year S&T Engineering Analysis activity, efforts were devoted to development of improved understanding relative to establishing the technical basis for ES and subsequent transportation. The FY 2013 multi-laboratory team included Oak Ridge National Laboratory (lead), Idaho National Laboratory (INL), Pacific Northwest National Laboratory (PNNL), and Sandia National Laboratories (SNL), as well as representation and contributions from the Department of Energy (DOE).

The scope of the S&T Engineering Analysis Control Account for FY2013 included performing analyses related to the following technical gaps:

- Thermal Profiles (Rank 1)
- Stress Profiles (Rank 1)
- Drying Issues (Rank 6)
- Burnup Credit (Rank 7)
- Cladding H2 Effects: Hydride Reorientation and Embrittlement (Rank 7)
- Cladding - Creep (Rank 11)
- Cladding - Annealing of Radiation Damage (Rank 12)

Specific activities and milestones, and their associated status, for each of the laboratories that support the above scope are provided below.

2.1 OAK RIDGE NATIONAL LABORATORY

The work ORNL performed for the ST Engineering Analysis Control Account in FY2013 was broken down into three main areas:

1) **Activity FT-13OR0810012** *Quantify Sensitivities and Uncertainties in UNF Characteristics*
2) **Activity FT-13OR0810011** *Provide Strategy and Coordination for Control Account*
3) **Activity FT-13OR0810016** *Provide Source Terms to Support Thermal Analyses*

Deliverables completed in FY2013 are identified as follows with brief descriptions of the work provided below.

- M4FT-13OR0810013—Report documenting covariance data development
  Completed on schedule.
- M3FT-13OR0810014—Report quantifying sensitivities and uncertainties in UNF characteristics
  Completed on schedule.
- M4FT-13OR0810015—End of Year Report on S&T Engineering Analysis Accomplishments (this report)
  To be completed on schedule, 09/30/2013.
- M3FT-12OR0810031 Report on the Identification of specific applications for early analysis
  Completed 12/7/2012.
- A journal publication was prepared for consideration in a nuclear engineering journal, and will be submitted in early FY2014. Although not identified as a formal deliverable in FY2013, this publication represents a significant accomplishment as a result of some of the work being performed in collaboration between ORNL and the Swedish Nuclear Fuel and Waste Management Company (SKB) that operates the Swedish Central Interim Storage Facility for Spent Nuclear Fuel, Clab.

Quantify Sensitivities and Uncertainties in UNF Characteristics

Complete nuclear analyses of UNF engineering systems require calculations of the UNF quantities of interest and also the assessment of the uncertainties in those calculated quantities. Uncertainties in predicted UNF characteristics have relevance to decay heat for thermal analyses, radiation source terms relevant to geologic disposal considerations, and isotopic compositions relevant to burnup credit criticality analyses.

Under this activity, nuclear data and the computational tools necessary to implement an automated uncertainty analysis methodology for used nuclear fuel (UNF) calculations was developed, implemented, and tested. The uncertainty methodology is based on the stochastic (Monte Carlo) sampling of the uncertainties in the underlying nuclear data (cross sections, fission product yields, and nuclear decay data) used in computational models. This task required the development of new covariance (correlated uncertainty) data for the generation of fission products from fission and uncertainty data for nuclear decay (documented in milestone report *M4FT-13OR0810013*). This work was performed in collaboration with international nuclear data uncertainty activities. In addition to predicting uncertainties in calculated UNF properties due to nuclear data, the uncertainty tools developed under this activity also allow for the analysis of uncertainties in the design, dimensional, and operational information used in the models, enabling an assessment of manufacturing tolerances, dimensional distortions (e.g., changes during irradiation in the reactor) and other uncertainties associated with the reactor conditions. This activity expanded beyond the original scope of work to include implementing a prototype of the uncertainty toolset in the SCALE nuclear systems analysis code systems. This uncertainty quantification tool will be released publicly with the SCALE version 6.2 next year.

This capability can potentially reduce reliance on large-scale experiments to measure UNF properties and characteristics, the conventional approach used for code validation, by being able to quantify uncertainties for fuel designs and characteristics that lack the experiment data necessary for code validation. Also, UNF uncertainties for cooling times where no measurements exist, e.g., times of extended dry fuel storage, transportation, and final disposition, can be quantified using this physics-based methodology. This approach has the added benefit that the predicted uncertainties will often be smaller than those obtained by experiments since they are not subject to the sometimes large uncertainties in integral measurements. Smaller uncertainties will reduce the required margins for safety and positively impact the nuclear system performance, safety, and economic margins. The status of preliminary studies to develop nuclear data uncertainties and covariance files required for UNF uncertainty analysis and the initial implementation of these data in a methodology for uncertainty quantification for used fuel studies is documented in milestone report *M3FT-13OR0810014*.

Additional work has been proposed to move the uncertainty analysis toolset from a SCALE prototype to full production, and perform additional validation that could be used to support application of the uncertainty results in licensing applications. Specific development needs include: 1) refinement of the fission product yields covariance file to improve fission product uncertainty estimates, 2) update of the decay library uncertainty data formats, and 3) complete implementation of a parallel computational capability to speed up uncertainty calculations.

Provide Strategy and Coordination for Control Account

Work in this area is to ensure that the different activities of the laboratory staff members between the ST Experiments, Engineering Analysis, Transportation, and Demonstration projects are coordinated to facilitate consistency throughout the project, and to ensure that the data and models that are developed can actually be applied at some future time to support development of the technical justification for extended storage and subsequent transportation of all fuel, including high burnup fuel. In support of this activity area, the milestone, *M3FT-12OR0810031* was completed in FY2013. Multiple laboratories—Los Alamos National Laboratory, Oak Ridge National Laboratory, and Pacific Northwest National Laboratory contributed to the completion of this report that identifies early engineering analyses to evaluate potential near- and long-term solutions for demonstrating the safety of UNF during extended storage and subsequent transportation, and some inspection techniques that could be used for closing technical gaps if they can be effectively developed/deployed for in-situ measurements.   The FY2013 summary of activities is described in this report, milestone *M4FT-13OR0810015*.

Provide source terms to Support Thermal Analyses

The energy released from decay of radionuclides in UNF is an important design criterion for the thermal performance of engineering systems for transportation, pool storage, aging in extended dry storage, and ultimately repository disposition or reprocessing. The energy release rate, or decay heat power, during aging is simulated using modeling tools and nuclear data libraries that calculate the transmutation of nuclides during irradiation and the decay over the timescales relevant to the UNF system. Validation of these tools against experimental data is a critical activity that underpins the system design basis. The validation procedure establishes the accuracy of the calculations and the results are used to define the safety margins necessary UNF engineering systems design.

Under this activity ORNL collaborated with the Swedish Nuclear Waste Management Company (SKB) in an experimental project to perform calorimetric measurements on modern high burnup fuel assemblies that reside at the Central Interim Storage Facility for Spent Fuel (CLAB) in Sweden. More than 120 different full-length fuel assemblies were measured at CLAB. The assemblies include both PWR and BWR assemblies with burnups up to about 51 GWd/MTU and cooling times from 12 to 27 years after discharge from the reactor. The experimental data was used to validate calculations performed with the ORIGEN code, implemented in the UFD used fuel analysis tool to predict decay heat for COBRA cask analyses and nuclide compositions for KENO criticality calculations. The mean bias in the calculations was demonstrated to be <<1%, with uncertainties of ±1.2% for the PWR assemblies, and ±2.4% for the BWR assemblies evaluated. These results indicate that additional margins for safety associated with the modeling uncertainty are very small, and may lead to increased cask storage capacities and improved economic performance, and improve the flexibility in allowable fuels and storage configurations.

Additional work on this activity in FY2014 is recommended as additional measurements are planned at CLAB this year to include fuels with increased burnup, longer cooling times of importance to the design of fuel aging systems, and more modern BWR assembly designs. Continued collaboration with SKB will provide access to the measurement data and the fuel design and operating information necessary to benchmark the calculations. In addition, the SKB experimental program provides an opportunity to potentially obtain more reactor operating data, and measurement data beyond decay heat, such as the local radiation environment important to UNF aging.

2.2 IDAHO NATIONAL LABORATORY

The work Idaho National Laboratory (INL) performed for the ST Engineering Analysis Control Account in FY2013 was broken down into three main areas:

1) Providing thermodynamic calculations representing free energy curves for the Zr-H system. Composition range – between Zr and ZrH1.6 will be adequate for temperatures between 400 and 200 C.

2) MD (molecular dynamics) or other calculations including the PV (pressure – volume) term for the phase transition from Zr with dissolved H to ZrH1.6. This may require calculations to estimate the exact crystal structure of Zr and ZrH1.6.
3) Characterize morphology of the hydrides in the Zr. Identify the size and shape of the ZrH1.6 platelets at a couple of different precipitation stages.

One deliverable was completed in FY2013 and is identified as follows with a brief description of the work provided below.

- M4FT-13IN0810041—Status report on FY13 activities and proposed work for FY14
  Completed 9/11/2013.

Regarding zirconium-based alloys used as cladding materials for light water reactor fuels (LWR), efforts were expended in FY2013 to further develop the scientific understanding of the underlying material degradation mechanisms, both in working conditions and in storage of used nuclear fuel. The report—Modeling of Some Physical Properties of Zirconium Alloys for Nuclear Applications in Support of UFD Campaign—*M4FT-13IN0810041*, contributes to these efforts by constructing the thermodynamic models of Zircaloy-4 and Zircaloy-2 alloys, and providing the respective phase diagrams, and oxidation mechanisms. A special emphasis was placed upon the role of zirconium suboxides in hydrogen uptake reduction and the atomic mechanisms of oxidation. The thermodynamic properties of phases in the Zr-H system were used to support the Sandia National Laboratories hydride reorientation model development activities that are discussed in Section 2.4.

Proposed work for FY2014 is related to integration of the hydride precipitation and reorientation model developed by SNL into the MOOSE-BISON-MARMOT (MBM) suite of codes. Proposed activities are are provided as an attachment to this report.

2.3 PACIFIC NORTHWEST NATIONAL LABORATORY

The work PNNL performed for the ST Engineering Analysis Control Account in FY13 was broken down into four main tasks—Thermal Analysis, Thermal Sensitivity, Radiolysis Modeling, and Structural Sensitivity—to complete the following work scope:

1) Perform thermal analyses on the two additional DCSS that EPRI will inspect and compare model predictions with actual results. Exact dates of and whereabouts of EPRI inspections are not yet known. Perform analysis of Prairie Island HBU cask. Prepare two Level 3 reports, one for each system, but dates may change based on when EPRI performs the inspections.
2) Perform sensitivity analysis on the parameters within the thermal analysis of different DCSS to inform the S&T Experiments Control Account which data is most important and what has the largest impacts on cladding and system temperatures. Account for possible fuel relocation due to degradation in the thermal analyses. Prepare a Level 3 report.
3) Modify the radiolysis model prepared for the disposal cask and adapt to conditions during storage and determine if radiolytic degradation of cladding or DCSS components may be of concern. Prepare a Level 3 report.
4) Modify structural models to incorporate degraded materials properties and perform analyses for design basis seismic events, cask tipover, normal transfer/handling, and normal conditions of transport to determine if SSCs maintain their ability to meet safety functions. Prepare a Level 3 report.
5) Provide experimental statistical matrix design to minimize tests to be performed.

Deliverables completed in FY2013 are identified as follows with brief descriptions of the work provided below.

- M3FT-13PN0810025—Perform Sensitivity Analysis Report
  Completed 9/24/2013.
- M3FT-13PN0810022—Report on Inspection 1
  Completed on schedule.
- M3FT-13PN0810027—Radiolysis model report
  Completed on schedule.
- M3FT-13PN0810029—Modify structural models report
  Completed on schedule.
- M3FT-13PN0810023—Report on Inspection 2
  Delayed. Tracked in FY14 under milestone M3FT-14PN0810035 to be completed 3/28/2014.

Thermal Analysis

The purpose of the Thermal Analysis work package was mainly to support the Thermal Profiles gap that was ranked a priority 1 in the *Used Nuclear Fuel Storage and Transportation Data Gap Prioritization (*FCRD-USED-2012-000109). Since almost all degradation processes are temperature dependent, it is important to determine accurate and realistic temperatures and temperature profiles. Industry typically calculates temperatures assuming that a dry cask storage system is loaded at its maximum design basis heat load. In reality, systems have typically been loaded to less than 60% of the design basis, although that is expected to change with newer systems having better heat dissipation and because industry is now loading more and more high burnup fuel.

In FY13, the focus was supporting the in-service inspections organized by EPRI under the Field Demonstration control account. A COBRA-SFS model of the HI-STORM 100S-218 Version B storage modules of interest at the Hope Creek Nuclear Generating Station Independent Spent Fuel Storage Installation was developed and run. The model was used to predict the peak temperatures of various structures, systems, and components in the four systems of interest for inspection. Results using both ORIGEN decay heat predictions and decay heats predicted using the RG3.54 methodology were reported. The main focus of the results is on the axial temperature profiles of the canister outer shell. A draft of the pre-inspection model results had been provided to Hope Creek, Holtec, and EPRI for comment, which resulted in major reworking of the model because Hope Creek had not provided all the necessary parameters initially. All results were documented in the report *Preliminary Thermal Modeling of HI_STORM 100S-218 Version B Storage Modules at Hope Creek Nuclear Power Station ISFSI,* FCRD-UFD-2013-000297 in fulfillment of milestone M3FT-13PN0810022. This report was also provided to the industry partners to better guide their preparations for the actual inspection.

The inspection was originally scheduled for July2013, but has been postponed until November 2013 at the earliest. As such, the report documenting the final model and comparison against measured temperatures has had to be delayed. Milestone M3FT-13PN0810023 thus has been delayed until after this inspection occurs and will be tracked in FY14 under the Milestone M3FT-14PN0810035. Similarly, the EPRI-led in-service inspection of systems at Diablo Canyon has been delayed into FY14. To date, PNNL has not received any information to begin building the model for the Diablo Canyon inspection, but there is a possibility that inspection will occur in December 2013.

Thermal Sensitivity

Because of the importance of calculating accurate and realistic temperatures and temperature profiles over the period of extended storage, the thermal sensitivity task was initiated to examine how uncertainties in various parameters as well as changes in those parameters as a result of potential degradation over time would affect temperatures. The task was also created to help inform the Experiments control account of what parameters might need additional R&D.

Models for typical horizontal and vertical storage casks were used to calculate the temperatures and temperature distributions of various structures, systems, and components over a period of 300 years. These temperatures and distributions were calculated over a range of total initial decay heat load to show the wide range of temperatures that can be realized depending on the loading of the systems.

The sensitivity of component temperatures to

- degradation of the canister backfill gas from pure helium to a mixture of air and helium, resulting from postulated leakage due to stress corrosion cracking of canister welds
- uncertainties or changes in surface emissivity of system components, resulting from corrosion or other aging mechanisms, which could cause potentially significant changes in temperatures and temperature distributions and

- the effect of fuel assembly position with the basked cells on fuel cladding and basket temperatures in the canister

were examined using a computational fluid dynamics model of a site-specific NUHOMS module containing a 24P dry storage canister. The results are documented in the report *Thermal Performance Sensitivity Studies in Support of Material Modeling for Extended Storage of Used Nuclear Fuel,* FCRD-UFD-2013-000257 in fulfillment of Milestone M3FT-13PN0810025.

At lower heat loadings, many of the variations in the parameters have relatively small effects. Still, it was shown that for systems such as the one modeled, temperature gradients in the canister outer shell may be used to identify if leakage of helium has occurred. It was also shown that uncertainties in the emissivity of cladding, especially because it is unknown for high burnup cladding or for the newer cladding alloys, could result in significant temperature differences. The work showed some limitations of the CFD models. Follow-on work has been proposed to continue this work using the more robust COBRA-SFS model applied to both horizontal and vertical systems.

Radiolysis Modeling

The data gap analysis identified drying issues as a very high priority because there is little to no data on how much water might be left in a canister even after a successful drying campaign following approved procedures. Remaining water could result in corrosion or degradation of internal structures and the cladding. One concern was that radiolysis of water and water vapor remaining in the cask could result in flammable gas mixtures and has led some regulators, such as in France, to require monitoring of packages for hydrogen. Other concerns were raised as to whether radiolysis of water and water vapor exterior to the canister as drawn in by natural convection with the air cooling the canister could result in radiolytic products that would accelerate corrosion of the canister or concrete overpack.

The report *Radiolysis Model Sensitivity Analysis for a Used Fuel Storage Canister,* FCRD-UFD-2013-000357 was submitted in fulfillment of Milestone M3FT-13PN0810027. The model accounts for all of the reactions and kinetics of reaction of 40 radiolytic species, but did not account for any loss from reaction with canister components or fuel. Ignoring back reactions was shown to grossly overestimate the concentration of species of concern. The model predicts that hydrogen or hydrogen peroxide build up is not a concern unless large quantities of water remain. It is proposed to use the gas analyses from the Industry Demonstration to help refine and validate this model. However, there are no plans to continue this work in FY14.

Structural Sensitivity

The *Used Nuclear Fuel Storage and Transportation Data Gap Prioritization (*FCRD-USED-2012-000109) identified Stress Profiles as a priority rank 1 gap. Basically, this gap is a means to address external forces that act on structures, systems, and components (SSC) either during storage or transportation and determine if that SSC is still able to maintain its integrity and fulfill its safety function. It is also a means to determine how much degradation can occur before the SSC loses integrity or fails.

The FY13 scope for PNNL was to build a LS-DYNA model of a generic dry cask storage system to determine how it would behave under tip-over, handling drop, and seismic load cases. The focus was on the canister welds to determine if they would continue to maintain containment when subjected to these stressors. The results are presented in *Structural Sensitivity of Dry Storage Canisters,* FCRD-UFD-2013-000378 in fulfillment of Milestone M3FT-13PN0810029. It was determined that tip-over offers the strongest challenge to the containment boundary, although clearly vendor specific designs analyze for this design basis event and are licensed by the NRC. Still, the analysis showed that the behavior of welded stainless steel joints under high strain-rate conditions needs further examination. With the baseline and sensitivity cases built, potential follow-on work in this area would be to intentionally "degrade" a SSC (i.e., thinning the canister wall, having a small crack in the weld, etc.) and determine how much degradation could occur before the SSC failed. Similarly, this type of analyses could be applied to the canister internals with specific focus on the fuel assembly and cladding.

2.4 SANDIA NATIONAL LABORATORIES

The work SNL performed for the ST Engineering Analysis Control Account in FY2013 was related to model development to complete the following work scope:

1) Develop the modeling approach for assessment of hydride behavior in high burnup fuels.
2) Develop clad models for creep and annealing.

Deliverables completed in FY2013 are identified as follows with brief descriptions of the work provided below.

- **M3FT-13SN0810032—**Develop and write a roadmap for hydride precipitation *Completed 12/15/2012.*
- **M2FT-13SN0810031—**Report on methodology to estimate used fuel cladding hydride re-orientation during thermal excursions simulated during drying *Completed on schedule.*

The milestone, M3FT-12SN0810032, provides a five year plan on how the hydride reorientation modeling efforts for the different types of used fuel cladding will be conducted, and how the material property effects will be merged into a structural analysis code. This effort supports development of the technical justification regarding used fuel structural integrity after long term storage and under loads expected during normal conditions of transportation.

The report—Model for Simulation of Hydride Precipitation in Zr-Based Used Fuel Claddings: A Status Report on Current Model Capabilities—was completed to meet milestone M2FT-13SN0810031. This M2 deliverable documents the state of a meso-scale, microstructural evolution model for simulation of zirconium hydride precipitation in the cladding of used fuels during long-term dry-storage. The model developed in this work is a computational capability for the prediction of hydride formation in used fuel claddings. This document demonstrates a basic hydride precipitation model built on a hybrid of the Potts kinetic Monte Carlo and phase-field models. The capabilities incorporated are:

1. A realistic microstructure was generated for the Zircaloy-4 with both geometric and crystallographic texture.
2. The free energies of the two pertinent phases, alpha-Zr and, delta-$ZrH_{1.5}$ were calculated and incorporated into the hydride model. CALPHAD-type

thermodynamics calculations were used to generate free energy data for the Zr-H system with four phases, thematrix alpha-Zr and the three hydride phases gamma-ZrH, delta-$ZrH_{1.5}$, and epsilon-ZrH_2. The free energies of the two pertinent phases, a-Zr and, d-$ZrH_{1.6}$ were fitted to generate smooth free energy curves and incorporated into thehydride model. Furthermore, the chemical potential that drives the compositional and phase changes were up-graded in the model to simulate more complex materials with more components and more phases, as necessary, for future simulations.

3. The hybrid Potts-phase field model was modified to include crystallographic texture so that hydride precipitate nucleation andgrowth would occur along particular crystallographic directions.
4. The model can distribute nucleation sites in the microstructure to match known nucleation behavior. Nucleation is thought to occur at defects such as dislocation loops and near grain boundaries. These capabilities aredemonstrated in the model by treating the case of nuclei distributed randomly with uniform probability of occurring anywhere in the grains and preferentially occurring near grain boundaries.
5. Hydride precipitate growth in simulated in a stress-free claddings and one with a constant, uniaxial stress applied to shown that the hybrid model is capable of incorporating local micro-mechanical stress state.

Future work activities in this area are identified in the five-year plan provided as milestone M3FT-12SN0810032.

3. FY 2014 PLANNING

In FY2014, the Engineering Analysis Control Account will build upon the results and recommendations of the Modeling & Simulation and Experimental Integration task that was initiated in FY2013 to look at Normal Conditions of Transport (NCT) and expand it to design basis events and normal handling during storage to account for cumulative effects. It is expected that this work may include involvement in, and participation with international organizations and conferences that have particular impact with the UFD ST R&D objectives.

Technical gaps that will be addressed under the ST Engineering Analysis Control Account in FY2014 are:

- Thermal Profiles (Rank 1)
- Stress Profiles (Rank 1)
- Drying Issues (Rank 6)
- Cladding H2 Effects: Hydride Reorientation and Embrittlement (Rank 7)
- Cladding - Creep (Rank 11)
- Cladding - Annealing of Radiation Damage (Rank 12)

Given the list above, the overarching focus for the ST Engineering Analysis CA for FY2014 will be:

- Develop the framework to incorporate submodels for materials behavior
- Development of a model to assess hydride behavior in high burnup fuels

- Initiate uncertainty quantification (UQ) modeling methodology development
- Continue collaboration with industry on in-site storage thermal profiles
- Initiate annealing of radiation damage model development
- Continue analysis to characterize fuel response to normal conditions of transport and cumulative effects from extended storage

The planned FY 2014 activities and milestones for each of the laboratories supporting S&T Engineering Analyses are provided below. Note: the planning information below has been taken directly from the approved planning information in PICSNE.

Idaho National Laboratory

- **M4FT-14IN0810051** *Draft V&V strategy for hydride model integration into BISON* **10/1/2013 - 4/30/2014**
  Description: Develop an approach to show that the implementation of the hybrid model into BISON has been done correctly. Likewise, develop an approach to show that the integrated capability represents real phenomena.

- **M4FT-14IN0810052** *Demonstration of correct integration of hybrid model into BISON* **11/1/2013 - 6/30/2014**
  Description: Generate evidence (computational results) showing that the implementation in BISON gives similar answers as the native implementation.

- **M4FT-14IN0810053** *Future work planning* **4/1/2014 - 9/15/2014**
  Description: Draft development plan for inclusion of further capabilities. This could include mechanical strain due to volumetric changes associated with phase transformations, a list of possible future applications of the technology, additional V&V needs, applications for UQ, and other items as identified within the other ST work packages.

- **ActivityFT-14IN0810057** *Integration of reports into SNL M2 report* **5/1/2014 - 8/15/2014**
  Description: Iterate with SNL to integrate two M4 reports into SNL M2.

Lawrence Livermore National Laboratory

- **ActivityFT-14LL0810043** *Support UQ analysis* **10/1/2013 - 10/31/2014**
  Description: Support to UQ by performing analysis of the composition of available data (both experimental and numerical).

- **M4FT-14LL0810044** *Input to SNL report on composition of available data* **- 7/7/2014**
  Description: Input to SNL report

Oak Ridge National Laboratory

- **ActivityFT-14OR0810014** *Perform best estimate neutronics analysis of candidate fuel for high burnup demo* **10/21/2013 - 8/29/2014**

Description: Activity to develop best estimate neutronics models and results for thermal, dose, and radionuclide content of candidate high burnup demo fuel assemblies.

- **M4FT-14OR0810011** *Provide detailed thermal source terms for candidate fuel assemblies for high burnup demo to PNNL* **3/3/2014 - 3/31/2014**
  Description: Thermal source terms and distributions will be provided to PNNL for use in detailed thermal models in support of PNNL M2 deliverable on high burnup demo.

- **M3FT-14OR0810015** *Document neutronics analysis models for best-estimate calculations of high burnup fuel assemblies* **5/1/2014 - 6/20/2014**
  Description: Report documenting model development for best estimate neutronics models and results for thermal, dose, and radionuclide content of candidate high burnup demo fuel assemblies.
- **ActivityFT-14OR0810017** *Perform dose rate evaluation of high burnup demo fuel canister and cask system* **4/1/2014 - 8/29/2014**
  Description: Develop MAVRIC dose rate models for TN-32B canister system simulating transfer operations and after emplacement on storage pad.
- **M4FT-14OR0810012** *Status report on dose rate evaluation of high burnup canister system* **8/1/2014 - 8/29/2014**
  Description: Status report documenting state of model development and dose rate evaluation of TN-32B canister system during transfer and after emplacement on storage pad.

- **ActivityFT-14OR0810016** *Integration with other ST control accounts* **10/1/2013 - 9/30/2014**
  Description: Funding to cover overall project management, meeting attendance, planning, status reporting, and integration/interface activities with other ST work activities

Pacific Northwest National Laboratory

- **M2FT-14PN0810031** *Thermal profile analyses of in-situ industry storage systems identified for inspection.* **9/17/2014 - 9/17/2014**
  Description: This report will document the development and testing of a COBRA-SFS model of the TN-32B cask to be used for the Industry Demonstration project. The thermal analyses will be used to help identify which of the 37 potential assemblies should be loaded into the 32 spaces in the demonstration cask, identify sister pins for pre-test characterization, and help determine the location of thermocouple lances.

- **M3FT-14PN0810032** *Draft of M2 Report* **7/1/2014 - 8/20/2014**
  Description: Submit draft M2 report for comment.

- **ActivityFT-14PN0810033** *Integration with other Control Accounts* **10/1/2013 - 9/30/2014**
  Description: Integration with other Control Accounts

- **ActivityFT-14PN0810034** *Demo Thermal Analysis* **10/1/2013 - 6/27/2014**

Description: Perform posttest analyses for the Hope Creek inspection and write report (M3 deliverable from FY13 postponed because of the delay in the inspection)

- **M3FT-14PN0810035** *Hope Creek Analysis Report* **11/1/2013 - 3/28/2014**
Description: Hope Creek Analysis Report. Previously Fy13 M3FT-13PN0810023.

- **ActivityFT-14PN0810036** *Diablo Canyon Analysis* **11/1/2013 - 7/31/2014**
Description: Perform pre-test analyses and provide draft report to the industry team for comment for the third inspection (Currently planned to be Diablo Canyon)

- **M4FT-14PN0810037** *Pre-inspection report* **6/1/2014 - 7/31/2014**
Description: Submit pre-test thermal analyses report.

- **M3FT-14PN0810038** *Post-inspection report* **7/1/2014 - 9/29/2014**
Description: Perform posttest analyses and provide report on the third inspection.

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- **M2FT-14SN0810021** *Documentation of Hybrid Hydride Model for Incorporation into Moose-Bison and Validation Strategy.* **10/1/2013 - 8/15/2014**
Description: Documentation of Hybrid Hydride Model for Incorporation into Moose- Bison and Validation Strategy.

- **ActivityFT-14SN0810022** *Assess the best method for incorporating the hydride model into MBM. Verify and validate model in MBM* **10/1/2013 - 6/30/2014**
Description: Assess the best method for incorporating the hydride model into MBM - either as a new code or incorporated into an existing code. Identify verification exercises and verify hydride model in MBM. Identify validation exercises and necessary supporting experiments.

- **ActivityFT-14SN0810023** *Continue model development to improve simulation of the pertinent materials physics for hydride formation simulation* **10/1/2013 - 8/1/2014**
Description: Make the model higher fidelity.

- **M4FT-14SN0810024** *Draft of M2 report on integration of the hybrid hydride model into INL's MBM framework for review* **6/1/2014- 7/2/2014**
Description: Draft is for review by other labs and DOE

- **M4FT-14SN0810025** *Report on methodology to assess phenomena impacting UFD S&T R&D most highly* **- 9/15/2014**
Description: UQ methodology development to quantify degradation mechanisms during storage and transportation of high burnup fuels and rank the likely degradation mechanism while identifying data gaps associated with these

- **ActivityFT-14SN0810026** *Assemble multi-lab team and formulate approach for methodology development* **11/1/2013 - 1/30/2014**

Description: Identify team members from other labs and develop a framework for assessment of failure mechanisms.

- **ActivityFT-14SN0810027** *Develop and apply methodology for quantifying phenomena contributing to failure* **1/1/2014 - 9/15/2014**
  Description: Quantify likelyhood of failure by the different mechanisms.

4. SUMMARY

The S&T Engineering Analysis team has achieved considerable progress and significant accomplishments in FY2013 and expects to continue to do so in FY2014. Through the experiences gained over the first two years and a refined understanding of priorities, the inter-laboratory teams are working more closely together and will be able to be even more productive in FY2014 and beyond.

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July 30, 2013

John Scaglione
Project Manager, Hydride Formation in Zr-based Claddings
Oak Ridge National Laboratory
Oak Ridge, TN

Dear Dr. Scaglione:

This letter report provides an overall plan to integrate the hydride precipitation and reorientation model into the MOOSE-BISON-MARMOT (MBM) suite of codes. This plan fulfills a task required by the Roadmap for Developing a Computational Tool for Prediction of Hydride Precipitation and Reorientation during Long-Term Dry Storage.

Background:
The hydride precipitation and reorientation model uses a hybrid Potts-phase field method to simulate the precipitation of hydrides in zirconium-based cladding materials. The model is incorporated into SPPARKS, a Sandia-developed open-source framework designed as a particle-based kinetic solver. The code in the MBM suite that most closely matches the materials physics at similar time- and length-scales is MARMOT, a phase-field code that uses a finite element approach. Given the similarity between the hybrid model and MARMOT, the possibility of incorporating the hybrid directly into MARMOT becomes an obvious path forward to evaluate. The tasks suggested below follow this overall thinking.

Proposed Work:
Preliminary tasks consist of evaluating SPPARKS

1. Evaluate licensing issues associated with incorporating SPPARKS into the MBM suite. Address licensing issues for sharing the hydride code.
2. Download SPPARKS, compile, and test on INL hardware.

Determine the most effective method to incorporate hybrid capabilities into the MBM suite

1. Architectural options:
    a. Explore options for including Potts into MARMOT as a sub-model
    b. Create a new MOOSE-based application of Potts that couples to MARMOT
    c. Create a new MOOSE-based application that treats Potts and its hybrids exclusively

2. Architectural decision will be based on performance, flexibility and utility for a broad range of materials modeling capabilities necessary for hydride formation in Zr-based claddings:
    a. Assess the model capability by its ability to couple multi-physics at the meso-scale
    b. Evaluate the computational efficiency to determine the length- and time-scales that can be addressed

c. Determine flexibility to continue developing the model to incorporate and couple more materials physics
d. Evaluate ability to exploit the existing capabilities in the MBM suite

3. Design the framework for the architectural choice made:
    a. Potts model can become function(s) in MARMOT
    b. A coupled MARMOT – SPPARKS code or some variant of this
    c. A separate code that is based on SPPARKS or a variant of it

4. Outline a verification and validation strategy for the hybrid Potts-phase field capability in the overall MBM framework. The V&V plans will be integrated into the entire process from architecture selection to demonstrating the MOOSE-based hybrid capability.

5. Develop an updating strategy for the new capability:
    a. If SPPARKS-based, consider whether updates to the included SPPARKS code will be necessary. If necessary, provide a strategy to incorporate updates.
    b. If MARMOT-based, provide capabilities to continue to update capabilities as they are developed.

6. The final task to exercise the hybrid model on a demonstration problem will be contingent upon funds from a separate INL project. This task will consist of simulating growing hydride precipitates including the stress/strain induced by the volumetric change associated with the phase transformation.

Result:
Upon successful completion of the above work, a collaborative meso-scale materials modeling environment that combines the two leading microstructural evolution models with the vast capabilities of the MBM suite will enable the ability to simulate many materials processes that cannot be achieved by either of the leading models. It has the potential to then be used to study other phenomena (sintering, fission gas bubble formation and percolation, dynamic recrystallization thought to occur in the high burn-up rim region, component segregation and more).

Budget:
The estimated budget for the INL portion of this work in items 1 to 5 is $75k.

The estimated budget for the Sandia to support the entire effort from items 1 to 6 is $100k.

Sincerely,

Jason D. Hales

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Veena Tikare

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