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Aluminum Clad Spent Nuclear Fuel Task 3: Sealed and Vented Systems Episodic Breathing and Gas Generation Modeling Plan

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SUMMARY

This document presents the test plan for Task 3 of the *Aluminum Clad Spent Nuclear Fuel Long Term Dry Storage Technical Issues Action Plan*, which covers modeling and predictions of the generations of corrosive gases within both sealed and vented, subject to episodic breathing, storage systems. This includes aluminum clad spent nuclear fuel (ASNF) that is currently or may in the future be held in dry storage for an extended period. The overall objectives of the Task 3 modeling plan are to:

1. Comprehensively model the combined effects of episodic breathing in vented storage systems/canisters using INL INTEC CPP-603 facility as an example. Both bulk gas phase radiolysis reactions and aluminum cladding surface gas generation reactions will be included into a 3-dimensional computational fluid dynamics (CFD) model to model and predict long-term evolutions of the temperature and concentrations of corrosive gases within unsealed canisters subjected to episodic breathing.
2. Comprehensively model sealed and inert canister storage system using DOE standard canister as an example.
3. Closely integrate with Task 1 and Task 2 for identification of main gas-generation reactions and kinetics and provide simulation results back to Task 1 and 2 to further refine experimental designs.

This test plan lays out the technical activities that will be performed to achieve the test objectives described above. Simulations will be performed using the Idaho National Laboratory super computer Falcon.

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ACRONYMS

ASME	American Society of Mechanical Engineers
ASNF	Aluminum clad spent nuclear fuel
ATR	Advanced Test Reactor
CFD	Computational Fluid Dynamics
%RH	Percent relative humidity
HPC	High performance computing
LHS	Latin hypercube sampling
SNF	spent nuclear fuel
SNFWG	Spent Nuclear Fuel Working Group
SRNL	Savannah River National Laboratory

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1. INTRODUCTION AND OBJECTIVES

The possibility that radiolysis and corrosion in spend nuclear fuel storage canisters could result in the generation of hydrogen leading to flammability conditions and other corrosive gas species has be one of the main concerns associated with the long-term dry storage of aluminum-clad spent nuclear fuel (ASNF). Radiolytic species are generated at a rate that is determined by the dose rate and the concentrations of air and water vapor present. The temperature, vapor content (humidity), initial concentrations of gaseous species are the most important environmental factors that can have significant impact on radiolytic generations of corrosive species.

In addition, the physical and chemical behaviors of oxyhydroxide layers of ASNF fuels are also strongly influenced by the temperature, humidity and concentrations of gaseous species inside canisters. Hydration/dehydration of oxyhydroxides is strongly temperature dependent. Seasonal and daily temperature swings within the facility may impact corrosion by effecting the amount of moisture within the carbon steel canister. This is because internal temperature changes are reflected in changes of internal pressure that drives the transfer of gases and associated moisture in and out of the unsealed canisters. The net impact of this respiration on moisture within the canisters and its impact on corrosion is not fully understood yet.

Existing radiolysis model studies for used fuel storage canisters typically approximated the bulk compositions of the gas phase as a uniform system without accounting for localized hot spots and possible diffusive and convection flow. While such approaches might be valid for sealed canister where no mass/moisture transferring into and out from the sealed canister, they are inappropriate for the vented systems where processes such as episodic breathing of ambient air/vapor into the unsealed canister, diffusive/convective flow of gaseous radiolytic reaction products inside and outside the canister, and heat transfer are tightly coupled together, leading to a strongly nonlinear multiphysics problem.

Understanding the combined effects of such coupled episodic breathing and radiolytic generation of corrosive gases on the long-term dry storage of ASNF fuels requires detailed multiphysics computational fluid dynamics (CFD) modeling and long-term predictions of the spatial-temporal evolutions of the temperature field, moisture content (humidity/%RH) field, concentration fields of gaseous species both inside and outside canisters.

The activities performed in this Task are based on work performed by the Aluminum-Clad Spent nuclear Fuel Sub Working Group captured in the document *Aluminum Clad Spent Nuclear Fuel: Technical Considerations and Challenges for Extended (>50 Years) Dry Storage* [1]. Following this report, an action plan was formulated to address five areas where additional knowledge was needed to understand the implications of long-term ASNF interim dry storage, as outlined in the *Aluminum Clad Spent Nuclear Fuel Long Term Dry Storage Technical Issues Action Plan* [2]. The objectives of Task 3 and approach for the test plan are provided below.

1.1 Modeling Task Objectives

Task 3 attempts to comprehensively model the combined effects of episodic breathing (in the vented canisters) on extended dry-storage of unsealed and vented canister storage systems using Idaho National Laboratory's (INL's) INTEC CPP-603 as an example with the radiolytic gas generations on the aluminum clad, oxide layers, canister, and other system components. Diffusional and convective exchanges of reactive gaseous species and heat inside the canister with ambient air induced by episodic breathing in vented, unsealed storage system will shift the chemical equilibrium conditions inside the canister and affect the amount of radiolytic production of corrosive gases. The main concern with vented storage is the potential loss of cladding structural integrity due to cladding corrosion induced by chemical and radiolysis driven processes.

This modeling task will closely interact with Tasks 1 and 2 to identify the main gas-generation reactions and kinetics under both sealed (using the U.S. Department of Energy [DOE] standard canister as an example) and vented systems (using INL INTEC CPP-603 as an example) and implement radiolytic reactions into the canister-scale multiphysics CFD models for predictions of long-term evolutions of the concentrations of corrosive gases and moisture contents inside and outside canisters. The simulation results will be passed to task teams 1 and 2 for guiding their experimental designs.

Coupling episodic breathing and radiolytic production of gases with the CFD convective and diffusive transport models would help to better understand knowledge gaps in the storage system for any given design of canisters, storage configurations, and ambient air conditions, by answering the flowing questions:

- What are the detailed temperature field inside and outside canisters in both vented and sealed systems?
- What are the detailed water vapor concentration field and spatial-temporal evolutions inside and outside of canisters?
- What are the detailed concentration fields of H_2, O_2, N_2 and radiolytically generated corrosive products such as HNO_3, CO, N_2O and NO_2 inside and outside of canisters over an extended period of storage time?
- What is the correct amount of condensed water and spatial-temporal evolutions on the surfaces of carbon steel canister and aluminum cladding?

1.2 Task Description

The modeling work performed by this task will be primarily done in the CFD code STARCCM+, developed by Siemens/CD-Adapco. The code has the advantages that its transient solver is an implicit integrator with a segregated solver which allows for solving of the velocity fields with a pressure projection method. The implicit integrator in a segregated set up also allows for easy integration of the steady state flow characteristics into a transient simulation, as well as decoupling of the flow solver from thermal and chemical species equations, which allows for longer timesteps than could be obtained with a fully coupled implicit method, or timesteps obtained with an explicit solver due to CFL requirements. The full task description is broken down into 5 separate tasks to develop and refine the model from an early thermal-convective flow model to coupling kinetic reactions for long-term chemistry modeling, to full sensitivity studies, ending with a coupled model describing the full CPP-603 facility. The models break down into two distinct scales – canister scale modeling, and facility scale modeling.

1.2.1 Canister-Scale Conceptual Models

Two canister-scale CFD models will be developed in this project, one for the sealed canister storage system using DOE standard canister as example and one for the unsealed canister using INL INTEC CPP-603 facility as example. Development of canister-scale conceptual models includes: geometries of canisters and representative fuel packing configurations; define representative initial storage conditions (i.e., infill gas compositions, temperature); define decay heat loading rates (lower-limit, average, upper-limit); define initial bulk gas phase radiolysis reactions and kinetics (starting from the literature and improve from outcomes of other tasks); define surface gas generation reactions and kinetics on gas/Al cladding interface; define sensitivity simulation scenarios with various combinations of load configurations, heat loadings and limiting reaction rates; milestone report.

1.2.2 3D Canister-Scale Multiphysics CFD Models for Sealed Canisters

Development of 3-dimensional canister-scale multiphysics CFD models for modeling coupled gas flow-heat transfer-radiolysis reactions processes within sealed canisters, using DOE standard canister as model system: create 3D mesh with full geometrical complexities of loaded canisters; implement kinetic reaction models (both bulk gas phase and surface reactions as defined in the conceptual models) into the numerical model; preliminary model sensitivity runs for sealed canisters based on the sensitivity simulation scenarios defined in M3.1; pass sensitivity simulation results to other tasks for determining environmental constraints to experimental studies; milestone report.

1.2.3 3D Canister-Scale Multiphysics CFD Models for Vented Systems

Extending the canister-scale multi-physics CFD model for sealed canisters to vented system as seen in INL INTEC CPP-603 facility: define venting scenarios and ambient air conditions (in close interaction with Task 4); implement boundary conditions to allow exchanges of mass/heat between inside and outside of the canisters; milestone report.

1.2.4 Improve CFD Models Including Comprehensive Sensitivity Studies

Improve canister-scale multiphysics CFD models for both sealed and vented canisters and perform comprehensive sensitivity studies: implement new radiolysis reaction models and kinetics identified from other tasks (Task 1 and 2 in particular); refine model sensitivity simulation scenarios (for both sealed and vented systems); model validations with new existing and new experimental results; compressive sensitivity studies; milestone report.

1.2.5 Develop 3D Facility-Scale Coupled Multiphysics CFD Model

Develop 3D facility-scale coupled multiphysics CFD model for predicting spatial-temporal evolutions of temperature and corrosive gas concentrations (including vapor concentrations) over extended period of storage time, milestone report. This storage facility-scale CFD model provides physics-based predicative capability to guide facility designs/ optimizations and support the assessment of the performance and degradations of the fuel or canister in a range of environments.

2. ASSUMPTIONS AND RISKS

2.1 Assumptions

The modeling plan will cover a range of conditions relevant to INL INTEC CPP-603 dry storage facility. Ambient temperature conditions are important for assessing model boundary conditions. For the initial modeling, ambient temperature conditions that were assumed from EDF-2760 [3] will be used as bounds for the unsealed and vented storage system. This same document also outlines the maximum temperature to occur within the rack under an assumption of completed ventilation shut off, this value will be assumed as the maximum ambient temperature for modeling. The storage configurations for sealed DOE standard canisters are based on DOE/SNF/REP-011-Vol 1.1 report [4] and INL/EXT-07-12326 report [5].

The report specifying the decay heat of the ATR assemblies, EDF-10891, is correct for characterizing the range of decay heat to use in the modeling [6]. This EDF relies on the correctness of the shipper's fuel data, which cannot be verified upon receipt of the fuel. Using this characterization, the range of decay heat that is utilized in modeled is from one standard deviation below the mean to two standard deviations above the mean, this is assumed to cover the variation necessary across all the relevant SNF.

For modeling the cases over long periods of time, the CFD flow fields will be assumed to be quasi-steady state over prolonged periods such that large timesteps can be taken with respect to chemical species and thermal transport equations. This should be valid as the decay heat for the ATR fuel assemblies, as well as the response time of the ambient air conditions for the facility are of long time scales when compared to the recirculation within a canister. CFD fields are updated as necessary as chemical species & thermal fields are evolved.

2.2 Risks

The assumptions made on bounds of decay heat range, ambient temperature range, moisture content range and other pertinent modeling parameters will be on the conservative side of estimates in order to mitigate risk from utilizing any model predictions for actual storage scenarios.

3. SIMULATION DESCRIPTION

3.1 Simulations

This section defines the sets of simulations used to perform work scope described in Section 1. We envision that the developments of canister-scale models for both sealed and unsealed storage systems will be an iterative process, i.e., the initial model inputs used to construct the canister model, such as packing configurations, thermal loads, dose rates, reaction chemistry and rates, will be repeatedly updated when new data are obtained from all other experimental tasks, Tasks 1 and 2, in particular. In addition, the experimental results will also provide important model validation data by comparing the simulated and measured concentrations of reactive species. In addition, the measured data under Task 4- Performance of ASNF in Dry-Storage, such as in-canister temperature and gas species concentrations, will provide additional model validation data to calibrate the canister model. The calibrated and validated canister models will then be used for long-term predictions.

3.1.1 Sealed Canister Model

The sealed canister model is the first step of the development. The initial model of sealed canisters will consist of modeling the standard DOE 15-foot canister filled with 3 Type 1a baskets containing 30 ATR fuel assemblies. Constructing this model requires identification of representative ambient air conditions, identification of heat source terms as a function of fuel type, configuration, age, and storage history, identification of dosage of fuel types, configuration and storage history, identification representative of radiolysis reaction pathways and ranges of reaction models and parameters. The initial reaction model will focus on simplifications of the chemistry assuming that canisters are properly backfilled and the only gas present is Helium and trace water vapor, based on DOE/SNF/REP-104 report [7]. The construction of the canister-scale high resolution CFD models for the coupled heat/mass transfer and radiolysis reactions within the full geometry pack will rely heavily on utilizing INL's high-performance computing (HPC) resources. A preliminary diagram of the sealed canister model is shown in Figure 1.

Figure 1. Initial representation of sealed canister model.

3.1.2 Vented Canister Model

The vented canister model is the second step of the development. The initial model of vented canisters will consist of modeling the standard IFSF canisters with mixed ATR4/ATR8 buckets filled with ATR fuel assemblies. Other geometrical packings for ATR fuel assemblies or other fuel assemblies will be modeled as needed. Constructing this model requires identification of representative ambient air conditions, identification of heat source terms as a function of fuel type, configuration, age, and storage history, identification of dosage of fuel types, configuration and storage history, identification representative of radiolysis reaction pathways and ranges of reaction models and parameters.. The construction of the canister-scale high resolution CFD models for the coupled heat/mass transfer and radiolysis reactions within the full geometry packing will rely heavily on utilizing INL's high-performance computing (HPC) resources. The model for the vented canister will expand on the chemistry model used for the sealed canister model to include radiolysis and other chemical reactions occurring with the addition of air (N_2/O_2) and CO_2 into the system. A preliminary diagram of the vented canister model is shown in Figure 2.

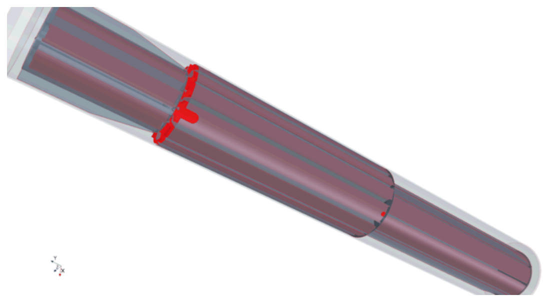

Figure 2. Initial representation of vented canister model.

3.1.3 Sensitivity Studies and Feedback of Other Tasks

Based upon the feedback of the other tasks which are studying the chemical reactions more in-depth, the kinetic chemical reaction modes that was built for the first two subtasks will be expanded upon and improved here to account for deviations from literature data as well as sufficient surface reaction data to characterize the problem. Sensitivity studies will determine the most pertinent parameters affecting the model outputs such as peak cladding temperature and maximum concentration of corrosive chemical species. If time permits, the sensitivity studies will also characterize a Latin hypercube sampling LHS study to determine cross-correlation effects between model input parameters.

3.1.4 Facility Scale Model

A facility scale CFD model will be developed representative of the CPP-603/IFSF building. This model will account for couple heat transfer, air flow, moisture changes within the entire storage facility for an array of canister conditions, with canister simplified as heat/mass volumetric source/sink terms for decay heat and reaction induced species. The important outcomes of such a facility scale CFD model include – detailed temperature and humidity fields with in the storage facility under various venting scenarios including daily/seasonal fluctuations, spatial variations of temperature and humidity within the storage facility under various venting scenarios, and predicted concentrations of various gas species – including radiolysis-generated corrosive gas species – at the venting outlets. A preliminary diagram of the facility layout to be modeled is shown in Figure 3.

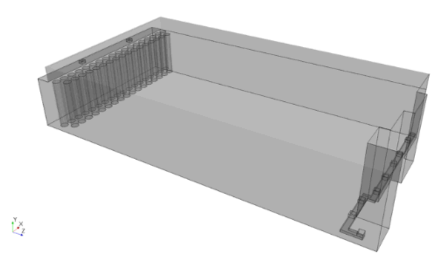

Figure 3. Facility preliminary geometry representation.

4. REQUIREMENTS

4.1 General

Model grid convergence and verification testing should be completed. Grid convergence to assess the uncertainty in the model from the size of the mesh, and verification of the kinetic model implemented into a test case of the CFD code conforming to the expected 0D result.

5. ENVIRONMENT, SAFETY, AND HEALTH

None.

6. QUALITY ASSURANCE AND DATA/RECORD MANAGEMENT

Quality assurance activities associated with Task 3 comply with all applicable requirements set forth in the INL Quality Assurance Program based on ASME NQA-1 2000. The software that is utilized, STARCCM+, has been shown by the software provider, Siemens, to meet ASME NQA-1 criteria. Final sets of simulations will be kept on the Falcon supercomputer storage drive as needed for reference to the data sets.

7. SCHEDULE

Table 1 provides the schedule for subtasks by quarter. The areas highlighted in blue indicate where that part of the project has scheduled activities. Descriptions of the subtasks are provided in Section 1.2.

Table 1. Schedule of activities by quarter.

Sub task #	Subtask	FY18 Q2	FY18 Q3	FY18 Q4	FY19 Q1	FY19 Q2	FY19 Q3	FY19 Q4
Task 3: Sealed and Vented System Episodic Breather and Gas Generation Prediction								
3.1	Canister-scale conceptual models.							
3.2	3D canister-scale multiphysics CFD models for sealed canisters.							
3.3	3D canister-scale multiphysics CFD models for vented canisters.							
3.4	Improve CFD models including comprehensive sensitivity studies.							
3.5	Develop 3D facility-scale coupled multiphysics CFD model.							

8. REFERENCES

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