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Problem Specification for FY12 Modeling of Used Nuclear Fuel during Extended Storage

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Reactor and Nuclear Systems Division

PROBLEM SPECIFICATION FOR FY12 MODELING OF USED NUCLEAR FUEL DURING EXTENDED STORAGE

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1. BACKGROUND

The Nuclear Energy Advanced Modeling and Simulation (NEAMS) program of the Advanced Modeling and Simulation Office (AMSO) of the US Department of Energy, Office of Nuclear Energy (DOE/NE) has invested in the initial extension and application of advanced nuclear simulation tools to address relevant needs in evaluating the performance of used nuclear fuel (UNF) during extended periods of dry storage. There are many significant challenges associated with the prediction of the behavior of used fuel during extended periods of dry storage and subsequent transportation [1]. The initial activities are focused on integrating with the Used Fuel Disposition (UFD) Campaign of the DOE/NE and a demonstration that the Advanced Multi-Physics (AMP) Nuclear Fuel Performance code (AMPFuel) [2–4] for modeling the mechanical state of the cladding after decades of storage.

This initial focus will model the long-term storage of the UNF and account for the effect, and generation, of radially and circumferentially oriented hydride precipitates within the cladding and predict the end of storage (EOS) mechanical state (stress, strain) of the cladding. Predicting the EOS state of the cladding is significant because it (1) provides an estimate of the margin to failure of the cladding during nominal storage operation and it (2) establishes the initial state of the fuel for post-storage transportation. Because there are significant uncertainties associated with the storage conditions, hydride precipitate formation, and the beginning of storage (BOS) condition of the UNF, this will also allow for the development of a rigorous capability to evaluate the relative sensitivities of the uncertainties and can help to guide the experimental and analysis efforts of the UFD Campaign.

This document is focused on specifying the problem that will be solved with AMPFuel. An associated report [5], documents the specifics of the constitutive model that will be developed and implemented in AMPFuel to account for the presence and predict the generation of the hydride precipitates. This report satisfies the deliverable for the DOE Office of Nuclear Energy, Advanced Modeling and Simulation Office, milestone M3MS-12OR0605083, "Definition of Problem Specification," which defines the problem to be solved that will satisfy milestone M2MS-12OR0605081, "Demonstration of the Advanced Multi-Physics (AMP) Nuclear Fuel Performance code for modeling UFD."

2. HIGH-BURNUP NUCLEAR FUEL ROD SPECIFICATION

The BOS state of the fuel assembly is dependent upon the specifics of the fuel rod, the irradiation history, wet storage conditions, and drying. To establish a baseline rod specification, we will utilize a pressurized water reactor (PWR) fuel rod that was part of a high-burnup demonstration program between Carolina Power and Light Co. (CP&L) and the fuel vendor, Framatome-ANP Richland, Inc. Twelve high-burnup rods were provided to the US Nuclear Regulatory Commission (NRC) for use in an extensive program of experiments at the Argonne National Laboratory for accident and long-term storage analysis.

2.1. FABRICATION AND IRRADIATION HISTORY

The particular rod used as the baseline for this report (A02 of Assembly S-15H) was irradiated in CP&Ls H.B. Robinson plant for seven cycles with a discharge burnup of 66.7 GWd/MTU (rod average).

The information in this section is primarily based on Reference [6].

The specifics of the as-fabricated state, core-average irradiation conditions, and cycle-specific irradiation conditions are provided in Tables 1, 2, and 3, respectively.

To provide supplemental information regarding the discharge internal pressure and the heat transfer through the fuel-clad gap, each of which have a significant impact on the thermo-mechanics of the fuel rod during storage, an Scale/ORIGEN-S simulation was performed to define the total fission gas generation. Reference [6] specifies a total fission gas release of 2.4%, which allows for an accurate specification of the total fission gas constituents in the plenum. Therefore, the fission gas concentrations generated and in the plenum are defined in Table 4.

Additional relevant information regarding Rod A02 of Assembly S-15H includes an average clad outer diameter of 0.4208 in (0.424 with the oxide layer included) and an oxide layer that varies from 43 to 115 μm.

2.2. BEGINNING-OF-STORAGE SPECIFICATION AND UNCERTAINTIES

The preceding section provides sufficient information to perform a single-rod fuel performance calculation to determine the discharge state of the fuel rod at 66.682 MWd/kgU. However, the report upon which it is based [6] refers to a supplemental core physics simulation that was used to model the entire core and provide estimates of the neutronics, power, and coolant state throughout the life of the fuel. In addition, we do not have specifics on the wet-storage or drying conditions. Rather than attempt to reproduce this work, we will specify some characteristics of the discharge state of the fuel.

From reference [7], it is clear that there are several significant factors that have a significant impact on the EOS state of the cladding. For these particular fields, we will specify their baseline values in this document, along with a range of uncertainty, so that a sensitivity study may be performed to determine the significance of their uncertainties. These baseline values and uncertainties were derived from reference [7].

The total hydrogen concentration in the cladding will affect the formation of hydride precipitates. Because the discharge burnup is 66.682 MWd/kgU, we will assume the mean wall thickness average hydrogen content in the cladding is 750 parts per million (wppm) with an uncertainty of +/-20%.

The BOS is defined as the time that immediately follows the drying stage of the fuel, which can contribute significantly to the concentration of radial hydrides and for which there is great uncertainty. In this report, we will assume a baseline of 100 wppm of radial hydride precipitates throughout the cladding with an uncertainty of +/-50%.

The circumferential hydrides form during irradiation, when the cladding is under compressive stress, but some can go into solution during the drying process as the cladding exceeds 400^{o}C. The hydrogen solubility limit in Zircaloy-4 at 400^{o}C is 210 wppm [7]. Therefore, we will assume that there is 300 wppm of circumferential hydride precipitates at BOS with an uncertainty of 75%.

Because of the internal pressure of the fuel rod, the cladding will creep out, which will increase the free volume in the tube and reduce the stress on the cladding, which is a major component of radial hydride precipitate formation during storage. However, the internal pressure is computed with a wide range of models in fuel performance codes and is sensitive to many factors during irradiation at the current state of the rod. Therefore, we will assume a baseline rod internal pressure of 4 MPa with an uncertainty of 10%.

2.3. DRY STORAGE CONDITIONS

The length of time that used fuel remains in dry storage is uncertain. Therefore, this study will establish a baseline storage condition and include a range of conditions. Once defined, there will likely be a small

Table 1. As-Fabricated Specification of the Representative Nuclear Fuel Pin

Region	Geometry	Unit	Value
Pin Specification	Pitch	in.	0.563
	Pin Height	in.	152
Clad Specification	Clad ID	in.	0.364
	Clad OD	in.	0.424
	Material		Zry4
End-Cap Specification	Height	in.	0.4
	Depth	in.	0.2
	Outer Diameter; extended	in.	0.3615
Fuel Specification	Fuel Height	in.	144
	Fuel Diameter	in.	0.3565
	Dish Volume (2 per pellet)	%	1
	Chamfer Volume		None
	Effective Fuel Volume	cm^3	230.9
	Material		UO_2
	Theoretical Density	g/cm^3	10.96
	Fraction of Theoretical Density	%	94
	Fuel Mass	kg[UO_2]	2.378
	Fuel Mass	gU/m	573.2
	Number of Pellets		527
	Effective Pellet Height	in.	0.27325
	Pellet Mass	g[UO_2]	4.51
	^{235}U Enrichment	wt%	2.9
	Open Porosity	%	<0.1
Insulator Specification	Insulator Height	in.	0.2
	Insulator OD	in.	0.3565
	Material		Al_2O_3
Spring and Plenum Specification	Material		Alloy 718
	Plenum Height	in.	6.8
	Plenum-to-Spring Volume Ratio		5.2
Fill Gas Specification	Material		^4He
	Helium Volume	cm^3	14.83
	Pressure	MPa	2
	Helium Mass	g	0.04715
	Helium Density	g/cm^3	0.00318
Grid Spacers	Number		7
	Height	in.	2.25

Table 2. Core Operational Description of the Irradiation

Region	Unit	Value
Coolant Pressure	MPa	15.5
Inlet Temperature	K	559.6
Outlet Temperature	K	590.5
Number of Cycles		7

Table 3. Cycle-Specific Operational Description of the Irradiation

Cycle Number	Length (Days)	Power (kW/ft)	Burnup (MWd/kgU)
1	302	6.8	11.8
2	310	6.2	22.8
3	307	5.9	33.1
4	296	4.8	41.3
5	305	4.3	48.8
6	392	4.3	58.4
7	393	3.68	66.682

Table 4. Fission Gas Distribution at Fuel Discharge

Constituent	Generated (g/kgU)	Released (g)
Xe	10.99	0.5528
Kr	0.591	0.0297
He	0.013	0.0007

uncertainty in these conditions during nominal operation of the facility, but assessing the sensitivity of the EOS state of the cladding to the particular storage conditions can assist in guiding the Campaign. 10 CFR 72.42(a) allows an initial license period of up to 40 years and license extensions of up to 40 years. This is combined with the NRC Waste Confidence Rule (10 CFR 51.23) that states that the Commission has confidence that fuel can be stored safely (wet or dry) for at least 60 years beyond the licensed life of the reactor without significant environmental effects. For a reactor that had an initial operating license of forty years and was granted a 20 year extension, this means the NRC has confidence that fuel can be stored for a total of up to 120 years. In addition, for its Generic Environmental Impact Statement to support the Waste Confidence Rule, the NRC is analyzing behavior up to 300 years. The baseline length of storage will be 200 years, with an uncertainty of +/-50%.

The cask heat transfer is a complex combination of conduction, natural circulation, and radiative heat transfer, which has been studied in other reports, but depends upon the ambient temperature of the final heat sink, which will have uncertainty based on the location of the facility and weather. Therefore, we will assume a baseline backfill coolant temperature, that is constant throughout the length of storage, of 350 K, with an uncertainty of 10% and a pin-to-backfill heat transfer coefficient of 1000 W/m^2-K, with an uncertainty of 50%. The baseline backfill pressure be assumed to be at atmospheric pressure.

3. DRY STORAGE SIMULATION

The physics occurring during the long-term dry-storage of nuclear fuel assemblies includes neutronics, heat transfer, and mechanics. The neutronics includes the heat generation based on radioactive decay (alpha, beta, and gamma), which is deposited locally (alpha and beta) and globally (gamma). The heat transfer component includes the thermal conduction within the structural and fuel components as well as the cooling of the fuel rods and structural components by conduction, convection, and radiation to the helium backfill and structural components. The mechanics of the system must account for the long-term creep of the materials due to thermal, mechanical, and gravity loadings. In addition, the microstructural changes that are occurring within the materials must be accounted for in the continuum-level constitutive models. The constitutive models used in the cladding for this analysis will be developed by Sandia National Laboratories and are described in detail in references [5, 7].

This section will describe the particular assumptions used in the modeling of the H.B. Robinson fuel rod during long-term storage. The initial (BOS) and boundary conditions were described in the preceding section.

3.1. GEOMETRIC DESCRIPTION

This initial evaluation will be modeling the thermo-mechanics of a single fuel rod over several decades. The geometric complexity of the fuel assemblies and storage cask will be neglected. For science domains for which the coupling is dominated by global (beyond a single pin) factors, such as fluid dynamics and gamma heating of the structures, will be neglected until this initial demonstration has been completed.

3.2. TIME INTEGRATION

Because of the extremely slow variation of the heat source and material properties with time, the fuel rod will be accurately modeled with a quasi-static approximation for all physics. The creep will be modeled with a implicit approximation, which will allow for a mesh refinement evaluation in time to determine the mesh independence of the solution.

3.3. HEAT SOURCE

The initial conditions for the decay-heat source term will be defined by the activities listed in Table 7-3 of reference [6]. The decay of these isotopes and heat generation will be modeled using the ORIGEN-S code within AMPFuel. For this initial study, it will be assumed that all of the heat is deposited locally (including gamma). Future analyses will need to consider the transport of photons to the assembly and cask structural materials.

3.4. HEAT TRANSFER

The conduction within the fuel, across the gap, and through the cladding will be modeled using standard finite-element technology. The thermal conductivity of the cladding and fuel will use the standard model for Zircaloy-4 and UO_2 fuel within AMPFuel, with a static burnup of 66.682 MWd/kgU. The gap heat transfer coefficient will be defined using a model derived from FRAPCON, which accounts for the gap pressure, temperature, gas constituents, gap thickness, and surface temperatures. The coolant will be modeled as a static temperature with a static heat transfer coefficient. A spatial mesh refinement study will be performed to evaluate the mesh independence of the solution.

3.5. MECHANICS

At high burnups, the fuel and cladding will be in full contact and chemically bonded during irradiation. After irradiation, as the fuel rod cools and it is placed in storage at atmospheric pressure, the cladding often remains bonded to the fuel. However, the magnitude of this chemical bonding and stress required for separation (lift-off) is not well characterized for storage conditions. Therefore, we will assume that the cladding and fuel are not in contact at BOS and because this lift-off has occurred during wet storage; future studies will be required to evaluate the significance of this approximation.

Because the fuel will be approximated as mechanically separated from the cladding at BOS and the internal pressure will lead to cladding creep away from the fuel, the mechanical deformation of the fuel can be neglected entirely. The anisotropic, elastic-plastic deformation of the cladding will be modeled using a standard finite-element technology, with reduced integration, and updated Lagrangian to model the large deformations. In addition to the time mesh refinement study associated with implicit creep, a spatial mesh refinement study will be performed to evaluate the mesh independence of the solution.

4. SENSITIVITY AND PARAMETRIC STUDY

Because there are significant uncertainties associated with the storage conditions, hydride precipitate formation, and the BOS condition of the UNF, we will also provide an initial parametric study to evaluate the relative sensitivities of the uncertainties associated with the problem to help guide the experimental and analysis efforts of the UFD Campaign.

The constitutive model developed by Sandia [5] will include the ability to perturb the coefficients in the model that describe the formation of hydride precipitates and their effect on the stress-strain relationship of the Zircaloy-4 cladding. Therefore, a basic parametric study will be performed to evaluate the relative sensitivities of a variety of inputs and the coefficients in the hydride model on the EOS mechanical state of the cladding. Using the representative uncertainty estimates of the input parameters (described in Sections 2.2 and 2.3 and collected in Table 5), an estimate of the uncertainty of the EOS mechanical state of the cladding will be determined.

Table 5. Input Parameters and Uncertainty Estimates for the Parametric Study

Parameter	Baseline	Units	Uncertainty
BOS Hydrogen Content	750	wppm	20%
BOS Radial Precipitates	100	wppm	50%
BOS Circumferential Precipitates	300	wppm	75%
BOS Rod Internal Pressure	4	MPa	10%
Storage Time	200	Years	50%
Coolant Temperature	350	K	10%
Oxide-to-Coolant Heat Transfer	1000	W/m^2K	50%

5. CONCLUSION

This document should provide sufficient detail to model a high burnup PWR fuel rod to provide an estimate of the EOS mechanical state of the cladding. The fuel rod and irradiation history are based on seven cycles of irradiation in the CP&L H.B. Robinson nuclear reactor, which achieved a discharge burnup of 66.682 MWd/kgU. The fuel has been experimentally examined for storage conditions by Argonne National Laboratory for the NRC. In addition, we have compiled a list of key factors that have been shown to strongly influence the EOS state of the fuel and have identified baseline values and ranges of uncertainties that will be considered. The simulations that will be performed have been described in detail and include the modeling assumptions and boundary conditions.

6. ACKNOWLEDGMENTS

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