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Report on UQ and PCMM Analysis of Vacuum Drying for UFD S&T Gaps

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Report on UQ and PCMM Analysis of Vacuum Drying for UFD S&T Gaps

Used Fuel Disposition Campaign Milestone M4FT-15LL0810022

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Table of Contents

List of Tables

List of Figures

Acronyms and Units

BRC	Blue Ribbon Commission
BWR	boiling water reactor
CWSRA	cold-worked and stress relief annealed
DCSS	dry cask storage system
FCT	fuel cycle technologies
HBU	high burnup
HLW	high-level nuclear waste
ISG	interim staff guidance
LWR	light water reactor
ISFSI	independent spent fuel storage installation
MBM	integration of MOOSE, BISON, and MARMOT that enables atomistically informed multiscale simulations of nuclear fuel microstructure
NRC	Nuclear Regulatory Commission
NUREG	publication prepared by staff of the U.S. Nuclear Regulatory Commission
PCMM	predictive capability maturity model
PWR	pressurized water reactor
RCT	ring compression test
RHT	radial hydride treatment
RHCF	radial hydride continuity factor.
RXA	recrystallized and annealed
SNF	spent nuclear fuel
SRA	stress relieved annealed
SSC	structures, systems, and components
UFD	used fuel disposition
UNF	used nuclear fuel

Units

GWd/MTU	gigawatt-days per metric tonne of uranium
MPa	megapascals
psi	pounds per square inch
wt. ppm	weight parts per million

Symbols

σ'_{th}	lower threshold stress
σ''_{th}	upper threshold stress

1 Introduction

This report satisfies the Lawrence Livermore National Laboratory (LLNL) Level 4 milestone: M4FT-15LL0810022 for the Storage and Transportation Analysis area of the Used Fuel Disposition (UFD) Campaign, funded by the U.S. Department of Energy's Office of Nuclear Energy (DOE-NE). The work was performed under UFD work-package FT-15-LL081002. The information in this report will provide input to a parent Sandia National Laboratories (SNL) milestone.

The UFD Campaign within the Department of Energy's Office of Nuclear Energy Fuel Cycle Technologies (FCT) program has been tasked with investigating the storage and ultimate disposition of the nation's used nuclear fuel (UNF) and high-level nuclear waste (HLW). Following the Blue Ribbon Commission (BRC) report on America's Nuclear Future (BRC, 2013), additional emphasis is placed on science based approaches to develop the technical bases in support of continued safe and secure storage of UNF for extended periods, subsequent retrieval, and transportation. UNF is currently housed in two different types temporary storage: (a) indoor pool storage at reactor sites and (b) outdoor cask storage. Storage within outdoor casks occurs both at currently operating nuclear facilities and in independent spent fuel storage installations (ISFSIs). The BRC recommends the implementation of a centralized interim storage facility to locate UNF prior to disposal. In order to assess the safety of UNF during transportation between sites and during storage at sites, the degradation of fuel, assemblies, canisters and casks must be considered.

This report discusses two phenomena that could affect the safety, licensing, transportation, storage, and disposition of the spent fuel storage casks and their contents (radial hydriding during drying and water retention after drying) associated with the drying of canisters for dry spent fuel storage. The report discusses modeling frameworks and evaluations that are, or have been, developed as a means to better understand these phenomena. Where applicable, the report also discusses data needs and procedures for monitoring or evaluating the condition of storage containers during and after drying. A recommendation for the manufacturing of a fully passivated fuel rod, resistant to oxidation and hydriding is outlined.

2 High Priority Phenomena Relevant to the Drying of Used Fuel Canisters

This report focuses on the dry storage of commercial light-water reactor uranium-oxide fuel with zirconium alloy cladding. Much of the fuel currently discharged from today's reactors exceeds the burnup threshold of 45 gigawatt-days per metric tonne of uranium (GWd/MTU) and hence is identified as high burnup fuel, defined by NRC as 45 to 62 GWd/MTU. These high burnup fuels make use of advanced zirconium alloys such as ZIRLO™ and M5® for which there is limited information about their SNF performance.

When UNF is removed from a reactor it is initially stored in water-filled pools where it cools and is shielded by the water. These pools eventually reach their safe storage capacity and the fuel assemblies must be removed. Since there is no operating repository on-site dry storage has become the default means for dealing with the spent nuclear fuel

(SNF). The transfer to dry storage canisters or casks takes place in the storage pool and hence the storage container must subsequently be dried.

There are two main categories that describe dry storage casks: the direct load cask where the UNF or SNF assemblies are loaded directly into a basket that is integrated into the cask; and canister based systems where the UNF assemblies are loaded into a basket inside a thin walled cylinder (called the canister) that is contained within a transfer cask and where the canister is subsequently transferred into a storage overpack. Today cask systems are designed to hold about 10 to 15 MTU of UNF. Cask dimensions are about 15-19 feet high and 8 feet in diameter with a weight of 100 to 120 tons.

Bare fuel casks are placed into the spent fuel pool for loading. Once loaded, the bare fuel cask is sealed and lifted out of the pool. Water is removed through a drain tube, the outer surfaces are decontaminated, and the cask is then transferred to the drying location. For the canister-based systems, the empty canister is loaded into the transfer cask and the two are lowered into the spent fuel pool for loading. Once loaded, the canister and cask are removed from the pool and the water is drained enough to weld the top onto the canister. Like the bare fuel casks, the system is then drained, decontaminated and dried. Most systems use vacuum drying (e.g., ASTM C1553-08) in which the decay heat of the fuel is used to help drive off water. Other systems use a flow of dry helium to remove residual water. The vacuum drying process often produces the highest cladding temperatures experienced during the dry storage process, and NRC guidance limits the peak clad temperature to 400°C under normal conditions (NUREG-1536, Rev. 1, Section 8.4.17 [NRC 2010b]) to meet the regulations in 10 CFR 72.122.

This report discusses two phenomena associated with the drying of the canister: water retention and/or water that has not been sufficiently removed from the container; and hydride reorientation as a result of the drying and backfill procedure.

2.1 Water Retention After Drying

A possible chemical stressor is water that may have not been sufficiently removed from the container during the loading and drying process. *The occurrence of potentially significant amounts of water within the container is considered an off-normal condition.* Assembly hardware is subject to corrosion during the off-normal condition of moisture presence inside the canisters due to inadequate drying or waterlogged rods. Water in the dry storage container can possibly impact fuel cladding, fuel assembly hardware, and the fuel basket. Water remaining in the canister could cause corrosion of the fuel cladding and internal structures or may create a flammable environment within the canister if radiolysis creates free oxygen and hydrogen.

2.1.1 Vacuum Drying Method

NUREG-1536 Section 9.5.1 [1] states that an accepted method is to drain the cask of as much water as practicable and then to evacuate to less than or equal to $4.0.10^{-4}$ MPa (3 torr) followed by back filling with helium. Acceptable water removal is verified if pressure is maintained in the cask/canister at this level after isolating the vacuum line and checking for a pressure rebound. An overview of vacuum drying methods and the factors affecting the quantity of residual water after drying has been prepared by Miller *et al.*, for the NRC [2]. NRC provides only general guidance to licensees concerning the

implementation of vacuum drying. In particular, NUREG–1536 [1], states that NRC staff accepts vacuum drying methods comparable to those recommended in Pacific Northwest National Laboratory Report PNL–6365 [3], which specifies less than 0.25 volume percent oxidizing gasses in the canister. When vacuum drying is implemented, licensees have a technical specification directing that the canister be evacuated to below a certain pressure with demonstration that the pressure will remain stable for a period of time after the canister is isolated from the pumping system.

The recipes developed by cask vendors for vacuum drying are similar to one another. The overriding goal is to decrease pressure in a step-wise manner with a hope of preventing ice formation by providing time for the residual heat to bring the system to equilibrium. This raises questions about situations where the residual heat is low. The bulk of the water in the canister is removed with a centrifugal pump connected to the siphon port of the canister. Pressurizing the canister with dry helium, allowing the helium water mixture to be exhausted through the siphon port, carries out a blow down process. This blow-down process is repeated until visual observation indicates a minimum amount of water being exhausted.

As mentioned, the important aspect of the subsequent vacuum drying is for it to be carried out in a step-wise manner (hold points). At each hold-point the canister is isolated from the pumping system for about 30 minutes during which time water and other volatiles evaporate. The typical number of hold-points varies between three and seven. As mentioned already, the final pressure to which the canister must be evacuated is in the range of 3 to 10 torr. The canister must not exceed this qualification pressure for a period of 30 minutes after being isolated from the pumping system. Helium is backfilled into the chamber system so as to pressurize it, couplings are removed and/or sealed, and then the canister is evacuated and refilled with helium a second time to several psi. During these vacuum drying procedures cladding temperatures can increase, and as we will discuss later, care must be taken to establish drying time limits to ensure that peak cladding temperatures do not exceed the allowable temperature of 400°C (NUREG-1536 [1]).

2.1.2 Uncertainty Quantification

Drying has been identified as a cross-cutting need for extended storage of UNF [4]. The need is characterized such because: *many degradation mechanisms are dependent on or accelerated by the presence of water. Even if proper drying procedures are followed, some water could remain, given the tortuous path water may follow, in addition to the contribution from physisorbed and chemisorbed water that may not be removed under the drying conditions.* The importance of R&D in this area is identified as “high” with the approach being: *to perform tests and develop models to better quantify the amount of residual water remaining after a normal drying cycle.* Also in [4], and related to drying, is monitoring, which also is rated as a cross-cutting need with “high” importance for R&D. It is described thusly: *continued efficacy or acceptable performance of dry storage systems for relatively short-term storage can be demonstrated through accelerated tests to validate models and analyses. However, for extended storage, projection of continued efficacy or acceptable performance may not be possible without collecting data to validate the models developed using data from short-term tests. To collect the necessary data as part of the R&D program and engineering-scale demonstration, more effective*

monitoring systems must be developed to detect failures (or precursors to those failures) and to evaluate materials property changes that can be correlated to their structural performance. Where the approach to closing the gap is: *Develop systems for early detection of confinement boundary degradation, monitoring cask environmental changes, and data transmission without compromising cask or canister boundary.*

Water can accelerate many degradation mechanisms in dry cask storage systems (DCSS). The DCSS is loaded with fuel while in the pool and hence removal of as much water as possible is important to the drying process. The question remains rather what is the maximum amount of water that can be left behind and not compromise the DCSS. Water, water vapor and/or its decomposition products produced through radiolysis can interact with the fuel, assembly hardware, baskets, neutron poisons, and canister materials.

The hold up of water in the canister may result from a combination of phenomena: insufficient vacuum drying of unbound water due to geometric characteristics of the fuel assembly and canister, or hold up of unbound water in water logged damaged fuel rod(s); and chemisorbed and physisorbed water. To quantify the water remaining in the canister after vacuum drying requires appropriate instrumentation: during vacuum drying, post vacuum drying, and in storage. The physical inspection of canister interiors that have been open after storage for extended periods of time will not routinely provide information about the remaining unbound water as such opening of casks is performed in pool. Nevertheless, such inspections can reveal consequences of wet corrosion such as corrosion of cladding, fuel assembly and canister components.

Quantification of the water content of a vacuum dried canister, once it has been sealed, would require breaching that seal and extracting an aliquot of the internal helium atmosphere that could then be subjected to quantitative analytical analysis for water vapor and other volatiles. Such a breaching would likely require a change in NRC regulations regarding dry-cask storage. An alternative is to qualify the actual vacuum drying procedure in such a way as to develop a statistical picture (data base) that could support an aleatoric uncertainty quantification analysis.

Miller and co-workers have outlined a test plan [2] for quantifying unbound water retention. For the two light water reactor (LWR) commercial fuel assembly designs, pressurized water reactor (PWR), and boiling water reactor (BWR), they identified creviced regions, guide thimble tubes in PWR assemblies, and creviced regions and the water-rod in BWR assemblies. They conclude that a plan should be developed to test for water hold-up in these areas of the fuel assemblies. They also considered test plans for canister designs, recommending that the test plan include evaluation of water hold-up on horizontal surfaces and pooling at the bottom of the canister past the end of the siphon tube. They note that fuel heat load is an important variable with regards to water ice formation that can block water removal and recommend varying the heat load of the fuel assemblies in a planned testing program. The possible hold-up of water in damaged fuel rods is discussed. Here the uncertainties are quite numerous, as icing will depend on the size/dimensions of the penetration, the pressure difference across the hole, and the location of the hole along the fuel rod. Various surrogate rods with holes of varying dimension and location be tested with respect to water hold-up as a means for quantifying this issue.

2.1.3 Predictive Capability and Model Maturity

An analysis of the consequences of cover gas impurities and their effects on the dry storage of LWR SNF was reported in (3). The study is based on gas analysis data for the cover gas composition taken from various dry cask storage systems at the time of the report and technical design information for four spent fuel storage casks taken from their operating manuals. The report considers how an assumed concentration of reactive impurity gases might potentially degrade the cladding either by reacting directly with the zirconium alloy or by reacting with exposed UO_2 fuel that is exposed due to cladding breaches. The non-inert impurities in the helium cover gas considered in this report are: O_2, H_2, CO_2, CO, and H_2O. The impurity gas concentrations theoretically available for reaction within the canister from these gases are, 0.075 mol/m^3 of O_2 and 0.085 mol/m^3 of H_2, where the dominant sources are O_2 itself and H_2O.

The report (3) does not consider details of reaction kinetics but rather considers bounding cases. Hydriding is dismissed as it is assumed that considerable hydrogen uptake has already taken place in the zircaloy cladding while in reactor service and that the small additional amount of hydrogen available from the cover gas is negligible. The report concludes that *O_2 will have no significant effect on the cladding unless all available O_2 reacts with the UO_2 fuel to produce lower density U_3O_8 at one or two cladding breaches*, thus expanding the breach significantly. However, the report notes that the zircaloy itself will *getter all the O_2 within the cask in one year if the temperature is greater than 300°C* resulting in a negligible decrease in the thickness of the cladding. It is concluded that less then 0.6 mol each of O_2 and H_2 is expected to be available for cladding degradation reactions assuming that the vacuum drying procedure is validated as described earlier. However, without a container specific analysis of the cover gas composition one cannot be sure that the statistically determined amount of reactive gas impurities is at a truly safe limit. Thus it is suggested that an *epistemic* approach is necessary if one desires to establish valid uncertainty quantification for vacuum drying and possible deleterious consequences resulting therefrom.

Table 1 General descriptions for PCMM table entries

MATURITY / ELEMENT	Maturity Level 0 Low Consequence, Minimal M&S Impact, e.g. Scoping Studies	Maturity Level 1 Moderate Consequence, Some M&S Impact, e.g. Design Support	Maturity Level 2 High-Consequence, High M&S Impact, e.g. Qualification Support	Maturity Level 3 High-Consequence, Decision-Making Based on M&S, e.g. Qualification or Certification
Representation and Geometric Fidelity What features are neglected because of simplifications or stylizations?	• Judgment only • Little or no representational or geometric fidelity for the system and BCs	• Significant simplification or stylization of the system and BCs • Geometry or representation of major components is defined	• Limited simplification or stylization of major components and BCs • Geometry or representation is well defined for major components and some minor components • Some peer review conducted	• Essentially no simplification or stylization of components in the system and BCs • Geometry or representation of all components is at the detail of "as built", e.g., gaps, material interfaces, fasteners • Independent peer review conducted
Physics and Material Model Fidelity How fundamental are the physics and material models and what is the level of model calibration?	• Judgment only • Model forms are either unknown or fully empirical • Few, if any, physics-informed models • No coupling of models	• Some models are physics based and are calibrated using data from related systems • Minimal or ad hoc coupling of models	• Physics-based models for all important processes • Significant calibration needed using separate effects tests (SETs) and integral effects tests (IETs) • One-way coupling of models • Some peer review conducted	• All models are physics based • Minimal need for calibration using SETs and IETs • Sound physical basis for extrapolation and coupling of models • Full, two-way coupling of models • Independent peer review conducted
Code Verification Are algorithm deficiencies, software errors, and poor SQE practices corrupting the simulation results?	• Judgment only • Minimal testing of any software elements • Little or no SQE procedures specified or followed	• Code is managed by SQE procedures • Unit and regression testing conducted • Some comparisons made with benchmarks	• Some algorithms are tested to determine the observed order of numerical convergence • Some features & capabilities (F&C) are tested with benchmark solutions • Some peer review conducted	• All important algorithms are tested to determine the observed order of numerical convergence • All important F&Cs are tested with rigorous benchmark solutions • Independent peer review conducted
Solution Verification Are numerical solution errors and human procedural errors corrupting the simulation results?	• Judgment only • Numerical errors have an unknown or large effect on simulation results	• Numerical effects on relevant SRQs are qualitatively estimated • Input/output (I/O) verified only by the analysts	• Numerical effects are quantitatively estimated to be small on some SRQs • I/O independently verified • Some peer review conducted	• Numerical effects are determined to be small on all important SRQs • Important simulations are independently reproduced • Independent peer review conducted
Model Validation How carefully is the accuracy of the simulation and experimental results assessed at various tiers in a validation hierarchy?	• Judgment only • Few, if any, comparisons with measurements from similar systems or applications	• Quantitative assessment of accuracy of SRQs not directly relevant to the application of interest • Large or unknown experimental uncertainties	• Quantitative assessment of predictive accuracy for some key SRQs from IETs and SETs • Experimental uncertainties are well characterized for most SETs, but poorly known for IETs • Some peer review conducted	• Quantitative assessment of predictive accuracy for all important SRQs from IETs and SETs at conditions/geometries directly relevant to the application • Experimental uncertainties are well characterized for all IETs and SETs • Independent peer review conducted
Uncertainty Quantification and Sensitivity Analysis How thoroughly are uncertainties and sensitivities characterized and propagated?	• Judgment only • Only deterministic analyses are conducted • Uncertainties and sensitivities are not addressed	• Aleatory and epistemic (A&E) uncertainties propagated, but without distinction • Informal sensitivity studies conducted • Many strong UQ/SA assumptions made	• A&E uncertainties segregated, propagated and identified in SRQs • Quantitative sensitivity analyses conducted for most parameters • Numerical propagation errors are estimated and their effect known • Some strong assumptions made • Some peer review conducted	• A&E uncertainties comprehensively treated and properly interpreted • Comprehensive sensitivity analyses conducted for parameters and models • Numerical propagation errors are demonstrated to be small • No significant UQ/SA assumptions made • Independent peer review conducted

reproduced from Oberkampf et al., 2007[5]

Table 2 PCMM graphic table for water retention in vacuum drying of canister/cask

PCMM		Level 0	Level 1	Level 2	Level 3
Representation and Geometric Fidelity (RGF)	Characterization				
	Computation Error				
	Verification				
Physics and Material Model Fidelity (PMMF)	Science basis for models				
	Model Accuracy				
	Extrapolation				
	Technical Review				
Code Verification (CVER)	Software Quality Engineering				
	Software Quality Assesment				
	Test Coverage				
	Computational Errors				
Solution Verification (SVER)	Numerical Solution Errors				
	Input/Output Verification				
	Technical Review				
Validation (VAL)	Validation Hierarchy				
	Model Accuracy				
	Extrapolation				
	Technical Rview				
Uncertainty Quantification (UQ)	Uncertainty Characterization and Interpretation				
	Sensitivity Analysis				
	Numerical Propagation Errors				
	Aggregation of Evidence for Characterization of Uncertainties				
	Completeness				
	Strong Assumptions				
	Technical Review				
Documentation and Archiving	Documentation and Archiving				

2.1.3.1 Maturity Model (PCMM) Quantification.

The Predictive Capability Maturity Model (PCMM) was developed by Oberkampf [5] and co-workers and is currently used to provide a qualitative measure of the overall UQ methodology task. For the purpose of this report we have adopted the methodology adapted in M4FT-14LL0810044 [6]. Table 1 describes the methodology while the numerical ranges are described in Appendix A. Table 2 shows the roll-up analysis of the PCMM for water retention modeling based on the studies in references [3] and [4]. The table reflects the fact that there are no models that attempt to quantify the amount of water remaining in a SNF canister after vacuum drying. The reasons for the lack of a model have been outlined above but in review we note that there are numerous canister types, each with different drying procedures defined by the manufacturer; the consequences and sources of water holdup in cracks, crevices and in breeched cladding have not been quantified; the actual amount of freezing or plugging is dependent on structural and procedural details and this is not quantified, and no attempt has been made to quantify the amount of bound water remaining in a generic vacuum dried canister.

2.1.4 Recommendations and Future Work

There is no direct evidence that the amount of water that remains in a cask after a normal drying process is of concern. However there is no data to validate just how much water remains despite the importance of water in some degradation processes. In a recent gap analysis the quantification of the amount of remaining water was deemed of high importance (4), and a series of tests and modeling efforts to better quantify the amount of residual water was recommended. If the efficacy of the drying process can be verified, a number of degradation processes for fuel, cladding, assembly hardware, and canister/cask internals can be ruled out. Validation of the drying process can lead to an aleatoric quantification of uncertainty with regards to degradation of fuel, cladding, and canister internals. In contrast, canister monitoring of the cover gas both shortly after drying and during storage is the only way to obtain an epistemic uncertainty quantification of the amount and hence the consequences of water hold-up (and other reactive gases) in the canister.

Ahn and co-workers have carried out a detailed assessment of the possible deleterious effects associated with vacuum drying inadequacy [7]. For their assessment they assumed the amount of residual water to be 55 moles, an order of magnitude greater than prescribed in NUREG-1536 [1] or used in an earlier assessment [3]. By introducing a time dependent model and considering radiolysis of the water, the assessment presents a picture that emphasizes the potential for cladding failure and fuel release into the canister as a result of cladding splitting. The assessment also suggests the possibility of flammability conditions within the sealed container if hydrogen is produced in molecular form as opposed to being gettered by the zirconium alloy cladding.

Experimental tests to measure the quantity of residual water that remains in the SNF canister following vacuum drying will contribute to a database that will identify best practices and qualify the drying procedure(s). The goal of such an experimental program is to provide additional confidence in the criterion recommended under NUREG-1536. In the report in reference [2] a review was made of canister types, fuel assembly types in an attempt to identify locations that might retain water. A conceptual test plan was

proposed with a more detailed plan subsequently released [8]. The following topics were considered:

- Fuel Assembly Designs
- Canister Designs
- Fuel Heat Load
- Damaged Fuel Rods

Measurement capabilities that would be needed for such a test program were also considered. The table from reference [2] outlining suggested measurement techniques is reproduced below as Table 3.

Table 3 Possible Measurement Techniques and Considerations (taken from reference [2])

Measurement Technique	Instrument	Use	Challenge
Visual observation	Window or camera	View ice formation	Limited field of view
Internal temperature distribution	External IR camera	View temperature deviations due to evaporative cooling and ice formation	IR transparent glass window required
	Internal IR camera	View temperature deviations due to evaporative cooling and ice formation	Vacuum rating
			Calibration for emissivity of internal fixtures
Internal temperature reading	Thermocouple	Detect presence of residual water/ice	Thermocouple wires can affect ice nucleation/sublimation rates
Internal water vapor content	Dew point sensor	Monitor drying process and water vapor rebound during 30-minute hold period	Water vapor partial pressure may be less than 3 torr [400 Pa] if other volatiles are present
External in-line water vapor concentration	Dew point sensor	Monitor drying process and water vapor rebound during 30-minute hold period	Water vapor partial pressure may be less than 3 torr [400 Pa] if other volatiles are present
	Cold plasma spectrometer	Provide direct measurement of water vapor content	Will require custom instrumentation and calibration
Vacuum measurement	Vacuum gauges or pressure sensors	Monitor total pressure during drying process and hold period	Accuracy over wide range of pressures
Mass flow	Mass flow meter	Monitor rate of water removal	Multiple meters for various flow rates
			Measurement sensitive to changing gas composition if multiple gasses present

Specific recommendations were made for factors to consider in a test plan. These were the operational parameters: number of hold points, final canister pressure; the physical locations: breached fuel rods, dashpot of PWR guide thimble tubes, BWR water rods,

crevices around assembly hardware such as grids, nozzles, and guides; the fuel condition: decay heat load.

It is the recommendation of this report that the experimental test program described in references [2 and 8] be executed so as to provide the statistical data needed to validate recommended vacuum drying procedures for dry storage of SNF.

2.2 Radial Hydride Precipitation During Drying

It is well known that canister/cask vacuum drying can lead to radial hydride precipitation in commercial nuclear fuel zircaloy cladding and that this in turn reduces the cladding DBTT. Radial hydride formation during drying depends on details of the drying process, the as manufactured microstructure of the zircaloy cladding, and the burnup level to which the cladding has been taken. Recrystallized and annealed (RXA) cladding appears to exhibit more radial hydride formation than cold-worked and stress relief annealed (CWSRA) cladding at high burnups (9). Hydride dissolution and reprecipitation as radial hydride is also extant under vacuum drying conditions for these two classes of zirconium alloys. It has been reported that Nb-bearing cladding alloys and RXA alloys are more susceptible to radial-hydride precipitation than Sn-bearing CWSRA alloys (Aomi et al. [10] and Burtseva et al. [11]). In the gap analysis of reference [4] the degradation mechanism of hydrogen on embrittlement (lowering the DBTT) and associated hydride reorientation is called out as having "high" R&D importance. Specifically the approach to closing the gap is: *a comprehensive experimental and modeling program to examine the factors that influence hydride reorientation with a focus on new cladding materials and high burnup fuels.* Cladding hydride reorientation and embrittlement are areas that have been recommended in a recent DOE report [12] for additional R&D within the next 3 years

2.2.1 Vacuum Drying Method

A standard review plan (NUREG-1536 Rev. 1)[1] prescribes guidelines for vacuum drying in an attempt to minimize the dissolution of hydrides and the precipitation of radial hydrides in the zircaloy cladding of commercial reactor fuels. NUREG-1536 Rev 1. Sec 4.4.2 states: *To guarantee cladding integrity of zirconium-based alloys, the maximum calculated fuel cladding temperature should not exceed 400°C (752°F) for normal conditions of storage and short-term loading operations, including cask drying and backfilling. A higher temperature limit may ONLY be used for low burnup spent nuclear fuel (SNF) (less than 45 GWd/MTU), as long as the applicant can demonstrate that the best estimate cladding hoop stress is equal to or less than 90 MPa (13.1 ksi) for the temperature limit that is proposed. During loading operations, repeated thermal cycling should be limited to less than 10 cycles, with cladding temperature variations* ~~*more than*~~ (*(less than)* is consistent with more recent guidance [13]) *(65°C (149°F). For off-normal and accident conditions, the maximum zirconium based cladding temperature should not exceed 570°C (1058°F).* As noted in ASTM C 1553-08 (14), the process of vacuum drying must not damage the fuel because the thermal cycling during the drying process for commercial LWR SNF may drive the hydride re-orientation process in the zircaloy cladding.

2.2.2 Uncertainty Quantification

The formation of radial hydrides in zirconium alloy fuel cladding during vacuum drying depends on the details of the manufacturing and the in-reactor history of the cladding. With the advent of new corrosion resistant claddings such as ZIRLO™ and M5®, which were developed for higher burnup up to 62 GWd/MTU, used fuel hydrogen contents and temperatures have become much more variable than in the past. Major questions regarding radial hydride formation for any particular used fuel cladding are the consequences of temperature cycling and peak temperature, hoop stress and peak hoop stress, solvated and precipitated hydrogen and radiation damage accumulation. Only recently have drying simulation tests been conducted on irradiated cladding in such a way as to simulate the variable pressure (radial hoop stress) with temperature cycling that the cladding experiences during vacuum drying cycles [15].

Prestorage drying-transfer operations subject cladding to higher tensile hoop stresses induced by higher temperatures and pressure relative to in-reactor operation and pool storage. During slow cooling radial hydrides may precipitate and introduce an embrittlement mechanism if the resulting cladding temperature decreases below the DBTT at some time in the future when the fuel has cooled sufficiently. In ([15] the relationship between hoop stress loading and DBTT as manifested through radial hydride formation during vacuum drying is investigated. Current interim guidance for HBU SNF is found in Interim Staff Guidance – 11, Revision 3 (ISG-11, R3) [13]. Limits set are similar to those in [1]: peak cladding temperature of 400°C, less than 10 repeated heatup and cooldown cycles, hoop stress less than 90 MPa with temperature variations that are less than 65°C.

2.2.3 Predictive Capability and Model Maturity

Because of their unique combination of low neutron capture cross-section, good mechanical properties, and corrosion resistance, zirconium alloys are preferentially used for commercial reactor nuclear fuel cladding. Hydrogen finds its way into the zirconium alloy fuel rods of LWRs as a consequence of waterside corrosion. For HBU fuel, oxide thickness of up to 100 μm and hydrogen contents in excess of 600 wt. ppm have been observed. The deleterious role of hydrogen pickup has been a concern in the application of zirconium alloy fuels from their inception. The pickup of hydrogen, its low solubility, and the eventual formation of platelet-like hydrides is an ongoing and only partially understood degradation mechanism of zirconium alloy cladding that is known to lead to mechanical failure. While the formation of both circumferential and radial hydrides is operative during in-core use of the fuel, the formation of additional radial hydrides of significant continuity/length so as to significantly reduce the DBTT are produced through a mechanism of hydride dissolution and reprecipitation resulting from the temperature cycling during the vacuum drying process. Thus, experimental data and modeling of sufficient quality and accuracy is needed to reduce the uncertainty of cladding failure of SNF in dry storage due to the vacuum drying process.

2.2.3.1 Experimental Results

Ultimately model maturity depends on experimental data that identifies the relevant phenomena and mechanisms of radial hydride formation during vacuum drying, and that also serves as a means to validate such models.

An important goal of hydride reorientation experiments is to develop a model description of the roles of hydrogen concentration, temperature, stress and temperature cycling, all of which are important but not independent variables that determine the kinetics of hydride dissolution and reprecipitation. In an experiment reported by Chu and co-workers stress-relief annealed specimens of (SRA) Zircaloy-4 cladding were hydrogen loaded by a diffusional method in the range of 100 to 600 wt ppm [16]. The experiment involved comparing the reorientation of the hydrides due to temperature cycling under constant stress in an autoclave with a corresponding isothermal treatment. A particularly good

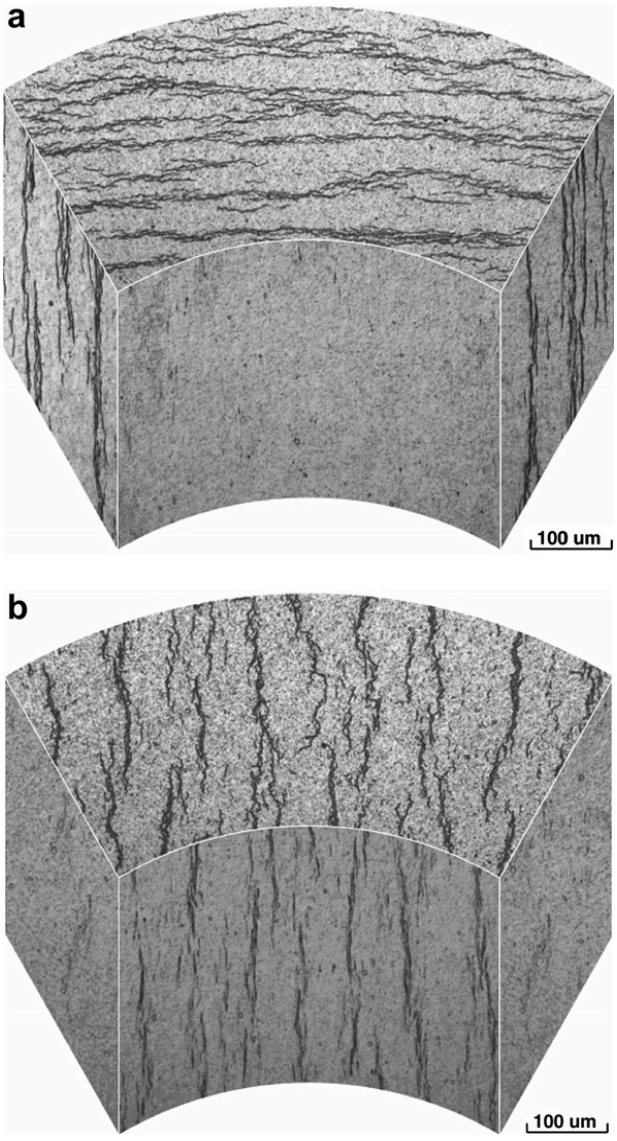

Fig. 1 Micrograph showing orientation of hydrides in Zircaloy-4 cladding of ~230 ppm: (a) as-hydrided and (b) after 8 cycles of thermal treatment. *From Ref [16]*

micrograph of the transition from as hydride to thermal treatment showing the for mation of radial hydrides is seen in Fig. 1. To explain their results Chu and co-workers developed a thermodynamic model that estimates the threshold stress for hydride reorientation a function of solution temperature and hydrogen concentration. According

to the model, the bounds of stress and temperature to stress reorientation of hydride precipitates were explained. The threshold stress for hydrides to reorientation was a function of solution temperature and specimen hydrogen concentration.

Dynamic in situ kinetic studies of hydride dissolution and hydride reprecipitation have been performed using synchrotron x-ray radiation [17]. The material examined was hydrogen charged (by high temperature gas diffusion) unirradiated recrystallized Zircaloy-2 and cold-rolled stress relieved Zircaloy-4. The measurements were performed under stress and at temperature and yielded a threshold stress for reorientation of 75 to 80 MPa. Extension of this work to irradiated zirconium alloys would be very useful in providing realistic and relevant numbers on which vacuum drying guidance could be based.

A brief review of the mechanisms for hydride initiated fuel failure (cladding failure) of zirconium alloys was provided by Motta and Chen [18]. In this paper it is noted that the hydrogen terminal solid solubility is different when measured in dissolution or in precipitation with hydride dissolution occurring at a higher temperature than hydride precipitation [19]. Fig. 2 illustrates this phenomena as well as comparing results from differential scanning calorimetry (DSC). This hysteresis effect establishes the recommended temperature cycling limit found in [13] for vacuum drying of SNF canisters/casks.

An important question is: does enough data exits in order to adequately inform model development and model validation? Wile much has been accomplished in search of the understanding of hydride behavior in zirconium alloys, there are still significant knowledge gaps that require more experimentation. The underlying complexity of the behavior of hydrides in zirconium alloys derives from the coupling of chemistry, thermodynamics, stresses, and hydrogen diffusion. More experimental work that focuses on in situ measurements that provide information about the non-equilibrium processes and the underlying kinetics coupled with advanced computational methods such as phase-fiel holds out the possibility for developing the level of understanding required for predictive and prescriptive guidance in the handling of SNF.

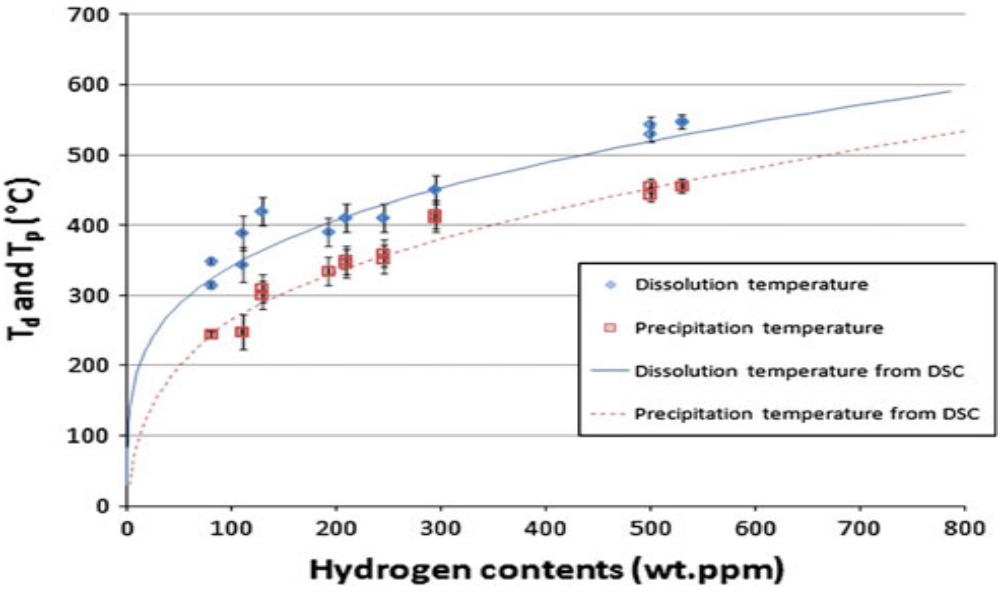

Fig. 2 Hydrogen dissolution and precipitation temperatures as determined using in situ synchrotron radiation diffraction and compared to DSC results. *From Ref [18]*

Recent experimental work from Argonne National Laboratory [15] has examined HBU reactor irradiated zirconium alloy claddings (Zircaloy-4 (ZRY-4), ZIRLO™, and M5®) by performing radial hydride treatments (RHT) at varying peak temperatures and varying peak hoop stresses. A noteworthy feature of the Argonne work is that it includes decreasing internal gas pressure and hoop stress with decreasing temperature, distinguishing the investigation from most other radial hydride precipitation and subsequent ductility studies. Ring compression tests (RCT) and extensive microscopy were employed in the Argonne work to deduce the radial hydride continuity factor (RHCF) and to estimate the DBTT. The results indicate that peak cladding temperatures may not exceed 350°C during vacuum drying and storage for canisters/casks containing HBU fuel assemblies, suggesting that a revision to ISG-11, R3 [13] should be considered for HBU fuels. The approach described in [15] thus serves as a model for future experimental investigations.

2.2.3.2 Modeling Results

In 1994 Bai and co-workers [20] proposed a quantitative model for evaluating the susceptibility to radial hydride formation under tensile stress. Threshold stresses were calculated with the lower threshold stress σ'_{th} = 95 MPa and the upper threshold stress σ''_{th} = 150 MPa which were in good agreement with XRD diffraction analysis of hydrided Zircaloy-4. The association of fracture with hydrides in zirconium is of particular concern. In two papers Shi and co-workers developed initial models for sharp crack tip [21] and shallow notch [22] fracture initiation due to delayed hydride cracking (DHC) in zirconium alloys. Expressions for the minimum stress intensity factor were developed along with its variation with hydride microstructure and temperature. The need for more accurate key parametric data is called out. In [22] the relationship to DHC in shallow or blunt notches under tensile stress and the need for the inclusion of hydrogen transport data are emphasized. The physics of hydride nucleation and growth are examined in some detail in a subsequent but related paper [23].

The reduction in the solubility of hydrogen in zirconium alloy cladding during long term storage is a consequence of lowering the temperature on the fuel. Hydride reorientation during long-term storage is a consequence of the combined effects of hoop stress and temperature lowering. While not directly related to hydride reorientation during vacuum drying, where hydride reorientation is understood to precede via hydride dissolution and reprecipitation driven by temperature cycling and hoop stress, the work of Chan [24] is important as it develops a micromechanical model for predicting hydride embrittlement in nuclear fuel cladding. Two important features of this work were: the capability to predict the orientation, morphology, and types of hydrides under the variables of time, temperature and stress, and the ability to predict the consequential mechanical effects of hydride morphology and orientation on the tensile ductility and fracture toughness of the cladding material.

A number of papers have focused on the kinetics and mechanisms of the formation of metal hydrides (see the review [25]) and others on the mechanical properties of zircaloy

alloys with hydrides and the mechanisms leading to crack propagation and failure of the zirconium alloy cladding [26, 27, 28, 29, 30, 31].

Papers focused on hydride reorientation are of particular importance to SNF vacuum drying of zirconium alloy clad fuel because radial hydride formation is a precursor to crack failure and is initiated by temperature and stress conditions encountered by zirconium alloy fuel cladding during vacuum drying of SNF canisters/casks. As noted in 2.2.3.1, Chu and co-workers developed a thermodynamic model from which one can extract the bounds of stress and temperature leading to hydride reorientation [16] based on the solution temperature and specimen hydrogen concentration. Such a model can assist in setting boundary conditions for vacuum drying of HBU SNF if the associated research were extended to the newer zirconium alloys such as ZIRLO™ and M5®.

Ultimately the goal of hydride modeling is to lead to engineering applications. To do so the models must deal with all the relevant concurrent and interacting phenomena in material that is subject to non-trivial histories of temperature and load [32]. Jenkvist and Massih have developed and validated a multi-field continuum based computational model for stress- and temperature-driven diffusion of hydrogen in hydride forming metals [32, 33] and extended this model to include fracture. Their model computes the volume fraction and mean orientation of hydride precipitates. They have taken this model and extended it to include local fracture properties and have been successful in validating the model against fracture tests on hydrogen charged Zr-2.5%Nb. They also have simulated crack initiation and growth by DHC. This is the first successful model to cover the entire process of material degradation in a zirconium alloy due to hydrogen while also linking material fracture with hydride reorientation.

Another approach that may be able to bridge all the phenomena associated with hydride formation and material degradation is the hybrid Potts-phase field model that has been developed to model coupled microstructural-compositional evolution. This new approach to the multi-physics modeling has been described recently [34, 35, 36, 37]. As implied the modeling method combines elements of the Monte Carlo Potts Model with those of phase field model. The goal is to simulate microstructural evolution processes that are kinetically controlled by long-range diffusion in multi-component systems. The specific challenge with respect to vacuum drying of storage canisters used for UNF zirconium alloy clad UNF is to include the phenomena of hydride dissolution and reorientation within the framework of the model.

2.2.3.3 Maturity Model (PCMM) Quantification.

The Predictive Capability Maturity Model (PCMM) was developed by Oberkampf [5] and co-workers and is currently used to provide a qualitative measure of the overall UQ methodology task. For the purpose of this report we have adopted the methodology described recently in UFDC milestone M4FT-14LL0810044 [6]. However, rather than evaluating one chart for each modeling approach related to hydride reorientation during vacuum drying of SNF we have qualitatively integrated the two model approaches which in our opinion are currently most advanced, the hybrid Potts-phase field model [34-37] and the multi-field model [32, 33]. Table 1 describes the PCMM methodology while the numerical ranges are described in Appendix A, reproduced from reference [6]. Table 4

shows the roll-up analysis of the PCMM for hydride reorientation modeling based on the current status of the two chosen models.

Table 4 PCMM graphic table for hydride reorientation in zirconium alloy cladding modeling arising from vacuum drying of SNF canister.

PCMM		Level 0	Level 1	Level 2	Level 3
Representation and Geometric Fidelity (RGF)	Characterization				
	Computation Error				
	Verification				
Physics and Material Model Fidelity (PMMF)	Science basis for models				
	Model Accuracy				
	Extrapolation				
	Technical Review				
Code Verification (CVER)	Software Quality Engineering				
	Software Quality Assesment				
	Test Coverage				
	Computational Errors				
Solution Verification (SVER)	Numerical Solution Errors				
	Input/Output Verification				
	Technical Review				
Validation (VAL)	Validation Hierarchy				
	Model Accuracy				
	Extrapolation				
	Technical Rview				
Uncertainty Quantification (UQ)	Uncertainty Characterization and Interpretation				
	Sensitivity Analysis				
	Numerical Propagation Errors				
	Aggregation of Evidence for Characterization of Uncertainties				
	Completeness				
	Strong Assumptions				
	Technical Review				
Documentation and Archiving	Documentation and Archiving				

2.2.4 Recommendations and Future Work

During the last 20 years modeling of hydride formation and hydrogen related mechanical failure of zirconium alloys has been steadily advancing. The challenge is not only, as already noted, multi-disciplinary, but also involves multi-length physics over variable time scales and different critical path processes each with its own non-equilibrium kinetics. The relevant issues in the order of their time evolution are: hydrogen diffusion, precipitation of hydrides, mechanism(s) of crack propagation (ductile or brittle), and finally the fracture mechanics and material failure. Overlaying and influencing these processes are the roles of stress and temperature as well as radiation damage accumulation. The issues introduced by vacuum drying of SNF canisters take place after significant in core accumulation of radiation damage and hydrogen pick-up so that the zirconium alloy cladding has developed hydrides (both circumferential and radial) if the hydrogen concentration has exceeded its solubility and if it has seen one or more temperature cycles due to normal operations.

Our recommendations are as follow:

- With respect to predicting hydride reorientation the multi-phase model [32, 33] appears to be more capable at the present time but additions to the Potts-phase field model are expected to provide a predictive capability for hydride reprecipitation orientation [37]. A "head to head" comparison of the two modeling approaches would be informative and improve the quantification of model uncertainties.
- Experimentally there is a need for more data such as that reported by the ANL group [11]. Experiments on used fuel cladding particularly advanced alloys, such as ZIRLO™, and M5®, with their higher burnups under conditions of temperature dependent stress are of particular importance. These experiments should be expanded so as to provide a two-sigma variation representative of the uncertainties of the details of the vacuum drying process.

3 Summary

A brief review of two phenomena associated with vacuum drying of SNF canisters/casks for dry storage was presented. The phenomena were, residual water left in the canister after drying and the potential for hydride reorientation as a result of the dryin procedure. The current status with respect to PCMM was presented for these two phenomena based on limited data and modeling. Recommendations for future work were made.

- It is the recommendation of this report that the experimental test program described in references [2 and 8] for vacuum drying and the quantitative determination of residual water be executed so as to provide the statistical data needed to validate recommended vacuum drying procedures for dry storage of SNF.
- The two advanced models for hydride formation, dissolution, and reprecipitation (the multi-phase model and the Potts-phase field model) should be validated in a head to head comparison to provide better quantification of model uncertainties.
- The scope of the ANL experiments should be expanded with the purpose of providing verification and validation data to present day and future models for hydride reorientation. The experimental matrix should encompass a two sigma variation to adequately represent the uncertainties associated with present day drying procedures particularly with respect to temperature variations due to fuel assembly power and the vacuum processing itself, and variation in hoop stress resulting from higher burnups.

4 Appendix A

Characteristics of PCMM Elements, General Descriptions of Levels and Scoring

Note Bene: This Appendix is copied from M4FT-14LL0810044 for the convenience of the reader.

For a complete understanding of the elements and general descriptions for each level in PCMM, and the subsequent scoring, information from Oberkampf et al. (2007) is reproduced here in Table A-1. Oberkampf recommends a score that matches the level (e.g. level 1, score = 1). In this work we have used scores that allow integer numbers to be generated for grading elements that possess some properties of adjacent levels (e.g. an element has aspects of both level 0 and level 1, score = 1). This scoring "spectrum" is illustrated in Figure A-1.

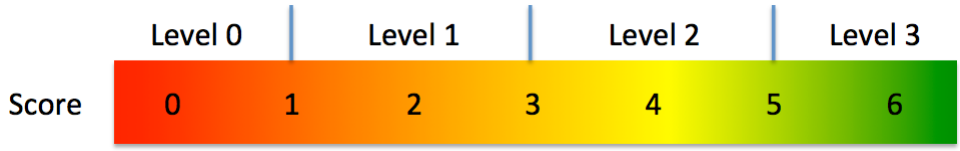

Figure A-1 Scoring "spectrum" for evaluating model and data maturity

In addition to scoring model and data maturity, the score-spectrum can be used to evaluate project maturity (Oberkampf et al. 2007):

- Green – the project assessment meets or exceeds the requirement
- Yellow – the assessment does not meet the requirements by one level or less
- Orange – the assessment does not meet the requirement by two levels or less
- Red – the assessment does not meet the requirement by three levels or less

Table A-1 General description of maturity levels in PCMM elements (Oberkampf et al. 2007)

Representation of Geometric Fidelity	
Level 0	Simplicity, convenience, and functional operation of the system dominate the fidelity of the representation and the geometry for the system being analyzed. There is heavy reliance on judgment and experience, with little or no expectation or quantification of representation and geometric fidelity.
Level 1	Quantitative specifications are applied to describe the geometry of the major components of the system being analyzed. Much of the real system remains stylized or ignored, e.g., gaps in systems, changes in materials, and surface finish.
Level 2	Quantitative specifications are applied to replicate the geometric fidelity of most of the components of the real system. Little of the real system remains stylized or ignored. For example, important imperfections due to system assembly or defects due to wear or damage in the system are included. A level of peer review, such as an informal review or an internal review, of the model representation and geometric fidelity has been conducted.
Level 3	The geometric representation in the model is "as built" or "as existing," meaning that no aspect of the geometry of the modeled real system is missing, down to scales that are determined to be relevant to the level of physical modeling chosen. An example is a

	complete CAD/CAM model for the real system as assembled and meshed for the computational model with virtually no approximations or simplifications included. Independent peer review of the model representation and geometric fidelity has been conducted, e.g., formal review by the M&S effort customer or by reviewers external to the organization conducting the M&S.
Physics and Material Mode Fidelity	
Level 0	The model is fully empirical, or the model form is not known. There is little or no coupling of models representing multiple functional elements of the system, and the coupling that does exist is not physics based. Confidence in the model is strictly based on the judgment and experience of the practitioner.
Level 1	The model is semi-empirical in the sense that portions of the modeling are physics based; however, important features, capabilities, or parameters in the model are calibrated using data from very closely related physical systems. The coupling of functional elements or components is minimal, or ad hoc, and not physics based.
Level 2	All important physical process models and material models are physics based. Calibration of important model parameters is necessary, using data from SETs and IETs. All model calibration procedures are implemented on the model input parameters, not on the SRQs. Important physical processes are coupled using physics-based models with couplings in one direction. Some level of peer review, such as an informal review or an internal review, of the physics and material models has been conducted.
Level 3	All models are physics based with minimal need for calibration using SETs and IETs. Where extrapolation of these models is required, the extrapolation is based on well-understood and well-accepted physical principles. All physical processes are coupled in terms of physics-based models with two-way coupling and physical process effects on physical and material parameters, BCs, geometry, ICs, and forcing functions. Independent peer review of the physics and material models has been conducted, e.g., formal review by the M&S effort customer or by reviewers external to the organization conducting the M&S.
Code Verification	
Level 0	Code verification is based almost entirely on the judgment and experience of the computational practitioners involved. There is little or no formal verification testing of the software elements. Little or no SQE practices are defined and practiced in the implementation, management, and use of the code.
Level 1	Most associated software is implemented and managed with formal SQE practices. Unit and regression testing of the software is conducted regularly with a high percentage of line coverage attained. Verification test suites using benchmark solutions are minimal, and only error measures are obtained in some SRQs.
Level 2	All associated software is implemented and managed with formal SQE practices. Verification test suites are formally defined and systematically applied using benchmark solutions to compute the observed order of convergence of some numerical algorithms. Some features and capabilities (F&Cs), such as complex geometries, mesh generation, physics, and material models, have been tested with benchmark solutions. Some level of peer review, such as an informal review or an internal review, of the code verification has been conducted.
Level 3	All important algorithms have been tested using rigorous benchmark solutions to compute the observed order of convergence. All-important features and capabilities (F&Cs), such as two-way coupling of multi-physics processes, have been tested with rigorous benchmark solutions. Independent peer review of code verification has been conducted, e.g., formal review by the M&S effort customer or by reviewers external to the organization conducting the M&S.
Solution Verification	
Level 0	No formal attempt is made to assess any of the possible sources of numerical error. Any statement about the impact of numerical error is based purely on the judgment and experience of the computational practitioner. No assessment about the correctness of software inputs or outputs has been conducted.

Level 1	Some kind of formal method is used to assess the influence of numerical errors on some SRQs. This could include a posteriori error estimation of global norms, iterative convergence studies, or sensitivity studies to determine how sensitive certain SRQs are to changes in mesh or temporal discretization. A formal effort is made by the computational practitioners to check the correctness of input/output (I/O) data.
Level 2	Quantitative error estimation methods are used to estimate numerical errors on some SRQs, and these estimates show that the errors are small for some conditions of the application of interest. I/O quantities have been verified by knowledgeable computational practitioners who have some level of independence from the M&S effort. Some level of peer review, such as an informal review or an internal review, of the solution verification activities has been conducted.
Level 3	Quantitative error estimation methods are used to estimate numerical errors on all important SRQs, and these estimates show that the errors are small over the entire range of conditions for the application of interest. Important computational simulations are reproduced, using the same software, by independent computational practitioners. Independent peer review of solution verification activities has been conducted, e.g., formal review by the M&S effort customer or by reviewers external to the organization conducting the M&S.
Model Validation	
Level 0	Accuracy assessment of the model is based almost entirely on judgment and experience. Few, if any, comparisons have been made between computational results and experimental measurements of similar systems of interest.
Level 1	Limited quantitative comparisons are made between computational results and experimental results. Either comparisons for SRQs have been made that are not directly relevant to the application of interest or the experimental conditions are not directly relevant to the application of interest. Experimental uncertainties, either in the SRQs and/or in the characterization of the conditions of the experiment, are largely undetermined or based on experience.
Level 2	Quantitative comparisons between computational results and experimental results have been made for some key SRQs from SET experiments and limited IET experiments. Experimental uncertainties are well characterized (a) for most SRQs of interest and (b) for experimental conditions for the SETs conducted; however, the experimental uncertainties are not well characterized for the IETs. Some level of peer review, such as an informal review or an internal review, of the model validation activities has been conducted.
Level 3	Quantitative comparisons between computational and experimental results have been made for all important SRQs from an extensive database of both SET and IET experiments. The conditions of the SETs should be relevant to the application of interest; and the conditions, hardware, and coupled physics of the IETs should be very similar to the application of interest. Some of the SET computational predictions and most of the IET predictions should be "blind." Experimental uncertainties and conditions are well characterized for SRQs in both the SET and IET experiments. Independent peer review of the model validation activities has been conducted, e.g., formal review by the M&S effort customer or by reviewers external to the organization conducting the M&S.
Uncertainty Quantification and Sensitivity Analysis	
Level 0	Judgment and experience are dominant forms of uncertainty assessment. Only deterministic analyses were conducted for the system of interest. Informal "spot checks" or "what if" studies for various conditions were conducted to determine their effect.
Level 1	Uncertainties in the system of interest are identified, represented, and propagated through the computational model, but they are not segregated with respect to whether the uncertainties are aleatory or epistemic. Sensitivity of some system responses to some system uncertainties and environmental condition uncertainties was investigated, but the sensitivity analysis was primarily informal or exploratory rather than systematic. Many strong assumptions are made with respect to the uncertainty quantification/sensitivity analysis (UQ/SA); for example, most probability density functions are characterized as

	Gaussian, and uncertain parameters are considered to be independent of all other parameters.
Level 2	Uncertainties in the system of interest are characterized as either aleatory and epistemic. The uncertainties are propagated through the computational model, while their character is kept segregated both in the input and in the SRQs. Quantitative sensitivity analyses were conducted for most system parameters, while segregating aleatory and epistemic uncertainties. Numerical approximation or sampling errors due to propagation of uncertainties through the model are estimated, and the effect of these errors on the UQ/SA results is understood. Some strong UQ/SA assumptions were made, but qualitative results suggest that the effect of these assumptions is not significant. Some level of peer review, such as an informal review or an internal review, of the uncertainty quantification and sensitivity analyses has been conducted.
Level 3	Aleatory and epistemic uncertainties are comprehensively treated, and their segregation in the interpretation of the results is strictly maintained. Detailed investigations were conducted to determine the effect of uncertainty introduced due to model extrapolations, if required, to the conditions of the system of interest. A comprehensive sensitivity analysis was conducted for both parametric uncertainty and model form uncertainty. Numerical approximation or sampling errors due to propagation of uncertainties through the model are carefully estimated, and their effect on the UQ/SA results is demonstrated to be small. No significant UQ/SA assumptions were made. Independent peer review of uncertainty quantification and sensitivity analyses have been conducted, e.g., formal review by the M&S effort customer or by reviewers external to the organization conducting the M&S.

Additionally, the aggregation of PCMM scores is detailed in Oberkampf et al. (2007), in which they recommend a set of three [or more] scores be combined using the minimum over all elements, the average of all the elements and the maximum of all the elements.

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