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LLNL-TR-659020

LLNL Input to SNL Report on the Composition of Available Data for Used Nuclear Fuel Storage and Transportation Analysis

M. Sutton, J. Wen

August 19, 2014

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This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

LLNL Input to SNL Report on the Composition of Available Data for Used Nuclear Fuel Storage and Transportation Analysis

Used Fuel Disposition Campaign Milestone M4FT-14LL0810044

Mark Sutton and Jiaxuan (Josh) Wen

Lawrence Livermore National Laboratory, 7000 East Avenue, Livermore
California 94550

August 14th, 2014

LLNL-TR-659020

Acknowledgements

The authors greatly appreciate the input of Charles Bryan at Sandia National Laboratory (SCC model), Harold Adkins at Pacific Northwest National Laboratory (thermal profiles), and both Cedric Sallaberry and Remi Dingreville at Sandia National Laboratories (PCMM and mathematical characterization).

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Acronyms

BC	boundary condition
BRC	Blue Ribbon Commission
BWR	boiling water reactor
CFD	computational fluid dynamics
CISCC	chloride-induced stress corrosion cracking
DOE	Department of Energy
DRH	deliquescence relative humidity
DSC	dry shielded canister
FCT	Fuel Cycle Technologies
HLW	high-level waste
ISFSI	independent spent fuel storage installation
LLNL	Lawrence Livermore National Laboratory
M&S	modeling and simulation
NE	Nuclear Energy
NOAA	National Oceanic and Atmospheric Administration
NRC	Nuclear Regulatory Commission
PCMM	Predictive Capability Maturity Model
PNNL	Pacific Northwest National Laboratory
PWR	pressured water reactor
QA	quality assurance
RH	relative humidity
SA	sensitivity analysis
SCC	stress corrosion cracking
SET	separate effects test
SNF	spent nuclear fuel
SQE	software quality engineering
SRQ	system response quality
SS	stainless steel
ST	storage and transportation
UFD	Used Fuel Disposition
UQ	uncertainty quantification

1. Introduction

This report satisfies the Lawrence Livermore National Laboratory (LLNL) Level 4 milestone: M4FT-14LL0810044 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-14-LL081004. The information in this report will provide input to a parent Sandia National Laboratories (SNL) milestone and will be supplemented with input from other organizations including SNL, PNNL and INL.

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 documents two phenomena that could affect the safety and licensing of dry spent fuel storage casks and their contents, and discusses modeling frameworks and evaluations that will are being developed and implemented. This work will continue in the remainder of FY14 and into FY15. The report also presents a method for evaluation and communication of model and data maturity, and an introduction to uncertainty quantification (UQ).

1.1 High Priority Phenomena of Used Nuclear Fuel Storage

The UFD Campaign has chosen to demonstrate the UQ framework on two previously identified gaps associated with the storage and transportation of used nuclear fuel, namely degradation-specific *atmospheric corrosion* leading to stress-corrosion cracking (SCC) of a welded cask/canister, and the crosscutting *thermal profile* phenomenon. The thermal profile affects the degradation rates of all of the structure, system and components, which include corrosion, creep, cracking and embrittlement, etc. Therefore, identifying and reducing the uncertainty in the thermal profile can positively impact the uncertainty of many other degradation mechanisms and licensing factors in the storage and transportation of casks, canisters and fuel assemblies. These two cases represent two extremes of phenomena (a) *simple* with the benefit in improving uncertainties in one degradation mechanism, and (b) *complex* with potentially large benefits in improving uncertainties across a wider range of degradation mechanisms affected by crosscutting phenomena. The phenomena and degradation mechanisms affecting storage cask safety and licensing are not limited to only thermal profile and SCC, which serve as high priority examples of knowledge, model and data gaps than can be addressed through UQ.

1.1.1 Thermal Profiles

Almost all degradation mechanisms for storage casks are sensitive to temperature and in some cases, temperature history (Cuta et al., 2013). The basis for the transfer of thermal energy from used fuel pellets to the outer surface of the storage cask is involves conduction, convection and radiation of heat from the fuel through concentric layers materials that span from cladding, assemblies and internal structures (e.g., basket) to the canister and cask components (e.g. vent, support array, wall, shielding etc.), the ground pad and the atmosphere. In addition, spaces (gaps) between fuel rods, fuel assemblies, baskets, canisters and casks exist, in some cases filled with an inert gas, while in others can be represented by a flow of air. Figure 1-1 (Suffield et al, 2012, courtesy of AREVA) and Figure 1-2 (Cuta and Adkins, 2014, courtesy of Holtec International) provide a visual example of different material layers and gaps that should be considered.

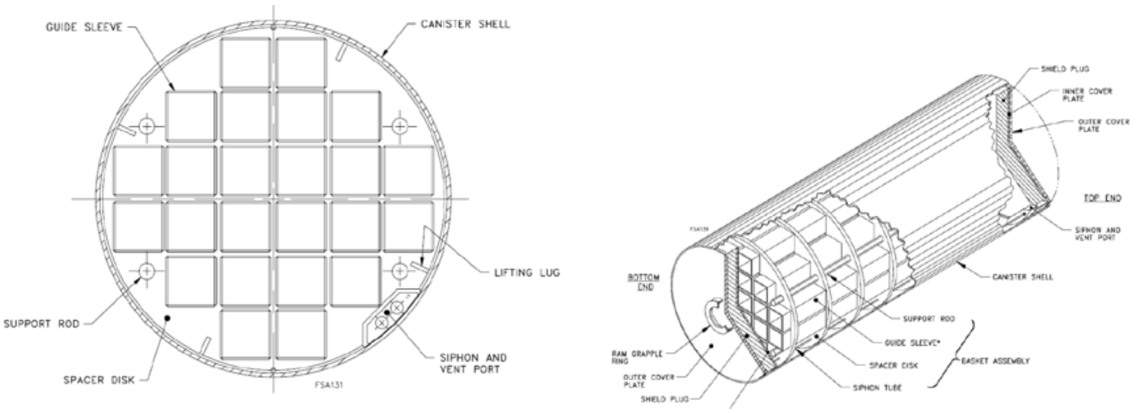


Figure 1-1. Illustrative diagrams of 24P DSC geometry (images courtesy of AREVA)

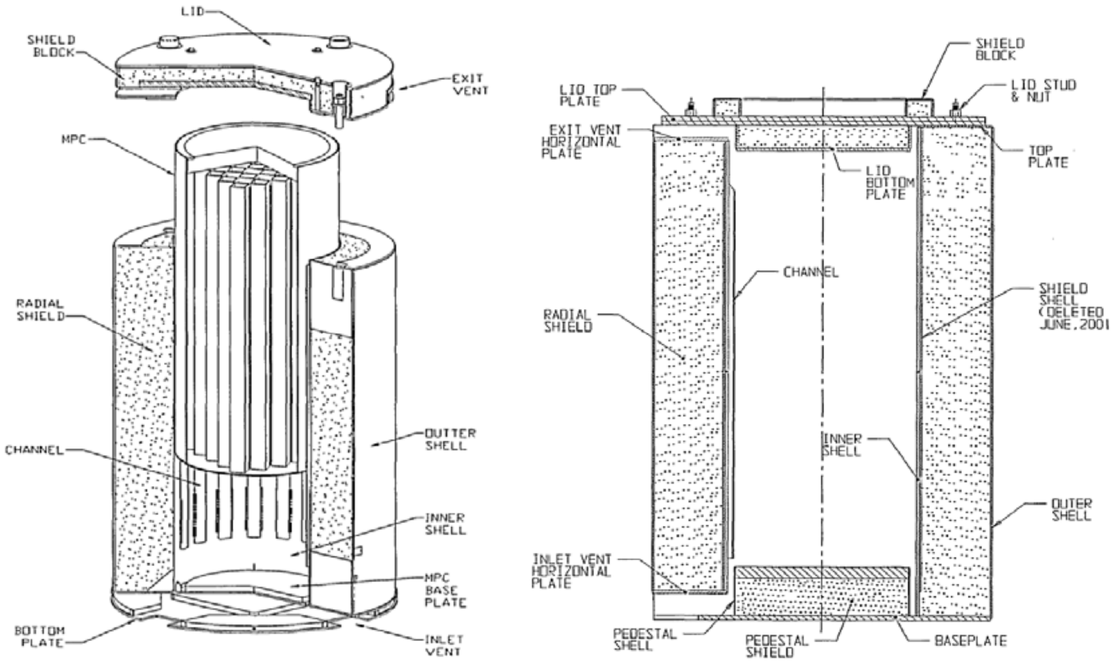


Figure 1-2. Typical HI-STORM 100S vertical storage module (image courtesy of Holtec International)

More information on the considerations of heat transfer on the thermal profile of storage casks and contents is given in Section 2.1.

In an evaluation of technical gap prioritization, all organizations and counties (with the exception of Spain and Japan) ranked both the consequence and the likelihood of thermal profile uncertainties affecting licensing ability as very high and that more thermal modeling is needed (U.S. DOE, 2012). Regulations in Japan limit peak cladding temperature to only 275°C, much lower than the 400°C peak cladding temperature limit in the U.S. (U.S. DOE, 2012). Further information can be found in the Mathematical Characterization document under revision for UFD's Storage and Transportation Analysis work package (WBS 1.02.08.10).

1.1.2 Atmospheric Corrosion of Welded Canisters

The atmospheric-induced SCC can be divided into 3 model levels, each of which are a condition that needs to be realized before SCC can occur:

1. Corrosive environment (including chemical environment on the surface of the canister, surface temperature and relative humidity; all of which are influenced by the geographic location of the storage cask)
2. Tensile stress (as observed in welded canisters)
3. Susceptible material (e.g. *201, 301, 302, 304, 309, and 316 steels, although –L steels have less susceptibility)*

Many storage cask designs utilize ventilation that allows decay heat to dissipate by thermal convection to the atmosphere. Cooler air is drawn into the cask ventilation, passing over the canister with warmer air exiting the cask. The flow of air over the canister also allows atmospheric dust to follow the same path, some of which is deposited on the surface of the canister. The geographic location of the storage facility impacts the composition of dust, with coastal sites containing higher amounts of chloride-bearing sea-salts (EPRI, 2005) and ammonium salts (Enos et al., 2013). Inland sites containing higher levels of silicate, carbonate and aluminate material impacted by local soil and geology. As the temperature and relative humidity fluctuate at a site, components of the deposited dust (particularly chlorides) can dissolve in absorbed moisture (deliquescence). The dissolved ions are then available to participate in corrosion of the canister. Research has shown that with deposited sea salt, a relative humidity at or above 15% can support deliquescence and subsequent corrosion of the canister steels.

Tensile stress can be either residual (pre-existing) or exerted. Residual stresses are the most prominent and problematic of the two stress components in the case of storage canisters and occur after welding of the canister. During fabrication, two cylinders are cold-rolled from sheet steel. The edges of the cylinder are joined using a double-V longitudinal (axial) weld to form complete cylinders. The two cylinders are joined using a double-V butt-joint circumferential weld and a further circumferential weld is used to apply the bottom plate to the cylinder. The canister is then closed with a single-V circumferential weld. The welding leaves the steel vulnerable to intergranular corrosion and high residual stresses are known to be present in the heat-affected zone (HAZ) of the welds (Ferry et al., 2013; Kusnick et al., 2013).

Enos and Bryan (2012) identified key materials for construction of welded interim storage containers, including shell and lid. The materials include 304, 304L, 316, 316L, "steel" and "coated carbon or stainless steel". Jones (1996) states that austenitic stainless steels such as those listed here in chloride hot environments are perhaps the most widely known and intensely studied examples of SCC. Jones (1996) also notes that although relatively rare, SCC at ambient temperature in the presence of concentrated chlorides and strong oxidizers (McIntyre and Dillon, 1985; Dillon, 1990).

Another factor that can affect corrosion (including SCC) is the presence of gamma radiation from the encased fuel leading to the formation of radials and molecules after radiolysis of the water (and brine) on the surface of the waste canister. Some of the species are highly oxidizing and their reactions in pure water are numerous. In brine solutions, the reactions (and shear number of species) is complex, including radials and molecules of chloride species. Farmer et al. (1988) reviews work performed on gamma irradiation of austenitic stainless steels (such as 304) in water and salt solutions, generally finding that the irradiation increased intergranular SCC even at low chloride concentrations.

In summary, the three requirements for SCC are presenet at the weld region of UNF canisters when chloride-containing salts deposit via deposition of dust during passive cooling. Additional information on each of these three requirements (and the understanding of each as they relate to SCC initiation) is given in Section 2.2 of this report. Once SCC is initiated, the environmental conditions need to be evaluated for propagation leading to a through-wall crack. The Nuclear Regulatory Commission highlighted the concern of chloride-induced SCC (CISCC) in a note sent to ISFSI license holders and applicants (NRC, 2012). In an evaluation of technical gap prioritization, all organizations and counties (with the exception of Spain) ranked both the consequence and the likelihood of SCC affecting licensing ability as very high (U.S. DOE, 2012). Spain ranked SCC resulting from atmospheric corrosion low due to planned vaults housing UNF canisters. Further information can be found in the Mathematical Characterization document under revision for UFD's Storage and Transportation Analysis work package (WBS 1.02.08.10).

1.2 Uncertainty Quantification

Both the thermal profile of storage casks and the degradation of the welded canister (from deposition and subsequent deliquescence of dust resulting in SCC) involve multi-physics processes. Uncertainties arise in simulation models due to a lack of precise knowledge about the physical processes, the model parameters, initial and boundary conditions, etc. As a result, the credibility of a model cannot be established without a thorough and rigorous uncertainty quantification (UQ) that can (Tong, 2008):

- characterize the output uncertainties of a simulation model (or, uncertainty analysis)
- identify the major sources of uncertainties of a model (or, sensitivity analysis, SA)
- establish the integrity of a simulation model (validation)
- tune a simulation model to match better with experiments (calibration)
- assess the region of the validity of a simulation model (risk analysis)
- provide information on which additional experiments are, needed to improve the understanding of a model (parameter exploration)

The first stage of the uncertainty quantification is to identify all of the input parameters and relevant multi-physics equations. The level to which the investigation will go should be determined at this stage, either back to basic principles or higher-level assumptions and knowledge.

The second task (which is the beginning of the UQ process) is to identify the model. This will involve compilation of detailed specifications including the simulation model, uncertainty parameters that will be varied, uncertain parameters which will be fixed in the current study but will affect the outcome of the analysis if they are varied, simulation output responses.

The third task is to characterize each of the parameters in terms of experimental data, literature data, expert judgment and any results from the validation feedback of the UQ process. Here is where parameters will be classified as aleatory or epistemic, which will determine the type of UQ model used.

The fourth task is to screen the parameters. This is important, since some parameters (and the associated uncertainty) will greatly affect the final result, while others will not. The degree to which the parameter affects the result is one consideration, while the amount by which the uncertainty can be reduced in any given parameter is another. There becomes a trade-off of the level of knowledge gained from UQ with cost and time at this point. If the first task has led to a large number of uncertain input parameters (e.g. significantly more than 100), it is recommended that a coarse down-select be performed (e.g. using the Plackett-Burman or low-resolution Morris-on-at-a-time "MOAT" experimental design) to result in less than 100 uncertain parameters. If the number of uncertain parameters is much larger than 10, an additional high-fidelity down-select is recommended using a multi-algorithmic approach such as Morris screening (means and standard deviations of the gradients to rank parameter importance) or Bayesian screening (using Gaussian process and Markov chain Monte Carlo to extract sensitivity information).

The fifth task is to develop a response surface by varying two parameters, overlaying physical experimental data and uncertainties, and interpolating over the validation domain. A space-filling sampling design is typically needed.

The sixth task is a focused uncertainty analysis in which output uncertainties are characterized in terms of means and standard deviations. The parameter sensitivities are then quantified and a risk analysis is performed based on design thresholds. Additionally, the model parameter may be tuned to better match known experimental data.

The first three stages of the process are described in this report. The method of characterizing relevant models and data associated with degradation and crosscutting phenomena was described by Dingreville (2013). For each degradation mechanism, we will identify applicable and associated models. These models will be characterized based their maturity and classified into five groups with increasing uncertainty:

1. Models directly available and applicable to storage and transport.
2. Abstraction/simplified models or discrepancy in model characterization.
3. Model yet to be developed based on theoretical understanding.
4. No model available but correlation between input and output available.

5. No model available (missing physics) requiring expert solicitation.

Data source will be categorized into four levels based on the appropriateness and confidence of the information:

I. Data directly applicable to transportation and storage.
II. Data from experiments and numerical models (need for up-scaling/extrapolation of the data).
III. No data available (expert solicitation)
IV. Categorical (no quantifiable data)

This effort will identify and compile the available data and models and characterize the associated uncertainty, with results and discussion documented in Section 2 and Appendix B (thermal profile) of this report.

1.3 Predictive Capability Maturity Model

The Predictive Capability Maturity Model or PCMM (Oberkampf et al., 2007) is being used to ascertain a qualitative measure of credibility within both the UFD ST Analysis UQ task and the overall UQ methodology. Used as a communication tool, PCMM will inform the UFD Campaign and stakeholders of the level of maturity of each of the model components and capabilities (in this case, thermal profiles and atmospheric chloride-induced SCC of welded canisters), identifying clear gaps and aiding decision making for focused research. These objectives are achieved through a multi-dimensional, qualitative metric that:

- determines the readiness of UFD Campaign UQ issues
- identifies gaps in credibility of the various models, and
- measures the progress of the integrated simulation effort.

There are six elements of the PCMM matrix as identified by Oberkampf et al. (2007) that should be used to contribute to decision making:

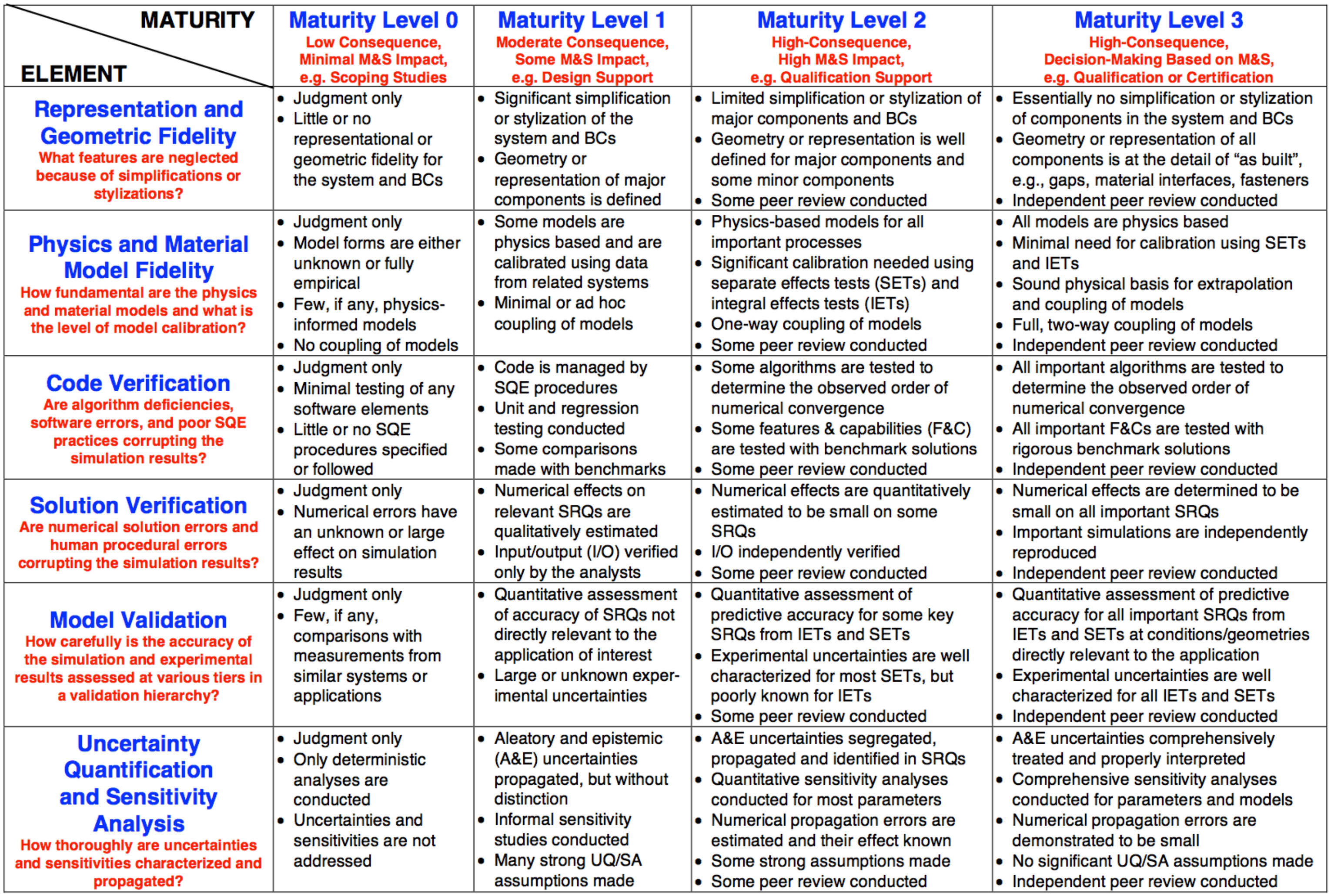
- Representation and geometric fidelity
- Physics and material model fidelity
- Model verification
- Solution verification
- Model validation, and
- UQ and sensitivity analysis

Each element is analyzed and given a maturity level score (from 0 to 3) based on accuracy, correctness and objectivity of intrinsic information, and the completeness, amount of available information and level of detail for contextual information (Oberkampf et al., 2007; Wang and Strong, 1996). The characteristics of each maturity level are (Oberkampf et al., 2007):

- Level 0 – Little or no assessment of the accuracy or completeness has been made; little or no evidence of maturity; individual judgment and experience only; convenience and expediency are the primary motivators. This level of maturity is commonly appropriate for low-consequence systems, systems with little reliance on modeling and simulation (M&S), scoping studies, or conceptual design support (0 points).
- Level 1 – Some informal assessment of the accuracy and completeness has been made; generalized characterization; some evidence of maturity; some assessment has been made by an internal peer-review group. This level of maturity is commonly appropriate for moderate consequence systems, systems with some reliance on M&S, or preliminary design support (2 points).
- Level 2 – Some formal assessment of the accuracy and completeness has been made; detailed characterization; significant evidence of maturity; some assessments have been made by an internal peer review group. This level of maturity is commonly appropriate for high-consequence systems, systems with high reliance on M&S, qualification support, or final design support (4 points).
- Level 3 – Formal assessment of the accuracy and completeness has been made; precise and accurate characterization; detailed and complete evidence of maturity; essentially all assessments have been made by independent peer-review groups. This level of maturity is commonly appropriate for high-consequence systems in which decision-making is fundamentally based on M&S, e.g., where certification or qualification of a system's performance, safety, and reliability is primarily based on M&S as opposed to being primarily based on complete system testing information (6 points).

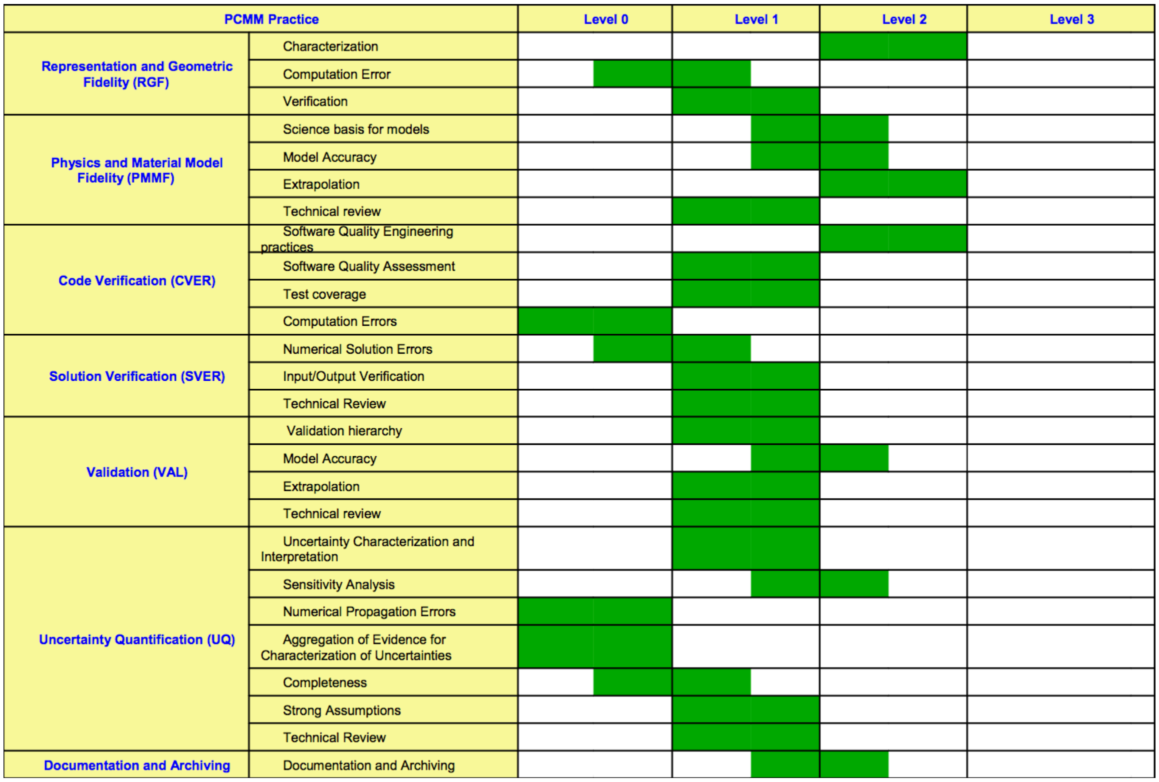
Table 1-1 (reproduced from Oberkampf et al., 2007) provides general descriptions for table entries within the PCMM framework. Additional descriptions for each PCMM element are reproduced in Appendix A.

Table 1-1. General descriptions for PCMM table entries (reproduced from Oberkampf et al., 2007)



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

Since assessment of maturity may not meet all criteria within a given level, the 2-points per level can be further divided to represent characteristics of two different maturity levels. For example, if a model has some maturity represented by Level 2, and other aspects are matured to Level 3, a score of 5 (between 4 and 6) can be awarded for each aspect of the 6 elements of PCMM. Additionally, since PCMM is used as a communication tool, the documentation and archiving of models and data is included in the PCMM score table. Figure 1-3 provides a graphical representation of how PCMM can measure and communicate model maturity and progress (Dingreville, 2014).



PCMM Practice		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 practices					🟩	🟩	
	Software Quality Assessment			🟩	🟩			
	Test coverage			🟩	🟩			
	Computation Errors	🟩	🟩					
Solution Verification (SVER)	Numerical Solution Errors		🟩	🟩				
	Input/Output Verification			🟩	🟩			
	Technical Review			🟩	🟩			
Validation (VAL)	Validation hierarchy			🟩	🟩			
	Model Accuracy				🟩	🟩		
	Extrapolation			🟩	🟩			
	Technical review			🟩	🟩			
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				🟩	🟩		

Figure 1-3. Example PCMM score table

2. Composition of Available Data and Models

2.1 Uncertainties in Thermal Modeling and Profiles of Used Fuel Storage Casks

As discussed in Section 1.1.1, three mechanisms exist for the transfer of thermal energy emanating from the used nuclear fuel to the waste canister and storage cask, namely conduction, convection and radiation heat transfer. The equations relevant to heat transfer in storage and transportation packages/casks are described by Wen and Hagler (2013).

Conduction is applied across gaps or through solid walls. For 1D conduction through a flat plate, Fourier's law describes the heat transfer rate,

$$Q = -KA\frac{dT}{dX}$$

where Q = heat transfer rate, K = thermal conductivity, A = area, T = temperature, X = length that heat flow through. The minus sign is a consequence of the fact that heat is transferred in the direction of decreasing temperature.

The heat flux $q = Q/A$ and the thermal resistance in linear conduction for length, L, is:

$$R_c = \frac{L}{KA}$$

For a cylindrical with radial thermal resistance (Figure 2-1), the heat transfer rate per unit length can be calculated as:

$$Q_L = \frac{Q}{L} = \frac{2\pi K(T_o - T_i)}{\ln\left(\frac{r_o}{r_i}\right)}$$

where r_i and r_o are the inner and outer radii of the cylinder, T_i and T_o are the temperatures at the inner and outer surfaces of the cylinder, and the heat source is central to the cylinder.

For radial conduction in hollow cylinders, thermal resistances over the length, L is of the form:

$$R = \frac{\Delta T}{Q_r} = \frac{ln\left(\frac{r_o}{r_i}\right)}{2\pi LK}$$

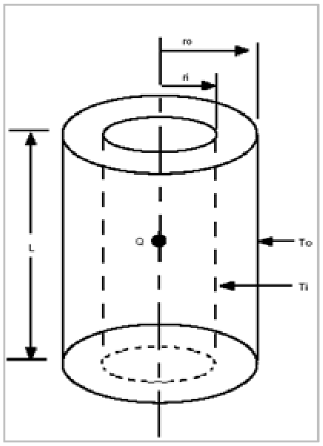


Figure 2-1 Schematic of conduction in a cylinder

If two pieces of material or components are bolted together, thermal resistance will exist at the joint.

Convection is applied in gaps or on external surfaces, where heat is transferred inside solid by conduction and convection at the solid-fluid interface. At the boundary, Newton's law of cooling is applied,

$$q = \frac{Q}{A} = h_c\left(T_s - T_f\right)$$

where q = heat transfer flux, h_c = convection coefficient, A = area, T_s = surface temperature and T_f = fluid bulk temperature.

The thermal resistance associated with convection can therefore be described by:

$$R_{conv} = \frac{1}{h_c A}$$

Heat is also transferred by radiation from a surface, either across gaps or from external surfaces, is scaled with absolute temperature. For storage casks, both concentric cylinder and parallel plate geometries are present. For exchange between long concentric cylinders, the following equation is used:

$$Q = \frac{\sigma A_1\left(T_1^4 - T_2^4\right)}{1/\varepsilon_1 + \left(A_1/A_2\right)\left(1/\varepsilon_2 - 1\right)}$$

For exchange between infinite parallel plates, the following equation is used:

$$Q = \frac{\sigma A_1\left(T_1^4 - T_2^4\right)}{1/\varepsilon_1 + 1/\varepsilon_2 - 1}$$

Radiation from a heated surface to surrounding environment can be described as follows:

$$Q = \sigma \varepsilon_{eff} F^{*}_{s-e} A_s \left(T^4_{surf} - T^4_e \right)$$

where Q = heat transfer rate, A = area, T = temperature (must be in absolute temperature K, if in metric unit), σ= Stefan–Boltzmann constant = 5.673 x 10^{-8} W/m^2 K^4 (0.1712 x 10^{-8} Btu/hr–ft^{2}R^4), ε = surface emissivity (emittance), and F^* = exchange coefficient (combined view factor and emissivities)

As can be seen from the equation, heat transfer by radiation is 4th order dependent on temperature, so uncertainties in temperature can greatly affect the calculation heat transfer.

Kirchhoff's law of thermal radiation for solid bodies relates absorptivity (α_λ, which is the ratio of the energy absorbed by the wall to the energy incident on the wall for a wavelength, λ) to the ε_λ is the emissivity at a wavelength λ,

$$\alpha_\lambda = \varepsilon_\lambda$$

Figure 2-2 shows a simplified cross-section of a storage cask (Cuta and Adkins, 2014) and a cask array (Easton, 2012), while Figure 2-3 shows a schematic sub-channel gap between fuel rods in a fuel assembly (McKinnon et al., 1992). These two figures demonstrate the two extreme scales of heat transfer across a gap within the confines of a used fuel storage cask.

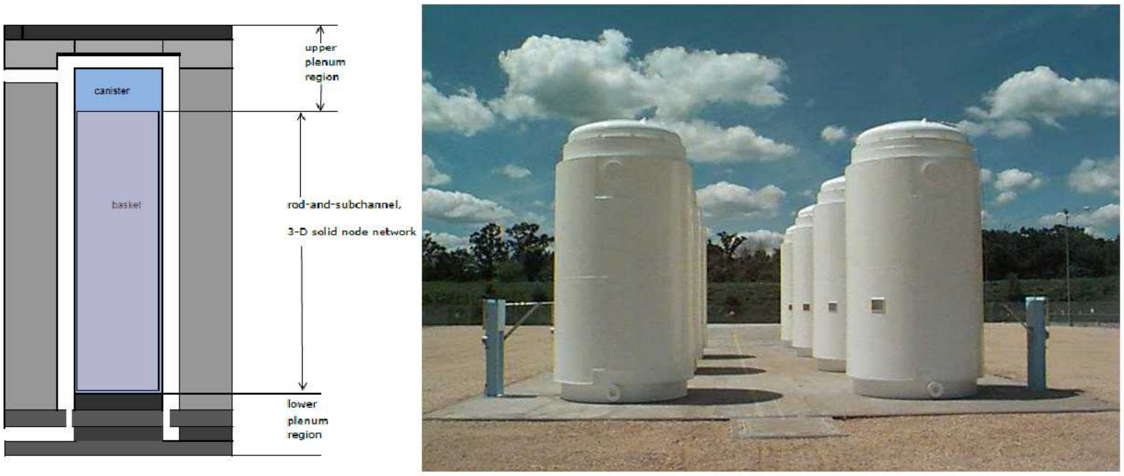


Figure 2-2. Cross-section view of a cask (Cuta and Adkins, 2014) and Cask Array (Easton, 2012)

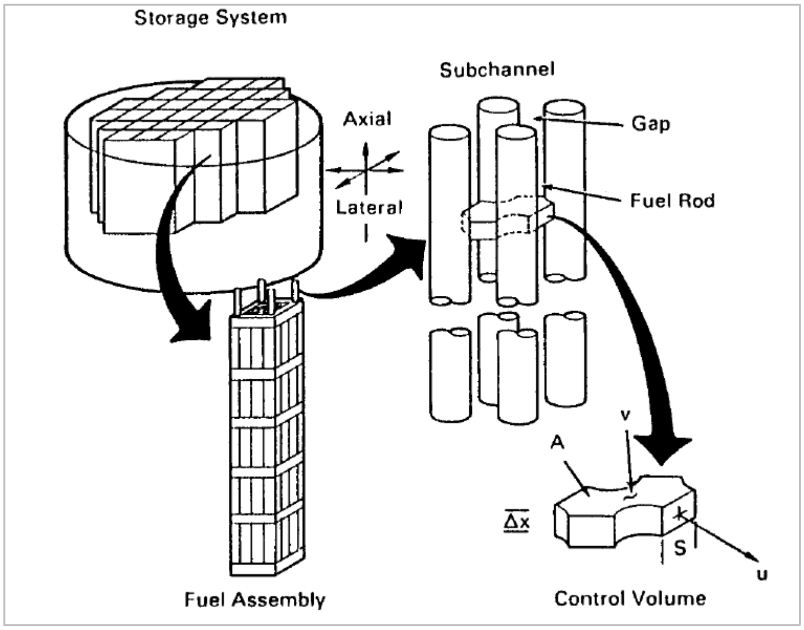


Figure 2-3. Schematic diagram of sub-channels in fuel assemblies (McKinnon et al., 1992)

In evaluating pertinent data and models, over 78 documents involving analyses (modeling) relevant to thermal profiles were found in the open literature (Adkins, 2012). The review of these documents is currently in progress with respect to understanding uncertainty and model/data maturity. A table identifying the documents reviewed so far, the type of study and cask configuration and associated identified uncertainties is given in Appendix B. Documents are characterized based on their maturity and classified into the 5 groups discussed in section 1.2, ranging from models that are directly available and applicable to storage and transport, to areas of missing physics where no model is available and requires expert solicitation is required. Uncertainty sources associated with thermal modeling to predict the maximum surface temperatures during storage are described below.

Uncertainties in Design / As-Build Geometry

Some cask vendors have provided design documents with geometries that have allowed more precise models to be generated. Modeling of other vendor/cask designs will rely on generic design geometry. Specifically, storage casks are licensed using a generic Safety Analysis Review for Packaging (SARP), for example those described in McKinnon et al. (1992), Suffield et al. (2012) and Cuta and Adkins (2014). Later, minor changes in dimensions and geometry are approved separately and SARPs are not always readily or publically available. This adds to the uncertainty in the ability to model thermal profile. Examples include changing a ventilation pathway, adding screening on ventilation ducts, and adding a flange to the base pedestal (Adkins, 2014).

Uncertainties in Material Thermal Properties

Uncertainties exist in the thermal properties of each of the component materials within a storage cask, from pellet and assembly to canister and cask. Such properties include the following:

- Density
- Specific heat
- Thermal expansion
- Thermal conductivity
- Thermal diffusivity
- Material strength
- Surface emissivity

The thermal conductivity and surface emissivity of cask component materials are given in Table 2-1 and Table 2-2. The average basket temperature was used to predict thermal expansion in McKinnon et al. (1989), and the gap conductance between fuel pellet and cladding is assumed constant (Rector and Michener, 1989).

Table 2-1. Thermal conductivities of cask components (Creer et al, 1987; McKinnon et al., 1986, 1989 and 1992; Rector et al., 1986)

Thermal Conductivities	Watt/m-°C	Btu/ft-hr-°F
Steel cask body	41.5	24.0
Polyethylene resin	0.2	0.1
Aluminum basket	206.0	117.0
Copper fins	337.3	218.0
Steel shell	41.5	24.0
Polypropylene	0.2	0.1

Table 2-2. Surface emissivity of cask materials

Material	Emissivity
Fuel rods	0.8 (Creer et al., 1987; McKinnon et al., 1986; Rector et al., 1986a; Rector et al, 1986b)
Stainless steel surfaces	0.2 (McKinnon et al., 1986)
Copper surfaces	0.5 (McKinnon et al., 1986; Rector et al, 1986b)
Lead surfaces	0.6 (McKinnon et al., 1986)
Fuel basket	0.4 (Rector et al., 1986a)
Nickel-plated surface	0.25 (Rector et al., 1986a)
Cask stainless steel inner liner	0.6 (Lombardo et al., 1986)
Cask surface (stainless steel)	0.3 (Rector et al, 1986b)

In addition to uncertainty in standard/reference values for thermal properties, there also exists uncertainty in the temperature dependence. Several of the thermal properties are also a function of temperature and therefore change over time as the cask (and contents) cools and is subject to changes in atmospheric temperature. For example, the thermal conductivity of stainless steel ranges from 14 W/mK at 0°C to 19 at 200°C (Hayes, 2014). The thermal diffusivity of 310SS can change from 3.352 to 4.075 mm^2s^{-1}, at temperatures from 25°C to 250°C. The specific heat capacity of 310SS increases from 0.483 to 0.525. The density decreases with temperature from 7.829 to 7.742 for the same temperature conditions (Hayes, 2014).

Similarly, the surface emissivity depends on temperature, fabrication and surface finish, including polishing and subsequent oxide buildup (Lombardo et al., 1986). The surface emissivity of polished 316SS increases from 0.28 at 24°C to 0.57 at 232°C.[*] The surface emissivity values were a major source of uncertainty in simulations in previous work, with low confidence in these values and small changes in the fuel tube emittance representing a large change in the radiative heat transfer to (and from) the fuel tube (Lombardo et al., 1986).

Another factor in the material thermal properties that should be considered (and which also changes with temperature) is the fill gas. If the canister were to incur a leak, helium would be replaced with air. The result would be a change in the density, thermal conductivity and specific heat capacity of the gas occupying the canister. Table 2-3 shows that there would be significant thermal changes that occur in the fill-space if the backfill gas was exchanged. Some models assume a constant value, unchanged over time (Cuta and Adkins, 2014).

Table 2-3 Density, thermal conductivity and specific heat capacity of gases at 200°C (Incropera and DeWitt, 1990)

Gas	Density (kg/m^3)	Thermal conductivity (W/m.k)	Specific heat capacity (J/kg.K)
Air	1.188	0.038	1,007
Helium	0.163	0.205	5,200
Argon	1.66	0.026	520
Nitrogen	1.67	0.018	1043

Uncertainties in the Manufacturing and Assembling Processes

Uncertainties exist in the manufacturing and assembly of the cask, canister and (after removal from the reactor and subsequent pool storage) the assemblies. Some uncertainty considerations include:

- the assumed straightness of fuel assembly and basket cells
- the assumed concentricity of the fuel assembly relative to the basket cell, and the basket relative with canister during assembly process
- the estimated gap size:

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[*] http://www.coleparmer.com/TechLibraryArticle/254

    - the gap between basket and inner cask wall dominates thermal resistance in radial conduction path (Creer et al., 1987; McKinnon et al., 1986)
    - conduction heat transfer between the basket and the canister wall was neglected (McKinnon et al., 1989)
    - the gap between basket and the cask wall is assumed to be nominal, 13mm (Rector et al., 1986a)
- the emissivity (considering view factor and finished condition) of the inside and outside surfaces of the fuel rods/assemblies and fuel basket are estimated to be 0.8, while the canister and cask are both estimated to be 0.9 (Creer et al., 1987; McKinnon et al., 1989)
- the estimated pressure applied at the joint contacts:
    - using separated laboratory components to determine contact resistance (McKinnon et al, 1986)
    - large uncertainties exist in the contact resistance between the heater rod and the flange, as well as the contact heat transfer area (Lombardo et al., 1986)

Uncertainties in Heat Generation in the Fuel Assemblies

Uncertainties exist in the heat generation in the fuel assemblies, due to uncertainties in burn-up (and the distribution of burn-up within an assembly). The following inputs to thermal profile are therefore affected, require estimation and are sources of uncertainty:

- total decay heat
- axial temperature profile
- assembly axial position
- averaged distribution of un-uniformed fuel assemblies with the canister

The total decay heat per canister is very sensitive to the maximum cladding temperature during early storage lifetime. Measured data rather than assumptions or estimates should be directly used in the analysis model.

Uncertainties in Heat Transfer to the Environment

In addition to heat transfer within the cask and canister, heat transfer to the environment (heat-sink) also requires estimation and therefore has associated uncertainties. The following factors are considered areas of uncertainty:

- using a constant ambient temperature rather than seasonal variations

- using average solar radiation on the flat and curve surfaces from 10CFR part 71.71
- estimating convection coefficients caused by wind
- estimating emissivity for the outside painted/coated surfaces of the cask
- conservatism in the cask-to-pad conduction values.

The use of actual measured local ambient temperature, solar radiation and wind-speed as well as cask surface temperature and emissivity in the models could show different thermal behavior in winter and summer months.

Uncertainties in Numerical Methods

Uncertainties exist in the implementation and design of numerical methods and models. For example, the simulated model results should converge as the improving mesh size. Since fuel assembly designs are typically complex, thermal models are often simplified and introduce uncertainties. Such models should be evaluated against actual thermal measurements on the surface of the cask and canister.

In most thermal codes, the analyst exercising the model may select an internal convection coefficient, *h* from some published correlation equations rather than actual values. Another example includes the use of computational fluid dynamics (CFD) codes, where the buoyancy effects that drive natural circulation of the backfill gas are calculated with a Boussinesq approximation with very small time-steps. Comparing internal convection and internal radiation should also be considered because of the temperature-dependency of thermal properties. Areas of uncertainty in numerical models include:

- choosing a coarse mesh size rather than a finer mesh
- absence of detailed the geometry and estimated effective material thermal properties
- estimating internal convection coefficients
- selections made in computational fluid dynamics
- estimating internal surface emissivity
- lack of validation against actual cask and canister measurements

2.2 Atmospheric Corrosion

UNF canisters are manufactured from austenitic stainless steels that are susceptible to chloride-induced stress corrosion cracking (CISCC). As discussed in Section 1.1.2, three phenomena are needed for CISCC, namely the presence of chloride, stress and susceptible material. Several factors that create the conditions necessary are known and do not need to be modeled. However, there are uncertainties associated with each factor.

One example of known information is the presence and concentration of chloride in atmospheric dust (either from dust analysis or rainwater analysis) at or near storage sites. A map of the current sites that store nuclear fuel is shown with an approximate overlay of chloride concentrations in rainwater in Figure 2-4. Blue points indicate sites with dry storage, solid red points indicate planned storage before 2015, open red points indicate sites with unknown plans or intentions for dry storage (NWTRB, 2010). Solid black points are rainwater analysis locations (EPRI, 2005). More detailed analysis of rainwater and dust composition can be found on databases including those managed by National Oceanic and Atmospheric Administration (NOAA)† and the National Atmospheric Deposition Program (NADP)‡. The data is available for each site, but must be collected before models of each site can be evaluated. There will be seasonal variations, and perhaps periodic highs and lows during years of severe storms or dry-spells.

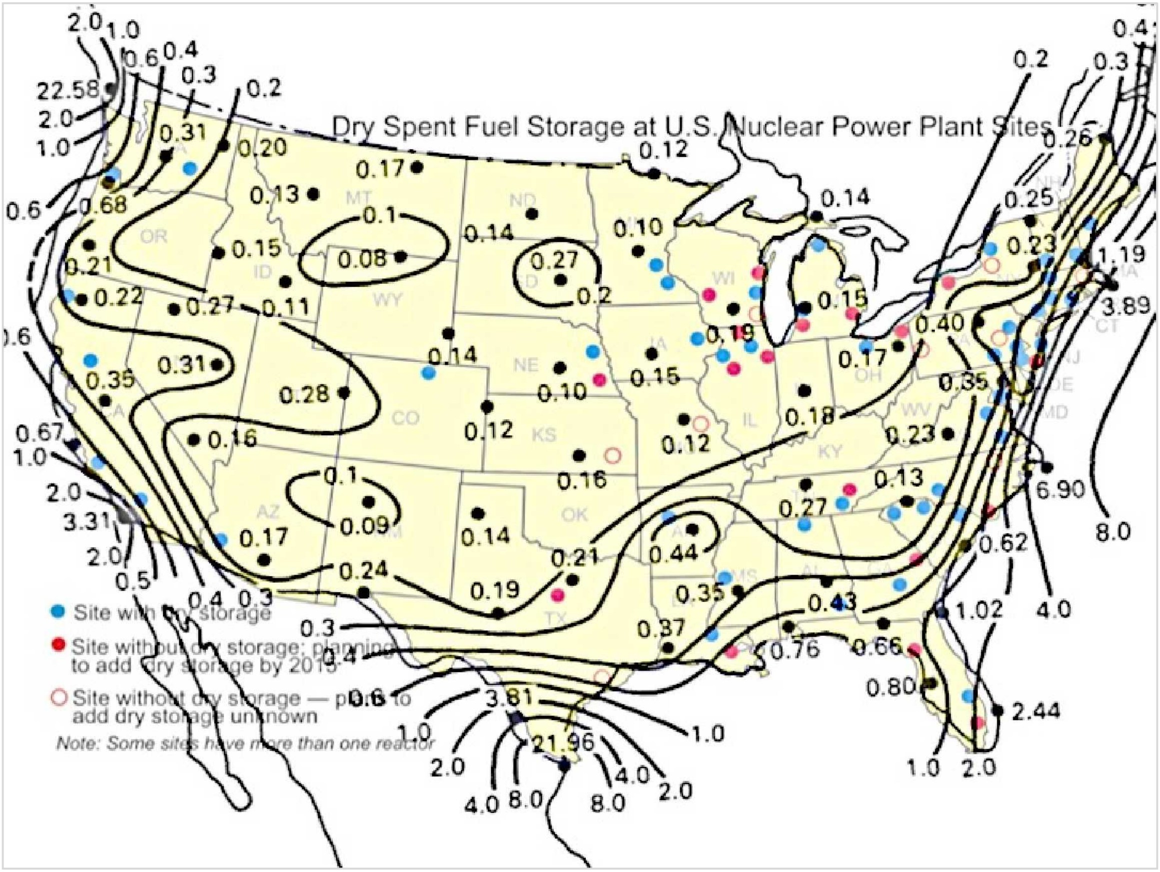

Figure 2-4 Overlaid storage site locations (NWTRB, 2010) and chloride concentration in rainwater (EPRI, 2005)

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† http://www.noaa.gov

‡ http://nadp.sws.uiuc.edu

Similarly, the historic temperature and relative humidity at or near sites is also known from meteorological data. Data are typically reported hourly or daily, weekly and monthly with highs, lows and averages that introduce uncertainty.

However, while the environmental conditions at the site are known, the dust deposition rate (and therefore the amount of dust containing potentially corrosive elements) is not well known. As with dust composition, seasonal highs and lows may exist, with anomalies for severe weather. Two methods are available to determine the amount of dust deposited, namely direct collection and measurement of the dust from example casks such as that previously performed by the UFD Campaign in collaboration with EPRI (EPRI, 2014), or deposition modeling using fluid dynamics to simulate where dust might deposit on the canister. The latter is significantly more difficult because the historical levels of dust in the atmosphere available to be deposited are not known and are a factor or particulate matter, temperature, wind velocity and direction, and precipitation.

The concentration of chloride needed to initiate CISCC on stainless steel is also well understood and has been the subject of much investigation over many years. Over 1000 articles on pitting, crevice corrosion and SCC of austenitic materials (including 304 and 316 relevant to this work) and potential waste package materials was reviewed by Farmer et al. (1988; 1999), including the basis for pit initiation as well as crack initiation and propagation. For pitting, Farmer et al. (1988) specifically highlights the work by Okada (1984a,b) where the pitting potential is derived from both the induction time and the critical size for a stable halide nucleus. Farmer et al. (1988) also highlight the work by Manning et al. (1980) in that pits can nucleate at inclusions in the alloy surface, and Chao et al. (1981) where pit initiation can be explained by a point defect model. The majority of the work was performed at room to moderate temperature (typically <100 degC) and in chloride solutions of concentrations ranging from 0.1 molar to 10 molar.

Farmer et al. (1988) notes the work of Hagn (1983) regarding the transition from pitting to corrosion fatigue through linear-elastic fracture mechanics. Hagn (1983) claims that the model is also applicable to SCC.

$$\Delta K_{ISCC} = \Delta\sigma(\pi a)^{1/2}.F(a,c)$$

where K_{ISCC} is the stress-intensity threshold for initiation of SCC, $\Delta\sigma$ is the alternating tensile stress, a is the pit depth and major axis of an ellipse, c is the minor axis of an ellipse, and $F(a,c)$ is a geometric factor calculated from a and c:

$$F(a,c) = {\left[1.13 - 0.07\sqrt{(a/c)}\,\right]}\Big/{\sqrt{1 + 1.47(a/c)^{1.64}}}$$

The equations can be rearranged to calculate the pitting depth threshold leading to SCC,

$$a_{th} = \left({}^{1}\!/_{\pi}\right)(\Delta K_{th}/F(a,c)\Delta\sigma)^2$$

The time to initiation a crack has been derived by Buck and Ranjan (1986), again with linear-elastic fracture mechanics,

$$t_{inc=} {}^{K_{ISCC}^{2} exp(-V_m/V_O)}\Big/_{\pi B\left(\sigma^2-\sigma_O^2\right)}$$

where σ is the applied stress, σ_0 is the stress needed to close the crack, *B* is a constant, -V_m is the electrochemical potential of the sample, and V_0 is the reversible potential.

It can therefore be concluded that the effect of temperature and chloride solution concentration on the initiation of CISCC can be modeled in such a way as to match experimental data and predict CISCC initiation.

Farmer et al. (1988) also notes that a review by Ford (1982) finds that SCC propagation mechanisms fall into three general classes: (a) pre-existing active-path mechanisms including intergranular stress corrosion cracking in sensitized steel, (b) absorption-related mechanisms including hydrogen embrittlement, and (c) strain-assisted active path mechanisms including transgranular stress corrosion cracking in non-sensitized steel, while Jones (1996) identifies SCC mechanisms as either anodic or cathodic.

Farmer et al. (1999) notes that once a crack is initiated, the crack will grow by SCC when the applied stress intensity factor (*K*) is equal to or greater than the SCC threshold (resistance) parameter, K_{ISCC}, which is material and environment dependent. For a crack to continue to grow by SCC, the following criteria must be met:

$$K = \alpha\beta\sigma\left[\pi\left(a_{pit} + \delta a\right)\right]^{1/2}$$

where a_{pit} is the depth of the pit, β is a geometric factor dependent on the shape of the crack and α is another geometric factor that accounts for the fact that the pit and the crack fissure do not constitute an idea crack.

Recent work by Charles Bryan and others at SNL has led to the development of a SCC model for dry storage canisters that includes many of the needed to demonstrate and evaluate SCC of welded canisters. The model evaluates the following aspects of SCC in the pitting initiation, pit growth, pit-to-crack transition and crack growth:

- Corrosive environment on the surface of the UNF canister
    - Presence of chloride

  - Aqueous conditions

- Susceptible canister material
  - Degree of sensitization
  - Cold-working
  - Surface finish
  - Presence of iron contamination

- Tensile stress

Key features and assumptions of the model are discussed here. The environment submodel consists of a chloride-presence option that utilizes estimated or site-specific aerosol compositions, as well as chloride deposition and loss using CFD and thermal models. The environment model also contains a submodel system to assess aqueous conditions, utilizing location-specific RH, canister surface temperature, storage system design, fuel-loading and burn-up (decay heat) at a known time out of reactor, weld locations and deliquescence relative humidity (DRH). For an example simulation, the model assumes a coastal storage site with chloride-rich marine aerosols that rapidly deposit on the UNF canister, representative of the majority of U.S. sites. The model case also assumes that chloride deposition is rapid compared to negligible loss by degassing. The model assumes a NUHOMS HSM-15 horizontal storage cask loaded with known burn-up fuel based on analysis and modeling by PNNL at Calvert Cliffs and stored from 2 to 20 years out of reactor. Environmental temperature and relative humidity data are taken from National Oceanic and Atmospheric Administration (NOAA) and the DRH is assumed to be greater than the limiting RH known to cause SCC in 304SS (>15%RH).

Other aspects of the Bryan et al. model include the degree of 304SS sensitization, which varies with weld temperature and position from the weld. This is performed by utilizing thermal models and including options for including cold-working and the presence of surface contamination that may increase the likelihood of SCC through development and stabilization of corrosive solutions on the surface of the steel. An example of the latter includes the presence of iron from steel work tool steel or rails, since analysis of surface dust deposited on tested UF storage casks showed the presence of iron. In practice, this is implemented in the Bryan et al. model as a multiplier on the likelihood of initiation. Additionally, the model can account for surface finish, which can impact emissivity and water capillary processes (although this will be ignored in early testing of the model).

The tensile stress in the Bryan et al. model is implemented based on the NRC models (Kusnick et al., 2013), evaluating axial and circumferential welds, with linear interpolation between the curves for the two models. Bryan et al. also note that an alternative conceptual model approach may be to assume that the tensile stress is equal to the yield stress through-wall, creating a conservative approach that is sometimes used by the NRC.

Once the three conditions needed for SCC are met, the pitting and crack growth leading to SCC in the Bryan et al. model are based on the work of Turnbull et al. (2006), in which a distribution of pit growth rates from previously published research is used to calculate pitting rather than measurement of individual pitting and corrosion parameters. The pit depth can be described by:

$$x = \alpha t^{\beta}$$

and therefore the pitting growth-rate is modeled as

$$\frac{dx}{dt} = \beta\alpha^{1/2}.x\left(1 - \frac{1}{\beta}\right)$$

where β is a derived constant that describes the shape of the distribution curve and the scaling factor α is unknown but is distributed normally. Both α and must be measured empirically, with many values needed to create a distribution. Each pit depth is selected at random and allocated a possible value of a (also selected at random). Bryan et al. identify that finding data to populate this function has been difficult, and instead opted for an observation that pits undergo transition to cracks at the 50-70 micron scale. The crack growth model selected by Bryan et al. incorporates key factors specifically calculating the rate of crack growth in CISCC:

$$\frac{dx}{dt} = \alpha f(K) f(R_a) f\left(\sigma_{ys}\right) f(T) f([Cl^-]) f(pH) \ldots$$

where α is the crack growth amplitude factor (or, the crack growth rate at a fixed reference set of conditions). Bryan et al. report that the value can be modified by many other factors, including material property factors such as the stress intensity factor (K), degree of sensitization (R_a), and yield stress (σ_{ys}), and environmental factors such as temperature (T), chloride concentration ($[Cl^-]$), and pH. Bryan notes that the effects of K and T are commonly included in the models (the other parameters are *sometimes* included) but that other factors are commonly included *implicitly*. For example, the effects of sensitization and yield strength are implicitly included if the reference corrosion rate used was derived experimentally from weld samples of the material of interest, which are sensitized to the approximately the same degree as the unknown conditions. Similarly, Bryan et al. notes the effects of both chloride and pH are implicitly included in the model in the reference corrosion rate only if the environmental conditions used to derive the reference corrosion rate match those of the unknown samples. Bryan et al. then concludes that for a model simply accounting for K and T, a power-law dependence is assumed for K, while an Arrhenius relationship is assumed for the temperature dependence. This yields:

$$\frac{dx}{dt} = \alpha \cdot exp\left[-\frac{Q}{R}\left(\frac{1}{T} - \frac{1}{T_{ref}}\right)\right] \cdot (K - K_{th}) \cdot f(R_a) f\left(\sigma_{ys}\right) f([Cl^-]) f(pH) \ldots$$

Each of the values has associated uncertainties, some of which can be derived by assessing prior experimental data, others must be estimated based on assumptions of distribution. The evaluation and scoring of uncertainties associated with inputs to the SCC model will be performed during the remainder of FY15 in collaboration with SNL.

Finally, preventing SCC generally requires elimination of one of the three required SCC factors, namely tensile stress, corrosive environment or susceptible material (Jones, 1996). However, in the case of dry-cask storage of welded canisters (especially those already loaded), the removal of stress, corrosive environment or canister material is largely impractical. While Jones points out that the use of coatings is often ineffective because they do not withstand the aggressive chemical or physical environments associated with SCC, we consider the potential application of amorphous metal or ceramic coatings (e.g. those developed by Blink et al., 2007) to both protect canister materials from atmospheric aerosol deposition with the added advantage of serving as a neutron absorber. Applying such a coating would require a thorough evaluation of the process, including the pros and cons of canister removal prior to application on currently stored canisters. Additional methods of prevention of SCC include cathodic protection, although this method can lead to accelerated hydrogen-induced cracking.

3. Summary

Two high-priority phenomena associated with the safety and licensability of used nuclear fuel storage casks are currently being evaluated. The data and models that contribute to the crosscutting thermal profile and potential chloride-induced stress corrosion cracking of welded used fuel casks are documented in this report. The deposition of dusts, particularly in coastal locations, can result in corrosive brines on the surface of waste canisters, leading to pitting and stress corrosion cracking at weld locations. Thermal models can be used to understand the temperature variation in (and on the surface of) waste canisters and storage casks, which can allow determination of a number of degradation mechanisms including the temperature on the surface of the waste canister that subsequently affects deliquescence of dust assemblages. Key data that strongly affect the thermal profile modeling where uncertainty could be improved include (a) specific design data beyond the generic design, (b) thermal properties of component materials, (c) radiation heat transfer with 4th order temperature dependence, and (d) improved surface measurements to validate thermal models. Key data that strongly affect the ability to provide a CISCC model where the associated uncertainty could be improved include (a) accurate determination of dust deposition rate, (b) validation of the model proposed by Bryan et al. including the a distribution of the number of canisters whose surface contains iron particle contamination (and the subsequent influence of the iron on the CISCC) as well as data to populate the Turnbull (2006) model.

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Appendix A – Characteristics of PCMM Elements, General Descriptions of Levels and Scoring

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.

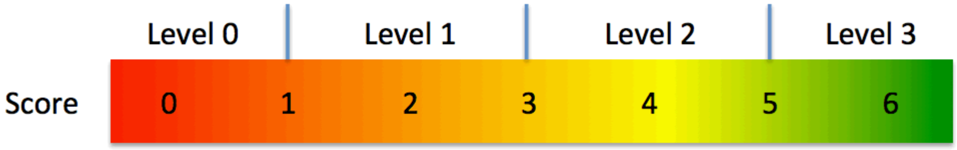

Figure A-1 Scoring "spectrum" for evaluating model and data maturity

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.

Appendix B – PCMM Table for Thermal Profile Models and Data

Key:

1. Models directly available and applicable to storage and transport.
2. Abstraction/simplified models or discrepancy in model characterization.
3. Model yet to be developed based on theoretical understanding.
4. No model available but correlation between input and output available.
5. No model available (missing physics) requiring expert solicitation.

Table B-1 PCMM Table for Thermal Profile Models and Data

V= vertical, H= horizontal

Lead Author	Study Type/ Cask Config.	Canister	Decay heat/ fuel	Uncertainties / limitation	1	2	3	4	5
Bates, 1986	1. test, PWR, V, air, He and vacuum	EMAD	1.17kW, actual fuel		Used for benchmarking				
	2. test, V or H, air, He and vacuum		15 x 15 array, 0.5kw or 1.0kw heater		Used for benchmarking				
Irino et al., 1986	Test V and H; He, N and vacuum				Used for benchmarking				
	Model with SICOH-3D			no detailed information		X needs further evaluation			
Creer, et al. 1987	Test V and H; He, N and vacuum	Single TN-24p	20.6 kW; 24 PWR actual fuel assembly		Used for benchmarking				
	Model with COBRA-SFS (2D)	Single TN-24p	Finite Difference	* difficult to determine thermal resistance of gap between basket and cask wall. (V); * assumed everything centered (V); * assumed no convection inside cask; *difficult to predict outside convection to ambient; lower plenum modeled as empty space filled with gas;	Good, benchmarked				

Lead Author	Study Type/ Cask Config.	Canister	Decay heat/ fuel	Uncertainties / limitation	1	2	3	4	5
Mckinnon et al., 1986	Test V and H; He, N and vac	REA 2023 BWR cask (or MSF IV)	15 kw, up to 52 assembly actual fuel, (copper basket)		Used for benchmarking				
	model with HYDRA; Finite Difference 3D			* The axial distribution of heat is based on core-average axial burn-up and applied it to all the assemblies. * geometry uncertainties of gap, straightness and flatness which affect the contact thermal resistance. * assumed gaps are evenly distributed. * the actual flow area below basket is not well defined.	Good, benchmarked				
	Model with COBRA-SFS, Finite Difference 3D			* Heat transfer from the cask surface to the ambient was copied from the test-measured value. * radiation to the ambient assumed to be black body. * radiation between 2 cask assumed to be grey body, the emissivity on painted and unpainted surfaces are taken from measured values.	Good, benchmarked				

Lead Author	Study Type/ Cask Config.	Canister	Decay heat/ fuel	Uncertainties / limitation	1	2	3	4	5
				* uncertainty of internal contact thermal resistance. * uncertainty of internal emissivity. * uncertainty flow resistances from contribution of fuel tube inlet and outlet flow losses..					
Mckinnon et al., 1989	Test V and H; He, N	single TN-24p	23.3kw PWR consolidated fuel, actual		Good, benchmarked				
	Model with COBRA-SFS			* difficult to determine thermal resistance of gap between basket and cask wall. (V); * assumed everything centered (V); * assumed no convection inside cask; *difficult to predict outside convection to ambient; lower plenum modeled as empty space filled with gas; * axial decay heat profile was not measured;		X needs further evaluation			

Lead Author	Study Type/ Cask Config.	Canister	Decay heat/ fuel	Uncertainties / limitation	1	2	3	4	5
McKinnon et al., 1992	Test V; He, N and vacuum	VSC-17 cask, PWR consolidated spent fuel	14.9 kw actual fuel assembly		Good, benchmarked				
	Model with COBRA-SFS			* the loss coefficient for the turbulent flow around a miter corner is estimated may not reflect real value. * assumes perfect centering of fuel pellets/rods, assemblies/basket cells, and baskets/canister. * thermal resistance of gas is estimated. * plenum is modeled as empty space filled with gas. * effect of heat transfer of rebar with concrete is neglected. * convection form cask outside surface to ambient is estimated. * axial decay heat profile is not determined by experiments.		X needs further evaluation			

Lead Author	Study Type/ Cask Config.	Canister	Decay heat/ fuel	Uncertainties / limitation	1	2	3	4	5
Rector et al., 1986a	Model with COBRA-SFS against measurement data which is not included in this report	Single CASTOR-1C Cask, backfilled with nitrogen	BWR 13.4kW	Steady-state 3D velocity, pressure and temperature distribution in the cask. * assumed constant thermal conductivities of cask wall is assumed, but that of basket is function of temperature. * treat fill medium as incompressible flows for internal convection. *sensitive to axial decay heat profiles. * gap between basket and cask wall is estimated as constant. * perfectly centered. * convection coefficient from cask outside surface to ambient is estimated. * the bottom od cask is assumed to be adiabatic.		X needs further evaluation			

Lead Author	Study Type/ Cask Config.	Canister	Decay heat/ fuel	Uncertainties / limitation	1	2	3	4	5
	Model with HYDRA			Steady-state 3D velocity, pressure and temperature distribution in the cask. * treat fill medium as incompressible flows for internal convection. *sensitive to axial decay heat profiles. Better agreement with measurement data than COBORA-SFS. * conductivity for mixed materials zone is estimated. * backfill is assumed to be vacuum. * mesh geometry is from design drawings which may not reflect as-built. *all centered. *use measured heat generation and axial profile as input. * convection coefficients on outside cask surfaces to ambient are estimated.	Good, benchmarked				

Lead Author	Study Type/ Cask Config.	Canister	Decay heat/ fuel	Uncertainties / limitation	1	2	3	4	5
Lombardo et al., 1986	Model with COBRA-SFS against measurement data which was not included in this report	Single PWR cask with an actual spent fuel assembly, backfilled with air, helium and vacuum vertical orientation;		*assumed that total radiation over the entire fuel was uniform. *symmetric rod heat flux model was used. * a new factor is introduced to correct the internal convection coefficient to agree with test data. * fuel tube emissivity is estimated.		X needs further evaluation			
		Single PWR cask with an electric heater backfilled with air, helium and vacuum vertical position and in vertical and horizontal orientation.	0.5 and 1.0 kW	* measured thermal power level and boundary temperature data inputted into the model. * assumed centralized fuel assembly even in horizontal orientation. * no buoyancy effect in horizontal cases. * fuel tube emissivity is estimated.		X needs further evaluation			
Rector et al., 1986b	Sensitivity analyses with COBRA-SFS	REA 2023 (MVSF-IV) cask and CASTOR-1C cask	Consolidated 8x BWR assemblies and unconsolidated BWR fuel assemblies, 0.8kw/assembly with N and He	Comparison between lumped model (combine rods and sub-channels) with detailed models		X needs further evaluation			

Lead Author	Study Type/ Cask Config.	Canister	Decay heat/ fuel	Uncertainties / limitation	1	2	3	4	5
			backfill gases						
Rector et al., 1989	Model with COBRA-SFS	TN-24P		Guides users to achieve accuracy of the calculation and dramatically reduce the complicity of model with COBRA-SFS code. * One limitation of the code was the absence of fluid shear stress terms in the momentum equations. As a result, the velocity distribution within the region may not have desired accuracy. *Another limiting aspect of the code was the upper and lower portions of storage casks, it was assumed that all fluid entering the region was uniformly mixed and that no temperature variation existed in the region. In addition,		X needs further evaluation			

Lead Author	Study Type/ Cask Config.	Canister	Decay heat/ fuel	Uncertainties / limitation	1	2	3	4	5
				heat transfer from each region to ambient conditions was modeled using two one-dimensional heat transfer paths.					
Rector et al., 1998	Model with COBRA-SFS			Report content not within the scope of interest					
Cuta et al., 2012	Model with COBRA-SFS	Single HSM-1 storage model and 24P DSC ; single HSM-15 storage model and 24P DSC ;	24 CE 14x14 spent fuel assemblies; total 10.8 kw in HSM-15 at-loading; total 4.1 kw in HSM-1 at-loading.	* geometry is based on generic design not site specific design data. * decay heat is calculated with ORIGEN based on the at-loading values. *axial decay heat profile is based on bounding generic PWR fuel. * detailed mesh for rod and sub channel are created.		X needs further evaluation			

Lead Author	Study Type/ Cask Config.	Canister	Decay heat/ fuel	Uncertainties / limitation	1	2	3	4	5
				* internal canister convection heat transfer is estimated by choosing transfer coefficient from correlation formula. *solar radiation load is based the average heat flux specified in 10CFR 71.71 and surface emissivity of painted external surface of over-pack is assumed to be 0.9.					
Suffield et al., 2013	Model with STAR-CCM+ (CFD code)	NUHOMS-HSM15 module, Horizontal and vertical orientations; helium backfilled	24P dry shielded canister (DSC), 24 CE 14x14 fuel assemblies; total 10.58 kW at loading	* CFD model is constrained by the limitation of using Boussinesq approximation for Buoyancy-driven flows for small density difference in the fill gas, rather than treating it as an ideal gas. * homogeneous effective conductivity is used in the CED model.		needs further study of internal convection and more detailed model for rod and sub channel			

Lead Author	Study Type/ Cask Config.	Canister	Decay heat/ fuel	Uncertainties / limitation	1	2	3	4	5
Cuta and Adkins, 2014	Model with COBRA-SFS	Single HI-STORM100S-218, Version B cask, vertical orientation, helium backfill gas	MPC-32 canisters, PWR 17 x 17 fuel assembly	* geometry is based on generic design not site specific design data. * decay heat is calculated with ORIGEN based on the at-loading values. *axial decay heat profile is based on bounding generic PWR fuel. * detailed mesh for rod and sub channel are created. * internal canister convection heat transfer is estimated by choosing transfer coefficient from correlation formula. *solar radiation load is based the average heat flux specified in 10CFR 71.71. and surface emissivity of painted external surface of over-pack is assumed to be 0.9. * ambient condition is still 50°F.		X needs further evaluation			
Adkins, 2012	History of validation development and UFD				Good reference				

Lead Author	Study Type/ Cask Config.	Canister	Decay heat/ fuel	Uncertainties / limitation	1	2	3	4	5
	Campaign								
Wen and Hagler, 2013	Presentation of SARP course sponsored by DOE				Used as a reference				

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