Criticality Consequence Analysis Roadmap for a Spent Nuclear Fuel Canister in a Repository

Spent Fuel and Waste Disposition

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Thomas M. Evans, Gregory G. Davidson, Steven P. Hamilton, and Kaushik Banerjee
Oak Ridge National Laboratory

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SUMMARY

This report discusses an initial criticality consequence analysis approach of commercial spent fuel canisters in a repository that will be developed to support a performance assessment (PA) of a repository with criticality events. A repository PA with criticality events may be needed to support direct disposal of currently loaded dual-purpose canisters. The ultimate goal is to develop a criticality consequence analysis model that can interface with any repository PA model. The criticality consequence analysis approach describes multi-physics coupling between neutronics, thermal hydraulics, and mechanics analysis codes. This report also discusses the sensitivity and uncertainty analysis approach for quantifying conservatism in the criticality consequence outcomes, as well as a defensible multi-physics validation approach to support any future licensing effort. This criticality consequence analysis approach will be refined in the future to support specific regulatory frameworks for a specific repository PA if needed.

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ACRONYMS

ANL	Argonne National Laboratory
BWR	boiling water reactor
CASL	Consortium for Advanced Simulation of Light Water Reactors
CFD	computational fluid dynamics
CURIE	Centralized Used Fuel Resource for Information Exchange
DOE	US Department of Energy
DOE-NE	DOE Office of Nuclear Energy
DPC	dual-purpose canister
ECP	Exascale Computing Project
FCRD	Fuel Cycle Research and Development
FEP	features, events, and processes
FY	fiscal year
GPU	graphics processing unit
NEAMS	Nuclear Energy Advanced Modeling and Simulation
ORNL	Oak Ridge National Laboratory
PA	performance assessment
PWR	pressurized water reactor
SFWD	Spent Fuel and Waste Disposition
SNF	spent nuclear fuel
SNL	Sandia National Laboratory
UQ	uncertainty quantification
TAD	transportation, aging, and disposal canisters
UNF-ST&DARDS	Used Nuclear Fuel – Storage, Transportation & Disposal Analysis Resource and Data Systems

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CRITICALITY CONSEQUENCE ANALYSIS ROADMAP FOR SPENT NUCLEAR FUEL CANISTER IN A REPOSITORY

1. INTRODUCTION

This report documents work performed supporting the US Department of Energy (DOE) Nuclear Energy Spent Fuel and Waste Disposition (SFWD) Spent Fuel and Waste Science and Technology under work breakdown structure element 1.08.01.03.05, "Direct Disposal of Dual Purpose Canisters." In particular, this report fulfills M3 milestone M3SF-18OR0103050111, "Repository criticality consequence analysis roadmap" within work package SF-18OR01030501, "Direct Disposal of Dual Purpose Canisters–ORNL."

As of August 3, 2018, there were 2,893 dry storage systems in use in the United States containing 121,920 spent nuclear fuel (SNF) assemblies [1], with the majority of those systems containing dual-purpose canisters (DPCs) or multi-purpose (e.g., storage and transportation) canisters. DPCs can accommodate up to 37 pressurized water reactor (PWR) assemblies and 89 boiling water reactor (BWR) assemblies, and they are designed primarily for storage and transportation. Direct disposal of DPCs has the potential to avoid or reduce the amount of repackaging of commercial SNF, which can have significant financial and dose liabilities. The DOE Office of Nuclear Energy (NE) is currently investigating the feasibility of direct disposal of DPCs in a geological repository to potentially offset the need to repackage currently loaded SNF into smaller disposable canisters. Although it has been indicated [2] that direct disposal of DPCs is feasible from a purely technical perspective, several engineering challenges, along with legal and policy issues, must be addressed to make DPC disposal a reality. One challenge is the potential for post-closure criticality in a repository time frame.

A repository performance assessment (PA) includes investigation of sequence of features, events, and processes (FEPs) that might affect the repository. Criticality is considered an event within the FEPs that has the potential to affect overall repository performance. The FEPs that can affect repository performance are screened for inclusion or exclusion in a PA. An FEP can be excluded based on a low-probability criterion, a low-consequence criterion, and/or by regulation. In the Yucca Mountain licensing application, criticality events were excluded from repository performance considerations on the basis of low probability of occurrence [3]. It has been demonstrated that many loaded DPCs have the potential to achieve critical configurations under specific conditions over a repository time frame of 10,000 years or longer. Therefore, reliance on the low probability criterion to support DPC direct disposal presents different challenges than the transportation, aging, and disposal canisters (TADs) that were evaluated for the Yucca Mountain repository site. Performance of the neutron absorber material inside the TAD was one of several key factors for excluding postclosure criticality from the PA on the basis of low probability. Existing DPCs were not loaded considering the requirements for disposal, and as such, they may not have the same capabilities as TADs to reduce the probability of criticality. DPCs can still meet disposal objectives, but the safety-basis options are more limited. One of the options to support DPC direct disposal is to perform a criticality consequence analysis to determine the impact of a potential criticality event on a repository PA.

This report presents an initial criticality consequence analysis roadmap that will be followed to identify and quantify the important parameters associated with potential criticality events internal to DPCs in a repository that will negatively affect the repository performance. This roadmap identifies a multi-physics coupling methodology and the analysis codes used to represent various interdependent physics aspects of DPC criticality events such as neutronics, thermal hydraulics, and mechanics. This roadmap follows the general criticality consequence analysis approach outlined in the criticality analysis methodology topical report [4]. Specifically, the roadmap serves the immediate purpose of conservatively gauging the impact of criticality events in terms of an increase in radionuclide inventory, temperature, pressure, and associated stress and strain to various engineered barrier systems such as the waste package (DPC inside a disposal overpack). Based on the initial findings and the future licensing needs for a specific repository and associated regulatory framework, the roadmap will be refined if needed.

This report is organized as follows. A brief background is presented in Section 2. Basic requirements for the criticality consequence approach are provided in Section 3. Section 4 presents the initial criticality consequence analysis approach. Section 5 describes sensitivity and uncertainty analyses, while Section 6 outlines a validation approach of the coupled-physics. Finally, Section 7 provides an overall discussion.

2. BACKGROUND

As-loaded criticality analyses of the currently loaded DPCs are being performed using the Used Nuclear Fuel-Storage, Transportation & Disposal Analysis Resource and Data System (UNF-ST&DARDS) [5]. As-loaded criticality analysis uses initial fuel characteristics such as assembly type, initial enrichment, and initial uranium mass; reactor irradiation histories such as effective full power day and outage intervals; decay time in the spent fuel pool; and DPC loading maps to calculate the realistic and time-dependent (up to ~22,000 years or second reactivity peak [6]) neutron multiplication factor (k_{eff}) of DPCs. As-loaded criticality analysis provides the uncredited criticality margin that is being used to offset postulated DPC degradation scenarios. For criticality analysis, it is important to assume that water enters a waste package at some point over the repository's time frame. While different geologic settings and material degradation mechanisms might yield a large number of potential configurations, two simplified, potentially conservative configurations are being used within UNF-ST&DARDS to assess DPC reactivity changes that may occur over repository time frames:

1. total loss of neutron absorber from unspecified degradation and material transport processes, and
2. loss of the carbon-steel internal basket structure (including the neutron absorber) resulting in elimination of assembly-to-assembly spacing.

Table 1. Summary of DPC as-loaded criticality analysis in calendar year 12,000.

Description	Value
Total DPCs analyzed	616
Total DPCs below subcritical limit with loss of neutron absorber (design-basis loading)	0 (0%)
Total DPCs below subcritical limit with loss of neutron absorber (as-loaded)	473 (~76%)
Total DPCs below subcritical limit with loss of neutron absorber and carbon-steel structures (as-loaded)	420 (~68%)
Total DPCs below subcritical limit with loss of neutron absorber and carbon-steel structures (as-loaded) considering misload	397 (~64%)

Note: Misload includes assemblies are placed in wrong location within canister [7]. Subcritical limit is defined by keff = 0.98 [7].

To date, UNF-ST&DARDS has completed as-loaded analysis of 616 DPCs [7]. Table 1 and Figure 1 show that even with detailed criticality analysis, a fraction of DPCs have the potential to form critical configurations in a repository time frame. Many of the DPCs that have already been analyzed are of the flux-trap design, which provides a relatively larger criticality margin compared to the modern high-capacity burnup credit DPCs. It is expected that the statistics related to number of DPCs with no criticality potential in a repository time frame presented in Table 1 will deteriorate as UNF-ST&DARDS performs analysis of more and more modern DPC designs. Hence, detailed criticality analysis itself will not be sufficient to support direct disposal of DPCs. Nonetheless, UNF-ST&DARDS detailed criticality analysis will be vital in defining the probability of criticality of a particular waste package within a repository PA.

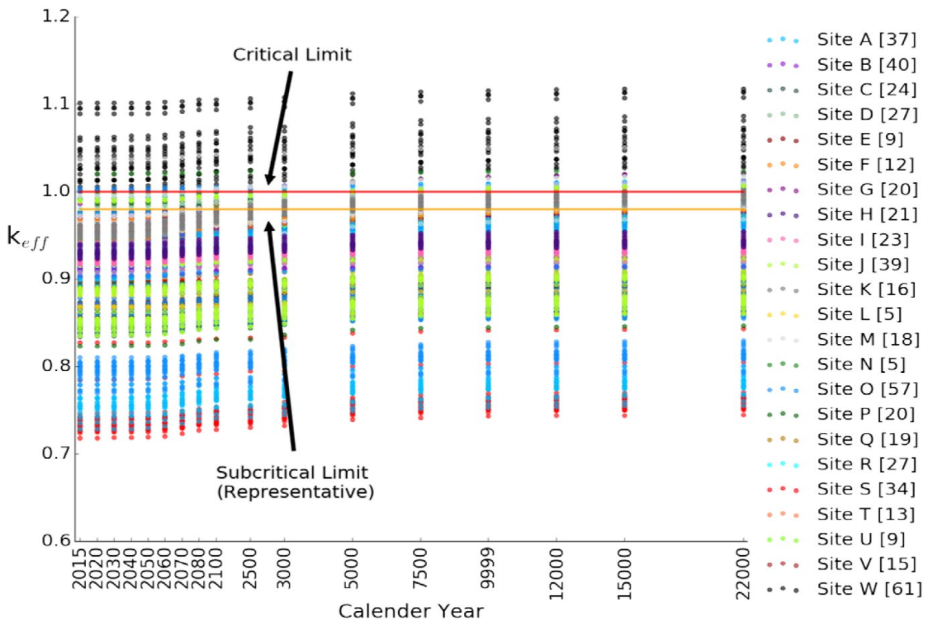

Figure 1. k_{eff} as a function of the calendar year (up to year 22,000) for 551 DPCs loaded at 23 sites (Postulated degradation scenario includes loss of neutron absorber panels from basket over repository time frame.).

Recognizing that as-loaded criticality analysis alone will not be able to demonstrate safe disposal of loaded DPCs, DOE Office of Nuclear Energy (DOE NE) began investigating other options for DPCs with criticality potentials in a repository time frame as determined by UNF-ST&DARDS. The two leading options include (1) preconditioning of DPCs with engineering filler materials that can be credited over a repository time frame to displace the moderator material and (2) analyzing the impact of potential criticality consequence on a repository PA.

To date, studies of repository criticality consequences [8, 9, 10, and 11] have been approximate and/or performed in an inefficient manner via development and use of problem-specific, unvalidated software that was applied to hypothetical, idealized configurations. A fully integrated criticality consequence analysis capability, which is defendable in the licensing space, is needed to enable risk-informed decisions for direct disposal of DPCs. The critically consequence analysis approach has been discussed in detail in the Yucca Mountain *Disposal Criticality Analysis Methodology Topical Report* [4], in which the following two criticality scenarios are postulated:

Steady state criticality is hypothesized as a sufficiently slow approach to criticality, permitting the negative feedback mechanism to hold the k_{eff} close to unity for a long time. This may be achieved at a temperature at which the moderator flow rate into the DPC will be similar to the moderator evaporation rate.

Transient criticality is hypothesized as the rapid approach (0.3–100 s [4]) to criticality in which the system k_{eff} will overshoot the value of unity, resulting in an exponential increase in power. The power excursion will be for a short duration, as the negative feedback mechanism should ensure k_{eff} to drop back below unity. This scenario can be caused by seismic events and or rock fall [4]. For example, this can be caused by a rapid reactivity insertion due to the sudden loss of the DPC basket structure, collapsing the SNF assemblies into a close-packed configuration as shown in Figure 2.

The criticality consequence analysis approach described in this report should be sufficient to model the above two scenarios.

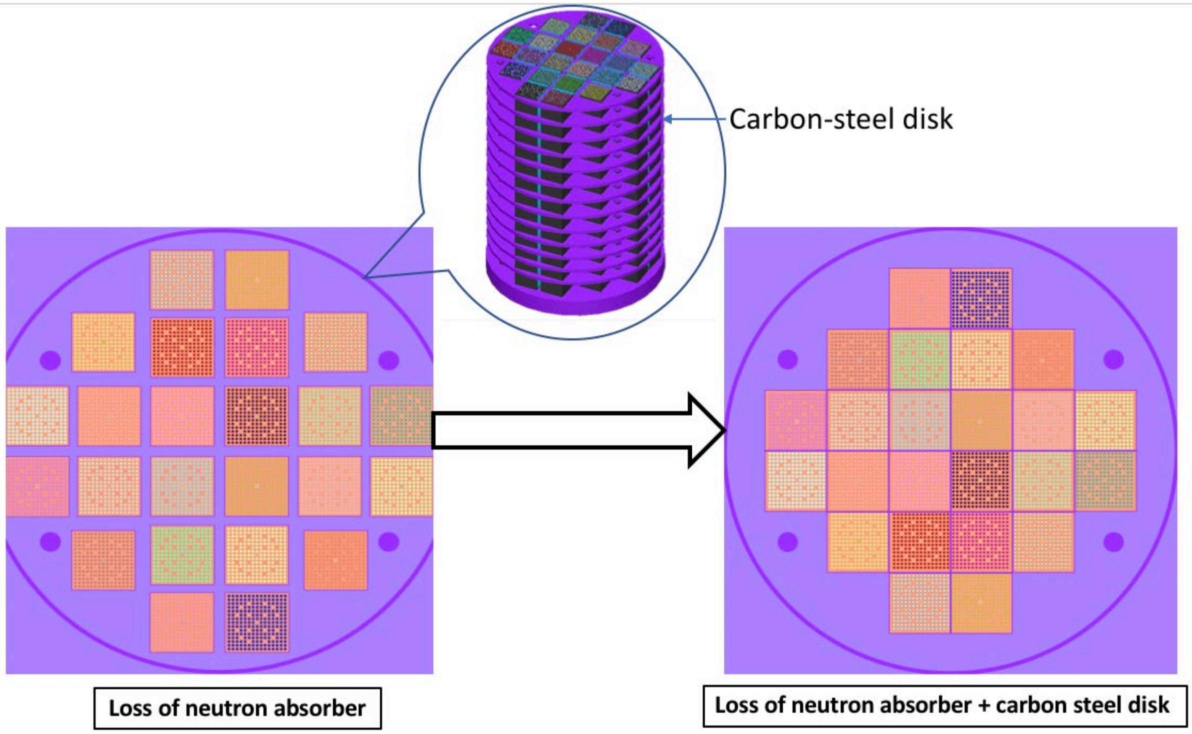

Figure 2. A hypothetical situation resulting in a rapid reactivity insertion.

3. BASIC REQUIREMENTS

The following basic requirements are identified.

1. The criticality consequence approach should be able to interface with any repository PA. A criticality consequence model should be able to receive initial parameter distributions from the PA model and provide criticality-related outcomes back to the PA model. A criticality consequence model developed following this roadmap should be able to function either as fully integrated within the PA or loosely integrated within the PA.

   a. **Fully integrated critically consequence approach.** In each time step t, the PA model will provide initial inputs (e.g., DPC configurations considering time-dependent and repository-specific corrosion mechanism, moderator flow rate, area of penetration to calculate temporal pressurization) and time interval (Δt) to the consequence analysis model. The consequence analysis model will perform consequence analysis for the time interval (Δt) by subdividing Δt as needed and will feed back important consequence-related changes such as an increase in radionuclides, temperature, or pressure to the PA model. For the next time step ($t+\Delta t$), the PA model will consider any changes to the initial inputs to the consequence model such as the flow rate based on criticality-related changes (e.g., temperature) from the previous time step. An increase in temperature due to criticality may also accelerate the engineered barrier corrosion rate and in turn the radionuclide mobility through a repository.

   b. **Loosely integrated criticality consequence approach.** Criticality consequence analyses will be performed outside the PA model to generate a table of various consequences such as an increase in radionuclides, temperature, or pressure etc., as a function of conservatively analyzed criticality scenarios such as DPC degradation scenarios or moderator flow distribution. The PA model will select appropriate consequence scenarios from this table based on other observations within PA.

2. The criticality consequence analysis methodology should be fully validated using applicable experiments, reactor operational data, and/or code-to-code comparison (in absence of real data).
3. The methodology should include uncertainty quantification (UQ) in criticality consequence distribution.
4. The criticality consequence model should identify a shutdown mechanism or duration of criticality excursion/event.

The criticality consequence model developed following this roadmap will initially be used to conservatively quantify various criticality-related parameters that negatively affect a repository PA. This initial step will determine any need for further improvement of the consequence analysis model.

4. CONSEQUENCE ANALYSIS APPROACH

The objective of this initial phase of the fully coupled application is to provide criticality analysis of the DPC. The coupled physics considered for this problem includes:

- ***neutronics*:** determination of the power, heat deposition, particle fluence, and nuclide number densities resulting from subcritical and critical fission inside the fuel assemblies;
- ***thermohydraulics*:** determination of the temperature, pressure, and density in the water inside the DPC; and
- ***mechanics*:** determination of stress and strain on the waste package components resulting from heat and pressure buildup over time.

The neutronics component of the physics is composed of *transport* and *depletion* calculations. Transport is used to calculate the space-energy distribution of neutrons and photons in the waste package. An additional step in the transport portion of the simulation is cross section processing. For a continuous-energy treatment of the interaction physics, this only requires assembling the constituent nuclide number densities into mixture tables that represent the compositions in the problem. However, when treating the energy using a discrete, multigroup approximation, the continuous-energy data must be processed to account for resonance self-shielding and other physical effects [12]. The inputs into the transport step are the nuclide number densities and material temperatures. The outputs are integrated power, reaction rates, and particle fluence.

The transport model used in this work uses the Monte Carlo method. The principal benefit of the Monte Carlo technique for neutron transport is that it can sample pointwise continuous representations of energy-dependent cross section data. This method drastically reduces the uncertainty in criticality calculations that result from the multigroup energy discretization.

The depletion step in the neutronics calculations uses input to the neutron reaction rates from transport and calculates updated nuclide number densities resulting from nuclide production, burnup, and decay. The outputs are updated number densities that represent the material composition of the waste package at a given point in time.

The thermohydraulics takes as input power and particle heat deposition from the neutronics and calculates water density, temperature, and pressure. In this work, a subchannel model is used to calculate the thermohydraulic behavior inside the DPC. The subchannel approximation is a simplified thermohydraulic model that characterizes the mass, energy, and momentum balance axially in one-dimension and radially using a bulk transfer between neighboring channels.

To perform a criticality analysis in a water-filled cask, the neutronics and thermodynamics must be coupled to properly calculate the state of the cask [13]. The coupling approach employed is illustrated in Figure 3.

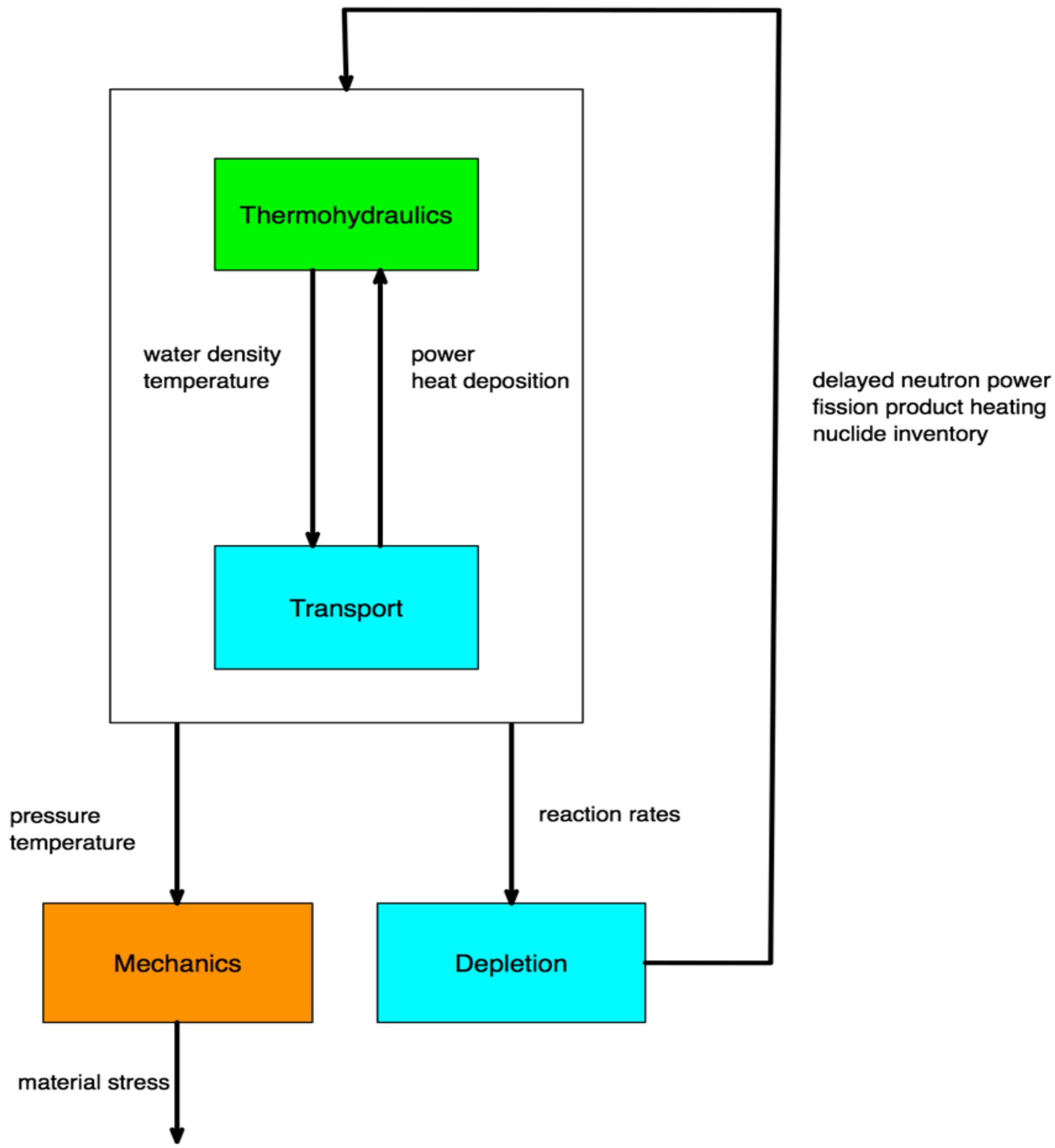

Figure 3. Coupling between neutronics (blue), thermohydraulics (green), and mechanics (orange).

Starting with a given nuclide inventory in the DPC and water level, the transport and thermohydraulics are iterated until water density, temperature, and power are converged. During these iterations, transport is assumed to be quasistatic, meaning that the neutron density and/or power is assumed to be constant during the timestep. After the iterations, the converged neutron reaction rates are passed to the depletion package to calculate nuclide burnup, decay, and production. Power and heating from delayed neutron and decay product gammas are also generated in this step.

A follow-on coupling effort will be to integrate mechanics into the solution sequence. This is a one-way coupling, as indicated in Figure 3.

4.1 Modeling and Simulation Tools

The following modeling and simulations tools will be used.

4.1.1 Shift

Shift is a high-performance, massively parallel Monte Carlo code featuring both continuous-energy and multigroup physics. Shift is capable of solving problems in both k-eigenvalue and fixed-source modes [14]. Shift can model coupled neutron/photon physics, including secondary particles born both by collisions and fission. Shift is also fully coupled to automatic cross section generation capabilities in the SCALE code package, as well as to ORIGEN for nuclide depletion and decay [15]. Shift has previously been used for used nuclear fuel cask dose analysis [16].

Shift is highly optimized to work on high-performance computing platforms using multiple parallelization strategies that can be tailored to the memory and performance requirements of the target architecture. Internode parallelism is managed using an MPI-based communication paradigm in which the problem is decomposed into N_s sets with N_b blocks per set such that the total number of processes is $N_s \times N_b$. Particles are decomposed across sets, while the spatial domain is decomposed across blocks. Thus, setting $N_b = 1$ reverts to the traditional *domain replication* parallelism model in which only particles are decomposed, while $N_b > 1$ implies *domain decomposition*. For problems with large tally requirements, which are typical in many full model depletion problems, multiple blocks can be used to enable the problem to fit within memory limitations on each process.

In addition, Shift has recently [17] been enhanced with an intranode transport algorithm that uses NVIDIA graphics processing unit (GPU) hardware. Recent performance analyses show that as the number of nuclides in the model increases, on the latest NVIDIA compute GPU (Volta V100) Shift achieves a particle tracking rate equal to between 100–175 IBM Power9 compute cores. Furthermore, the efficiency is highest when large numbers of particle histories are simulated. Therefore, Shift is ideally suited to efficiently run the large particle count simulations necessary to reduce statistical convergence below the minimum uncertainty bounds required by this work.

The depletion package within Shift is also optimized to work on high-performance computing platforms. The depletion package does not attempt to maximize parallelism by simply evenly distributing the depletion regions among all available processes, since this would require that the communication of the depletion results be global. Rather, the depletion package exploits Shift's multilevel parallelism to reduce the amount of memory and communication required during solution of the depletion equations. A process only performs the depletion calculation on the depletable regions within its local block, with the depletion regions in a block evenly distributed across all sets. This maximizes the parallelism within a block while minimizing block-to-block communication. This depletion method has been shown to scale well to 10,000 cores [15]; however, since the depletion only constitutes a few percent (< 5) of the total simulation time, this performance is considered sufficient for the work proposed here.

As part of DOE's ASCR Exascale Computing Project (ECP), Shift is being coupled to Nek5000, a spectral finite-element computational fluid dynamics (CFD) code [18] that can resolve turbulent flows using the large eddy simulation model. Capabilities developed during the ECP project will be leveraged for coupling to Cobra-SFS, including the use of on-the-fly doppler broadening of the cross sections, enabling tight coupling between the neutronics and thermodynamics.

Shift also has advanced hybrid deterministic/Monte Carlo capabilities for automatic variance reduction. This enables the rapid calculation of quantities of interest, even in low flux regions such as particle fluence on cask boundaries [19].

4.1.2 COBRA-SFS

COBRA-SFS is a program for steady-state and transient simulation of the thermal-hydraulic behavior of spent nuclear fuel systems [20, 21, and 22]. Similar to other codes in the COBRA family, such as COBRA-TF [23], COBRA-SFS solves a set of subchannel equations describing conservation of mass and momentum in the coolant flowing within fuel assemblies as well as energy conservation within the fuel rods and other solid structures in the system. COBRA-SFS retains the validation history of other codes in the COBRA series, but also provides additional validation specific to analysis of spent fuel systems. COBRA-SFS is distinguished from other COBRA variants by its treatment of features specific to spent fuel storage systems. This includes the ability to model natural circulation of coolant within a fuel cask, as well as simulation of radiative heat transfer between fuel rods and solid structures such as a spent fuel cask. It also extends the iteration scheme of other COBRA versions to be fully implicit in time to allow stronger coupling between equations governing fluid energy and heat transfer in solid components of the system.

4.1.3 Diablo

Diablo [24] is a three-dimensional, Lagrangian, nonlinear structural-thermal-mechanics code. It is part of the DOE NE Nuclear Energy Advanced Modeling and Simulation (NEAMS) project and is integrated into the SHARP multi-physics toolkit. Diablo is a finite-element code and has already been successfully integrated with Nek5000 as part of the NEAMS project. The coupling requirements between Shift and Diablo should be straightforward since Diablo and Shift are both coupled with Nek5000,

Nek5000 is a high-fidelity computational fluid dynamics code that resolves high-Reynolds number turbulent flows. Simulations using Nek5000 are computationally expensive and they require extensive user-intervention to generate the finite-element grids that are unique to each potential cask scenario. Furthermore, to properly capture the criticality conditions of the proposed problems, the added fidelity would likely not provide improved solutions over the more computationally inexpensive COBRA-SFS, which has been designed specifically for the simulation of spent fuel systems. Therefore, we believe the combination of Shift, COBRA-SFS, and Diablo will provide the best simulation solution for criticality consequence analysis of spent fuel casks. Nonetheless, Nek5000 remains an option for specific scenarios should the need arise, particularly for non-regular geometric configurations that may present in the course of specific analyses.

5. SENSITIVITY AND UNCERTAINTY ANALYSIS

A sensitivity analysis of the consequences to the variation of configuration parameters will be performed to quantify the conservatism in the approach. Sensitivity analysis and UQ for nonlinear, coupled problems is still an active research area. However, there are approaches that can be used to determine sensitivity and uncertainty for specific parameters. This is accomplished through the use of a sequence of calculations in which quantities of interest are manually perturbed. The Dakota (UQ) package [25] from Sandia National Laboratory provides a sensitivity and UQ framework for coupled physics simulations. Dakota provides a functional interface for perturbing specific quantities, running a series of calculations, and assembling sensitivities and uncertainties for the resulting model. There are open questions when applying a stochastic solution technique, such as Monte Carlo neutronics, inside of a global, sensitivity/uncertainty framework. These questions are the result of the statistical noise in the solution, which may exceed the sensitivities of the parameters. Dakota will be used to investigate the effect of the Monte Carlo statistical noise on UQ estimation.

6. VALIDATION APPROACH FOR COUPLED CRITICALITY CONSEQUENCE ANALYSIS

The objective is to leverage coupled thermohydraulics-neutronics model simulations performed in the DOE Energy Innovation Hub, the Consortium for Advanced Simulation of Light Water Reactors (CASL). CASL established a series of progression problems [26], including two specific problems with documented solutions dedicated exclusively to thermohydraulic-neutronics coupling. There are additional coupled benchmark problems in the literature, including BEAVRS [1], and other validation cases that apply to this problem will also be investigated. Finally, the DOE ECP is generating high-fidelity coupled thermohydraulic-neutronic simulations for natural circulating reactor cores in the ECP ExaSMR project. The ExaSMR simulations will provide an additional benchmark for the calculations proposed in this work.

7. DISCUSSION

This roadmap describes a criticality consequence analysis approach that will be used to support a repository PA with criticality events. The consequence analysis approach is based on multiphysics coupling between neutronics and thermal hydraulics analysis codes and a one-way coupling with a mechanics code. High performance Shift Monte Carlo code will be used for neutronics simulations (transport and depletion), and COBRA-SFS will be used to represent thermal hydraulic mechanisms internal to DPCs. Mechanics simulation will be performed using Diablo three-dimensional finite-element code. A criticality event internal to DPCs will only be considered in the initial phase. The criticality consequence approach described in this report should be capable of interfacing with any repository PA. This roadmap will be refined in the future as needed.

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