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Multiphysics Simulation of DPC Criticality: Scoping Calculations and Coupling Strategy

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Acronyms

CASL	Consortium for Advanced Simulation of Light Water Reactors
DPC	Dual-purpose canister (storage and transportation)
EBS	Engineered barrier system
FEPs	Features, events and processes
GWd	Gigawatt-day
MJ	MegaJoule
MT	Metric ton
MTU	Metric ton (uranium, or heavy metal)
MPa	MegaPascal
MW	Megawatt
NEAMS	Nuclear Energy Advanced Modeling and Simulation
ORNL	Oak Ridge National Laboratory
PA	Performance assessment
SNF	Spent nuclear fuel
SNL	Sandia National Laboratories
TAD	Transport-aging-disposal (canister)
TH	Thermal-hydraulic
UQ	Uncertainty quantification
WF	Waste form
WP	Waste package
YM	Yucca Mountain

Multiphysics Simulation of DPC Criticality:

Scoping Calculations and Coupling Strategy

WBS: 1.08.01.03.05
Work Package: SF-18SN01030507 – Multi-Physics Simulation of DPC Criticality – SNL
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1. Objectives for Multi-Physics Simulations

- **Provide a systematic framework for multi-process modeling** – Conduct parallel model development efforts that cover the technical areas needed to support criticality consequence screening in performance assessment (PA) and that will be more closely integrated as development proceeds.
- **Investigate separate effects** – Allow partitioning of the overall waste package (WP) internal criticality multi-physics modeling effort during development activities, for study of specific processes that can later be coupled if warranted from interpretation of results.
- **Study scaling and bounding approaches** – Where possible, represent criticality consequences in PA using simplification of uncertain criticality event frequency and magnitude, bounding of consequences for screening purposes, and scaling of consequences to multiple WPs.
- **Integration among participants** – Multiple modeling teams (mainly SNL and ORNL, and their collaborators) will work on different parts of the in-package criticality phenomenology. Insights generated this way will be combined for more realistic coupled modeling, and for validation.

2. Dual-Purpose Canister Disposal Concepts

For both saturated and unsaturated hard-rock settings (Table 1) dual-purpose canister (DPC) based packages would weigh approximately 95 MT (loaded DPC 55 MT, overpack with shielding 40 MT). The in-drift axial mode of emplacement would be used for safety in handling and efficiency of operations. Waste packages would be transported underground and emplaced using rubber-tire, diesel or electric powered equipment with personnel shielding (the last stage of emplacement would be remotely operated).

Saturated Hard Rock Setting – A low-permeability backfill would be used to inhibit flow along and parallel to repository openings. Packages would be placed on plinth structures fabricated from dry compacted clay-based material, then backfill would be emplaced remotely using a combination of pre-formed compacted blocks and dry granular material. Experimental studies have shown that clay swelling pressure causes homogenization and sealing of the backfill. Once the near-field engineered barrier system (EBS) is fully hydrated the corrosion environment would be chemically reducing. A layer of corrosion resistant metal would serve as the outer barrier on the disposal overpack. Passive alloys (e.g., Hastelloys) are effective in reducing conditions, as are naturally occurring materials such as pure copper. Localized corrosion and stress corrosion cracking of the outer barrier are potentially significant mechanisms, and would depend on surface treatment for stress mitigation, service temperature, and exposure to corrosive agents (e.g., chloride or sulfide) and protective species (e.g., nitrate for

Alloy 22). The outer barrier would be supported by a thicker inner vessel of welded, annealed SS316 which is strong and ductile, has lower cost, and also exhibits corrosion resistance. The DPC shell (typically welded SS304) would comprise a third layer of disposal packaging.

Unsaturated Hard Rock Setting – Disposal drifts would be un-backfilled to facilitate heat removal and dissipation (preclosure and postclosure), promote seepage diversion, and to serve other functions such as possible retrieval. Packages would be placed on low pedestals to help with emplacement and to stabilize them in the event of seismic ground motion. Additional engineered drip shields (as proposed for the Yucca Mountain License Application) would be installed over each package prior to closure. The drip shields would reduce the possibility of seepage entering WPs, and protect the packages from rockfall and drift collapse. The corrosion environment would be oxidizing, associated with barometric pumping of atmosphere from the ground surface. The corrosion resistant WP outer material would be a passive alloy (e.g., stress-relieved Hastelloy), and the inner vessel and DPC shell would be of stainless steel as discussed above.

Table 1. Comparison of disposal concepts for study.

Environment	**Unsaturated**	**Saturated**
Water Table	Deep	Shallow
Host Medium	Hard rock (e.g., granite, welded tuff)	
Depth	>200 m	>300 m
Ground Water Quality	Fresh Water (limited salinity)	
Waste Package Type	Corrosion Resistant (expected containment > 10^4 yr)	
Near-Field Chemical Environment	Oxidizing	Reducing
Near-Field Engineered Barriers	Drip Shield	Clay Buffer

3. Fuel Characteristics

The purpose of this section is not to specify details about nuclear fuels and fuel assembly designs, but to identify some broad descriptors to be used in selecting fuel characteristics for model development.

Multi-physics modeling of criticality related processes will focus initially on pressurized water reactor (PWR) fuel because previous studies have shown that PWR fuel in existing DPCs is more likely than boiling water reactor (BWR) fuel to be critical under repository conditions. This has been shown by as-loaded deterministic analysis (Liljenfeldt et al. 2017) which used current methods for representing axial burnup, and the geometry of fuel assemblies and baskets. Eventually, multi-physics modeling will extend to BWR fuel also. Axial burnup for BWR fuel is more difficult to model, and planned activities at Oak Ridge National Laboratory starting in FY19 will work toward improved burnup modeling.

There will be some failed cladding initially, which will affect mechanical strength and radionuclide release on exposure to ground water. The proportion of failed cladding is uncertain and inspection would be virtually impossible without complete disassembly. However, estimates of this proportion range up to about 2% on average (BSC 2005).

Cladding will be represented by the available types of Zircaloy (not distinguished unless required by models). Zircaloys are highly resistant to corrosion (more so than any other material in DPCs, at circum-neutral pH and without significant fluoride). Modeling will investigate the relative importance of mechanisms for mechanical deformation and failure (Section 8.2).

4. Previous Studies

The following studies represent a reasonably complete sample of previous scoping analyses for consequences of criticality. Many studies including some of those discussed below have developed probabilities for *initiation* of criticality, but that aspect is not compiled here. Rather, the focus is on estimates of power, energy, duration, and radionuclide inventory changes for steady-state and transient events, and the methods used for estimation.

The discussion below yields several insights. Mechanistic modeling of fuel and basket degradation in conjunction with nuclear criticality and thermal-hydraulics has not been attempted. Disaggregation of fuel, collapse of the basket, and/or draining of the WP (in an unsaturated environment) will ultimately turn off criticality. Without modeling processes that turn off criticality, steady-state approximations extrapolated over long durations can lead to relatively large changes in radionuclide inventory. Mechanistic simulations of criticality events involve intensive computational effort, and few cases have actually been run, which may improve using more modern tools. Both steady-state and transient analyses have been performed, and transient analysis may prove to be more realistic especially if it can be used to simulate the onset of conditions that lead to steady-state behavior.

Gottlieb, P., J.R. Massari and J.K. McCoy 1996. *Second Waste Package Probabilistic Criticality Analysis: Generation and Evaluation of Internal Criticality Configurations.* BBA000000-01717-2200-00005 REV 00. Office of Civilian Radioactive Waste Management, U.S. Department of Energy.

This study considered internal criticality for a WP consisting of corrosion resistant Alloy 625 on the inside, and corrosion allowance low-alloy steel on the outside. Many assumptions were used to quantitatively describe, in a limited way, the progression of corrosion, WP flooding, and degradation of neutron absorbers.

The approach relates corrosion rates to the availability of oxygen dissolved from air that circulates into the WP through breaches. It should be noted that experimental results such as those from Anderson et al. (2011) show that oxygen is not required to sustain corrosion reactions within a breached WP. The emphasis on oxygen in the model leads to speculation (and additional assumptions) about convective circulation in partially fluid-filled WPs.

Assumptions were also used to represent filling of a WP with ground water, including: flow focusing, dripping onto breaches, efficiency of seepage entry into breached packages, plugging of breach openings with corrosion products, and lack of corrosion penetrations on the lower side of the package (inside or outside). Other assumptions quantified mass exchange of oxygen entering and dissolved boron exiting the package at small breaches.

The authors proposed that boron (initially as boride, or intercalated with Fe) would partially remain trapped in Fe corrosion products, particularly magnetite, at 2 to 5% of the initial concentration in borated Type 316 stainless steel. The dissolved B would then be removed from the package by the assumed exchange process.

Simulations using the *MCNP* code were used to study the effect from boron removal. From a set of cases, the neutron multiplication factor k_{eff} was regressed against the amount of remaining B. The time to first criticality was estimated using an independently estimated degradation rate for neutron absorber material (subcritical limit $k_{eff} < 0.91$). Time to criticality was dominated by the borated stainless steel corrosion rate, fraction of B trapped in corrosion products (e.g., magnetite), and the hydrologic parameters affecting package filling and B removal. The trapped B fraction exhibited a threshold effect on k_{eff}, whereby at ~5% or greater residual B the time to criticality became much more sensitive to Fe solubility. The study proposed an inverse relationship between Fe solubility and the fraction of B in magnetite corrosion products.

The overall duration of cyclic criticality depends on feedback mechanisms, primarily the continued availability of water and the ability of the package to hold water, as well as the depletion of fissile nuclides and buildup of fission products.

The changes in activity for 36 radionuclides considered in the "TSPA-95" study for Yucca Mountain (YM) (expressed in Curies) were calculated for criticality averaging 2 kW over periods ranging from 1,000 to 10,000 yr, starting at 15,000 yr. The increase in radionuclides (comprising fission products and activation products) was as large as 24% at the end of criticality, decaying to 10% or less by ~50,000 yr, relative to the activity of low-burnup fuel (20 GWd/MTU with 3% enrichment). This result assumes that the configuration of fuel at the onset of criticality remains constant over the entire criticality period, and that other influences also remain constant such as the conditions that allow the package to remain flooded.

Rechard, R.P., M.S. Tierney, L.C. Sanchez and M.-A. Martell 1997. *Consideration of Criticality when Directly Disposing Highly Enriched Spent Nuclear Fuel in Unsaturated Tuff: Bounding Estimates*. SAND1996-0866. Sandia National Laboratories, Albuquerque, NM.

This study uses a heat dissipation argument (with WP at 100°C) to estimate 13 kW average power for each package. Various analogies are used to justify the power, energy, and duration of criticality events in a repository. This includes comparison to Oklo in scale, depletion, and number of fissions, and comparison to industrial criticality accidents in energy released. Some of the analogies may not fit commercial spent nuclear fuel (SNF) assemblies in a WP, which require additional moderation for criticality. For example, rapid compaction of an under-moderated mass of degraded spent fuel is not likely to increase reactivity.

McClure, J.A. and J.R. Worsham III 1997. *Criticality Consequence Analysis Involving Intact PWR SNF in a Degraded 21 PWR Assembly Waste Package*. BBAOOOOOD-01717-0200-00057 REV 00. Office of Civilian Radioactive Waste Management, U.S. Department of Energy.

This study used *MCNP4A* to represent criticality in a symmetry model of a horizontal WP containing 21 PWR assemblies. *MCNP4A* calculation results for infinite geometry were calibrated to *SAS2H* cases, to include buckling and geometrical loss effects. The *RELAP5/MOD3* code was used to model the time-evolution of power and other characteristics. The simulated configuration did not change (except for water level) and included:

- Fully degraded basket with iron oxide settled.
- Package initially filled, with the top 1.5 rows (of a 21 PWR stack) in pure water.
- Reactivity change represented by pure water vs. dispersed iron oxide.
- Reactivity insertion rate represented by sinking velocities for a range of particle size.

Temperature and water behaviors observed included:

- Fuel temperature transients increase before changes in water temperature-density.

- The water temperature and water pressure effects on reactivity are insignificant compared to the water density.
- Onset of boiling (steam void fraction) occurs at or near 100°C.
- Criticality events were terminated by voiding of water from the package
- Fuel temperature does not exceed 540°C.

Reactivity (estimated at $14.18) was inserted over times of 3,600 sec (lower rate) and 30 sec (higher rate). Model predictions for the low/high cases included:

- Approximately 1 to 50 MW peak power (low, high reactivity insertion rates)
- Total energy approx. 50 to 80 MJ per assembly.
- Peak fission power approx. 0.9 to 95 MW.
- Time when peak power occurred approx. 630 to 4 sec.
- Duration (termination time) 1,800 to 1,200 sec.
- Maximum pressure approx. 0.256 MPa.
- Change in burnup approx. 1.6E-3 to 1.8E-3 GWd/MTU per event.

These results differ from previous studies (Gottlieb et al. 1996; Rechard et al. 1996) in that transient events were simulated, and that the slow transient event represented a cyclic process that can be compared to steady state analyses. The study used significant geometrical simplification, for example intact fuel, flooding up to a prescribed level, and Fe-oxide mixed uniformly with water in the flooded region. Flow processes were simplified. The entire lengths of the assemblies were involved in the nuclear chain reaction, which scaled up the thermal and flow responses to criticality.

With transient reactivity the peak power is much greater than the constant steady-state criticality postulated by Gottlieb et al. (1996). However, a constant event acting over hundreds to thousands of years produces potentially much greater change in inventory. The transient events simulated by McClure et al. (1997) would need to repeat twice daily to produce as much average power, and do so for thousands of years to produce as much burnup, as the Gottlieb et al. estimates. This comparison highlights the importance of not only bounding the average power, which is straightforward using heat balance, but also the duration.

Mohanty, S., R. Codell, J.M. Menchaca, R. Janetzke, M. Smith, P. LaPlante, M. Rahimi and A. Lozano 2003. *System-Leval Performance Assessment of the Proposed Repository at Yucca Mountain Using the TPA Version 4.1 Code*. CNWRA 2002-5. Center for Nuclear Waste Regulatory Analysis, Southwest Research Institute, San Antonio, TX.

Steady-State

A scoping calculation of power output for steady-state criticality equated heat generation minus enthalpy gained by water flowing into a WP, to dissipation from the package by convection, conduction, and radiation from the WP surface to the drift wall. The result (4.8 kW) is comparable to other estimates. A bounding steady-state event at this intensity for each critical package was modeled beginning at 5,000 yr and running for an additional 10,000 yr. "Bathtub" type geometry was assumed whereby corrosion penetrations allowed liquid water into WPs at the top, but did not allow drainage at the bottom. The number of critical WPs was set to 32, which was the number of initially defective packages in the TPA model. Every one of these was assumed to be subject to seepage dripping.

A calculation with the ORIGEN code represented the change in radionuclide inventory, which varies from insignificant to a factor of 3 for different radionuclides depending on fission yield, and the half lives of fission products and activation products. Heat generation from criticality was implemented in order to include other effects from heating in the TPA model, by increasing the temperature of each critical package by 25°C, and increasing power generation by corresponding values (in W/MTU) appropriate for BWR and PWR fuel.

The dose effect from steady-state criticality in this analysis, totaled over all critical packages, and expressed for the entire repository, was a factor of 3 greater than a base case without criticality (Mohanty et al. 2004, Section 7.1.4). This may have been the first and only total system performance assessment published, that incorporated criticality.

Transient

A different scoping calculation included transient criticality. A transient event was assumed to have sufficient energy for an explosion that completely destroys the package containment and drip shield, and also ruptures adjacent WPs and their drip shields, and eliminates the waste isolation performance of the invert under all of these packages. Conceptually, the mechanism of transient criticality was assumed to result from sudden flooding of fuel that was intact except for loss of neutron absorbers. This might be caused by "sloshing" of water in a partially flooded package due to seismic ground motion, or by collapse of the fuel basket in such a way as to suddenly submerge intact, partially degraded fuel assemblies. Changes to radionuclide inventory were assumed to be negligible because although damaging, the transient event would produce a limited amount of energy and would not likely be repeated.

A single package was assumed to undergo transient criticality at 5,000 yr, also causing its neighbors, their drip shields, and the invert under all three packages to fail. The assessment focused on the relative magnitude of changes to the repository source term from these three packages. The calculated dose increased after the event by one order of magnitude compared to the base case with no criticality (Mohanty et al. 2004, Section 7.1.4).

It should be noted that these assessments were conditional, with the stated purpose of evaluating possible consequences from criticality. Likelihoods for transient and steady-state criticality events were not assessed. A number of conservative assumptions were made in estimating event consequences, so they could be considered as bounding for YM repository performance as represented by the TPA Version 4.1 code used.

Wells, A. 2007. Program on Technology Innovation: Yucca Mountain Post-Closure Criticality – 2007 Progress Report. Electric Power Research Institute, Palo Alto, CA. 1015128.

Corrosion of the transport-aging-disposal (TAD) neutron absorber material and collapse of a water gap flux trap structure are potential initiators for prompt critical transients.

Two transient criticality events were envisioned that could happen after 10,000 years, or if the bases for the low probability of criticality were changed (e.g., less robust neutron absorbers, less robust baskets, or less burnup than expected):

- Rapid water filling of a corroded zone in the neutron absorber of the TAD canister fuel basket could result in power levels of up to 85 to 280 times the full rated power of the fuel assembly, causing an energy release of 50 to 165 Megawatt-seconds.

- Collapse of a water gap flux trap structure, with a portion of the neutron absorber damaged, could result in power levels of 500 to 1500 times the full rated power of the fuel assembly, producing an energy release of 300 to 900 Megawatt-seconds.

These are transient event cases that are less likely than the steady-state, gradual-onset criticality events for which initiation probability was analyzed by DOE for features, events and processes (FEP) analysis.

Analysis of transient criticality is conditioned on WP flooding, fully or partially, which is unlikely in 10,000 years given the corrosion resistant WP outer barrier and drip shield, in the YM disposal concept.

The length of the corroded zone (neutron absorbers removed or flux trap geometry collapsed) need not be more than ~0.5 m for a prompt criticality to occur if water is rapidly introduced to the region. The most reactive part of the fuel core is the upper end. Corroded upper zone length of ~15 cm or less leads to delayed transients with flooding. Prompt criticality requires corrosion damage (neutron absorbers) for at least two assemblies, over a distance of 30 cm, with rapid flooding. When more assemblies are damaged (up to 9 were analyzed) the resulting prompt criticality event could produce pressure of 7 MPa and energy release of 50 to 165 MJ.

Collapse of 0.5-inch flux trap gaps in a basket with intact neutron absorber plates, could produce a prompt critical event with twice the power of the water redistribution case described above, and energy release on the order of 300 MJ. Collapse with degraded neutron absorber plates could produce an event with 6 times the power and release ~900 MJ.

All of the cases analyzed would require quite selective degradation of the package and basket, and the largest estimates would require simultaneous degradation of adjacent fuel cells in the basket (i.e., simultaneous corrosion damage or collapse of flux trap gaps). The steady-state type of criticality event, associated with gradual degradation, is more likely (although analysis has shown that it has low probability).

Gamma burst would be ~7% of the energy released by a transient criticality, directly heating the surrounding fuel and packaging.

5. Scoping Calculations

- How much energy would need to be provided by criticality, to drive the waste package temperature to 100°C (unsaturated) or 264°C (saturated, depth of 500 m) for a system that is steady-state and unthrottled? To estimate average fission power, estimates have assumed quasi-steady heat dissipation in the repository environment outside the WP, with a fixed temperature at the package surface. For example, for a 4-PWR (12-BWR) size WP temperature-regulated by boiling in a saturated repository at 500-m depth, approximately 13 kW could be dissipated on a long-term (>10 yr) basis (Hedin et al. 2013).

- For unsaturated repositories, estimates of steady-state power limited by boiling at 100°C include 13 kW (Rechard et al. 1997) and 4.8 kW (Mohanty et al. 2004).

- Gottlieb et al. (1996) used another approach to estimate the power of criticality events steady-state power in an unsaturated repository (Yucca Mountain). They assumed counter-flow of liquid water into a package and water vapor out (originating with evaporation within the package). Seepage inflow rate was balanced by evaporation, and temperature was extracted using an evaporation equation (Stefan's Law). For average package temperature of 57°C, the steady state heat generation rate was estimated to be ~2 kW accounting approximately for a mixture of heat losses from thermal radiation and conduction through rubble). Results from the exercise could be skewed by the low hydrologic flux values used (compared to YM flux distributions developed later), and the realism of counter-flow at small breaches in the package.

Additional scoping/bounding calculations will be evaluated to identify important processes and mechanisms, and as a check on more complex calculations. Potentially informative calculations include:

- Internal pressure: consider instantaneous heating of a closed container due to deposition of a quantity of heat, with thermal expansion of water and container, pressure expansion of the container, and compression of the water. This is bounding and corresponds to rapid heating without pressure relief, e.g., from a transient event at or near the beginning of the criticality event history for a package. High internal pressure could cause tensile damage to the canister shell and overpack layers, and impact the geometry of breaches in the canister shell and WP layers (temporary or permanent deformation).

- Relative degradation rates for neutron absorbers and basket structure, combined with episodes of degradation (e.g., driven by settling or seismic ground motion) will determine criticality event character and history. Criticality is likely to be terminated ultimately by collapse of the basket structure and fuel under its own weight. A DPC basket design combining the neutron absorption and structural functions in a single material (e.g., Metamic®) could collapse at about the same time that criticality became possible. Basket designs that combine different materials (e.g., steel or stainless steel with aluminum) would exhibit potentially different outcomes. Scoping calculations that compare neutron absorption and structural behaviors could help to evaluate the nature of criticality events, or whether criticality is possible.

6. Independent Review

An independent review of the technical feasibility studies led by Sandia from 2012 through 2017, for direct disposal of commercial SNF in DPCs of existing designs, was performed by Halim Alsaed of EnviroNuclear, LLC. The following discussion includes summary information and recommendations from the review report (Alsaed 2018). Several of these recommendations are being directly addressed by the modeling efforts described in Sections 8 and 9.

The purpose of this report is to document the technical review of past and ongoing SFWST activities in the area of criticality modeling and analysis in support of potential future direct disposal of DPCs. Additionally, this report provides recommendations that could advance the viability of direct disposal of DPCs. The reviewer was requested to address the following questions:

- What is the value of accumulating as-loaded fuel data and DPC design data for the existing fleet and future additions to the fleet of DPCs?

- What additional data could be collected to facilitate demonstration of disposal criticality control?

- What fraction of DPCs in the existing fleet is likely to be disposable with overpacks, but without other modifications? Is this likely to change significantly with future additions to the fleet?
- What DPC types currently in use are best/least suited for direct disposal?
- What reasonable modifications could be made in loading DPCs at the reactor sites to enhance the viability of direct disposal of DPCs?
- What effort is needed to follow through on the plan documented in *Criticality Analysis Process for Direct Disposal of Dual Purpose Canisters* (Scaglione et al. 2014)?

The reader is referred to the independent review report (Alsaed 2018) for specific findings with respect to these questions. The review was generally supportive, but also described a new direction for the work–consequence screening of postclosure criticality. The recommendations from Alsaed (2018) were:

1. Regulatory engagement for the development of guidance to address compliance with 10 CFR 72.236(m).
2. Probabilistic approach to k_{eff}, which is inherently probabilistic but has been represented by deterministic analyses.
3. Probability-weighted consequence screening, which could benefit from defining criticality FEPs to partition the variety of possible criticality events into categories that are readily analyzed and screened.
4. Credit for the stable Cs-133. Because the current analysis basis configurations assumed intact fuel pins, there is no path for release of Cs-133 from the fuel. Cs-133 is the highest yield fission product (6.8%) with a cross section of 28.9 b, and is a more valuable burnup credit isotope than most of the currently credited isotopes. Credit for Cs-133 is already accepted for storage and transportation.
5. Development of a burnup verification tool. Per ISG-8 Rev. 3 (NRC 2012), burnup confirmation would eliminate the potential for misload consideration for deterministic storage and transportation applications, which is one of the most significant vulnerabilities in the current analysis approach. With a probabilistic approach, a burnup confirmation tool would significantly reduce the probability of a misload.
6. Continue the evaluation of the viability of the use of a filler material that would be cost effective and meet the storage, transportation, and disposal structural, thermal, criticality, and retrievability requirements. This option is the subject of a follow-on deliverable and will be discussed in detail.
7. Continue to pursue methods for analyzing BWR SNF burnup credit.
8. Continue to gather the necessary data for DPCs to support as-loaded modeling.
9. Development of overpacks or overpack treatment that would reduce the probability of early failure (e.g., use additive manufacturing), where early failure would be more rigorously defined taking into account appropriate classes of defects and performance-based functions (e.g., maintaining moderator exclusion from the DPC with partial failures).
10. Simulate the degradation of DPCs to determine the composition of the water within the DPC, relocation of neutron absorbers and extent of failure.

The work described in the present report is responsive to the recommendation to pursue consequence screening (item 3), include Cs-133 burnup credit (item 4), and develop a degradation model for DPC internals (item 10).

7. Process Coupling Approach

This section gives an overview of process coupling, using influence diagrams which are a widely used graphical tool. The coupling approach will start with neutronic-thermal-hydraulic (N-TH) coupling, which was attempted by previous studies (Section 4). In parallel, a separate thrust will develop models of fuel/basket degradation (C-M-TH), with the objective to understand the longevity of configurations with the potential for criticality, and the likelihood of prompt criticality excursions to be initiated by seismic ground motion or another type of mechanical disruption. Interactions with the probabilistic consequence screening work package will help determine whether further coupling (e.g., N-TH-C-M, with disruptive events) is needed to terminate criticality. If so, then the details would be developed in a future revision to this workplan.

Multi-physics simulation is conceived as a 2 to 3 year effort focused on process-level support for consequence screening. Process models of criticality will help develop abstracted information to represent the uncertain power, energy, repetition rate, and overall sequence duration for criticality events. To support consequence screening, process modeling will help determine how differences among DPC-based WPs influence criticality, with the objective to estimate about how many WPs constitute a representative sample to represent the range of possible criticality events and their effects.

Coupled N-TH modeling will in part leverage technology from the Consortium for Advanced Simulation of Light Water Reactors (CASL) at Oak Ridge National Laboratory. The fuel/basket degradation modeling thrust will use mechanistic models to describe the evolution of fuel and basket materials, and the nature and timing of degradation and collapse that result. Some implementation details for both of these are described in Section 8.

The reference disposal conditions for this study assume hard rock (e.g., granite or welded siliceous tuff), hydrologically saturated (with a clay buffer) and unsaturated (with a drip shield but no buffer).

The degraded neutronic cases used for deterministic analysis of as-loaded DPC reactivity (Liljenfeldt et al. 2017) included loss of neutron absorbers (replaced by water), and basket degradation (eliminating neutron absorbers and basket components, and moving assemblies together). Coupling with TH will allow water or steam to by ejected from the WP, and to flow back in when criticality has subsided. Key variables in this scheme include the resistance to flow of water or vapor from/to the WP, to/from the near field.

The fuel/basket degradation model will combine corrosion processes, mechanical loading, and seismic ground motion to characterize the evolution of damaged states and the influence of model uncertainty and spatial variability. The histories of configuration generated will be studied for impacts on nuclear reactivity, and some configurations may be analyzed directly.

Progressively complex coupled modeling schema are described below using influence diagrams. Coupling (1-way or 2-way) is indicated also, using symbols "N" to represent neutron propagation; "H" or "TH" for thermal-hydraulics; "M" for mechanical responses of the fuel, basket, and container; "S" for seismic ground motion; and "C" for chemistry which could include corrosion conditions inside or outside the WP (near field), and radiolysis.

Coupling Influence Diagrams

The simplest N-TH diagram (Figure 1) represents the previous exploratory study by McClure et al. (1997). The circumstances of container breach and neutron absorber failure were described ad hoc, and the *RELAP5/MOD3* simulations (supported by *MCNP*) focused on temperature and pressure, and ejection of water. Few cases were run. This architecture could be a useful benchmark for comparison to other simulations, but it has limited utility for PA.

Adding feedback to degradation processes, and flow of water both within the package and in the near field (Figure 2) allows better representation of conditions necessary to sustain criticality, and better fidelity for transient events that depend closely on in-package TH conditions. Temperature and pressure effects from criticality on fuel and basket degradation, and WP breaches, are shown as ad hoc in Figure 2. This could be appropriate to test sensitivity, for example, of criticality excursions to the state of degradation. This scheme (with ad hoc or mechanistic coupling of degradation) is the primary target for planned work by ORNL discussed in Section 8.1.

The next diagram (Figure 3) shows how degradation of the fuel and basket, and WP breaches, could be modified by in-package temperature and pressure changes induced by criticality. Modification of the source term for radionuclide release is thought to be the principal effect from criticality on repository performance (see DOE 2003, Section 3.7) so this scheme will provide important support for probabilistic criticality consequence screening. Validated, mechanistic submodels for fuel/basket degradation and package breach behavior are needed.

The next iteration (Figure 4) couples independent information on near-field chemistry and seismic damage to the WP, to constrain the timing of breach leading to flooding. These influences represent variability in the corrosion environment, uncertain corrosion rates, and uncertain incidence of damage from disruptive events. All of these generally depend on site-specific information, but they are important influences on the number of packages that could be critical, and the overall timing of criticality events in a repository. Hence, they are potentially more valuable to probabilistic consequence screening than complexity in representing in-package degradation. This scheme would be implemented by combining criticality modeling or abstracted results with a PA model, and it will be addressed in future updates to this plan. In the interim, the modeling performed in FY18-19 (Section 8) will be repeated for a range of breach times as a check on reactivity changes throughout the performance period.

A more complete coupling scheme (Figure 5) would impose seismic accelerations on the fuel and basket. Depending on the nature of the seismic hazard, this scheme could be the chief cause of transient criticality events. The degradation model (Section 8.2) proposed for FY19 will be capable of including the influence from seismic acceleration.

Finally, the most complex scheme proposed here would couple chemical effects from in-package corrosion and radiolysis resulting from criticality, with near-field chemistry as a boundary condition, to constrain chemical degradation of the fuel and basket. This scheme is the endpoint recommended by independent review (Section 6). As depicted, the chemical processes would be represented along with multiphase flow, by a reactive transport code. However, more ad hoc constructions could be used to test sensitivity. This scheme is technically challenging and will be addressed in future updates to this plan.

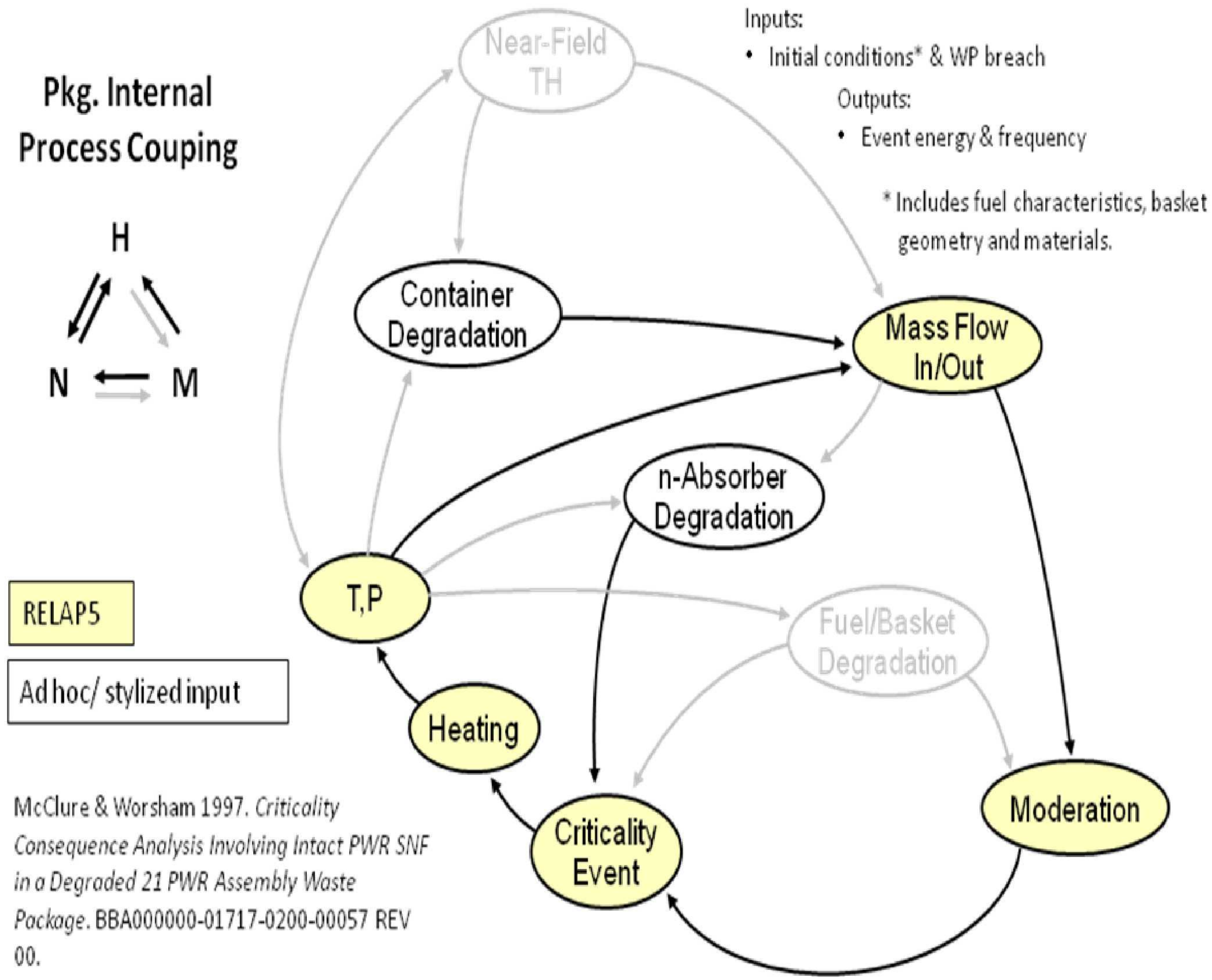

Figure 1. Influence diagram for previous criticality modeling (RELAP5/MOD3; McClure et al. 1997)

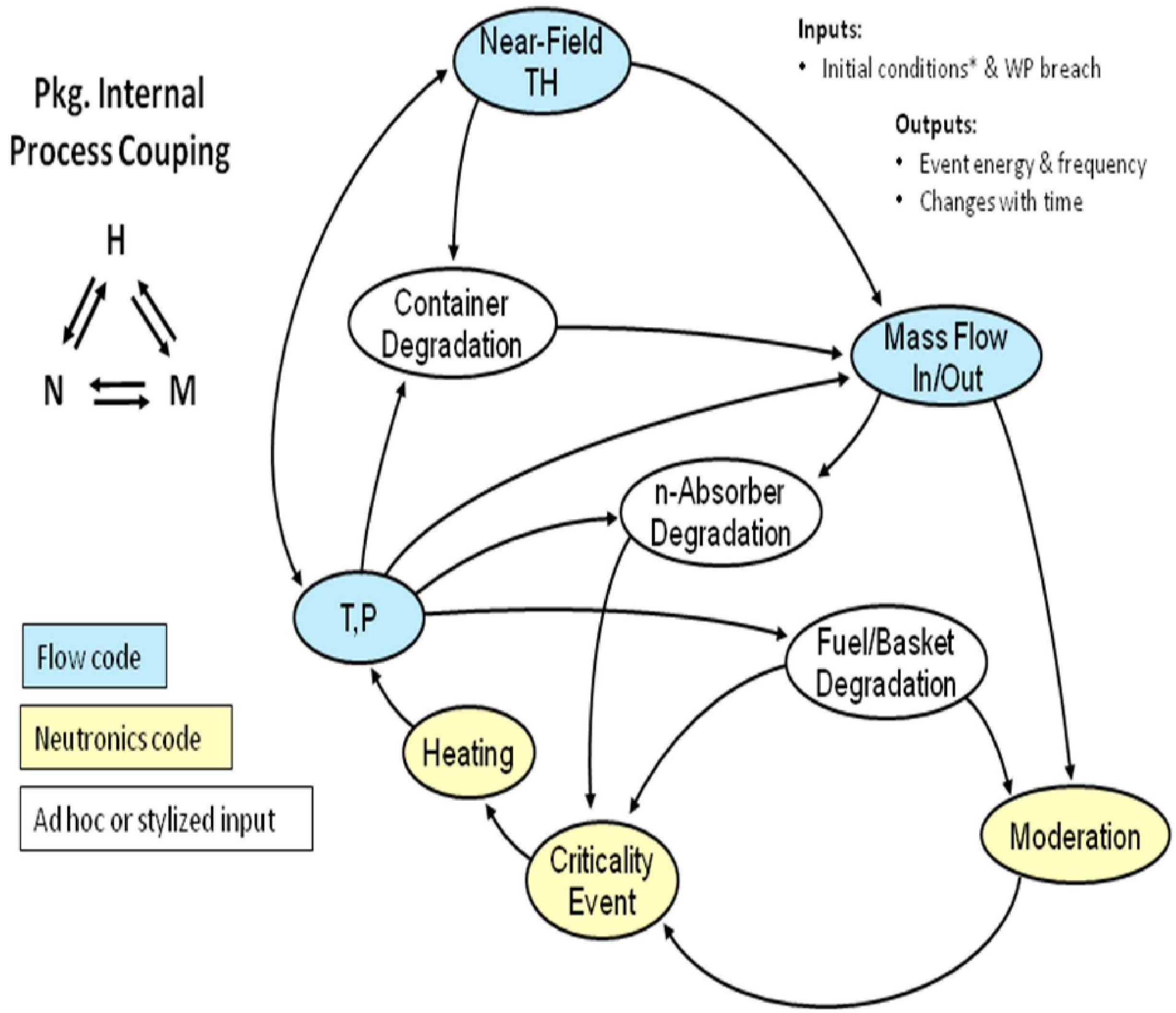

Figure 2. Influence diagram for neutronic-thermal-hydraulic-mechanical coupling (multi-code external).

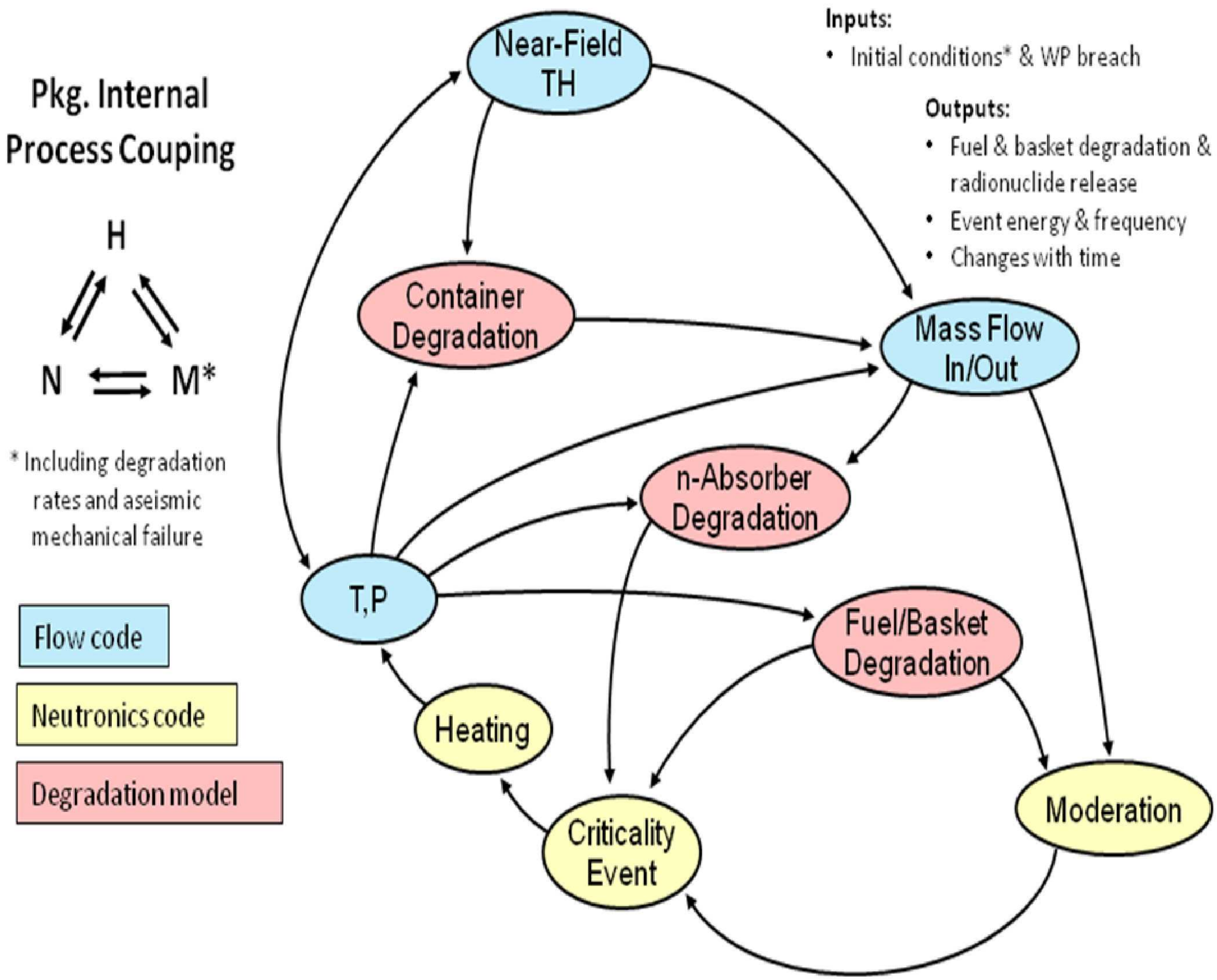

Figure 3. Influence diagram for neutronic-thermal-hydraulic-mechanical coupling (multi-code external).

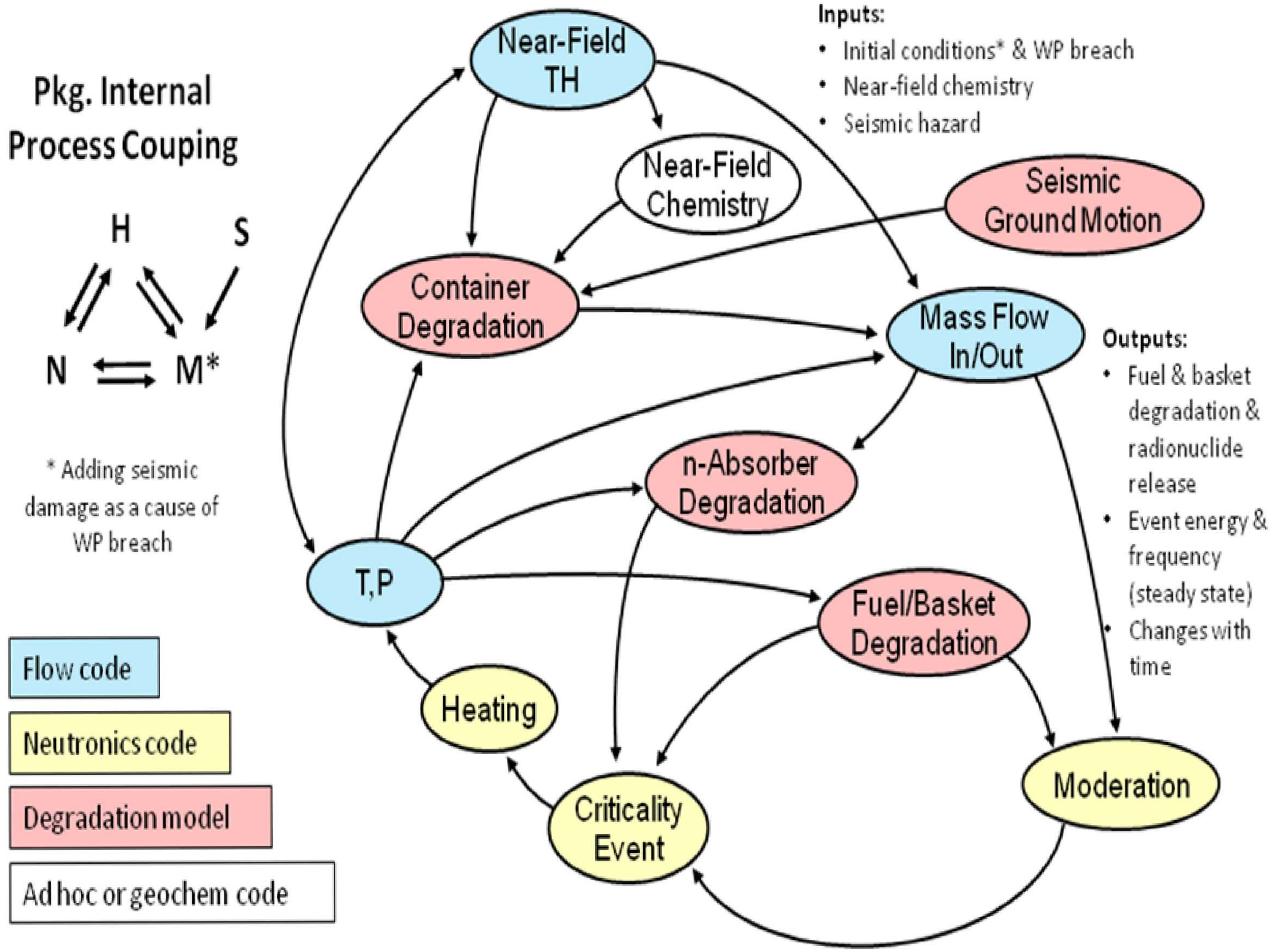

Figure 4. Diagram for neutronic-thermal-hydraulic-mechanical coupling with chemical/seismic degradation of waste package containment (multi-code external).

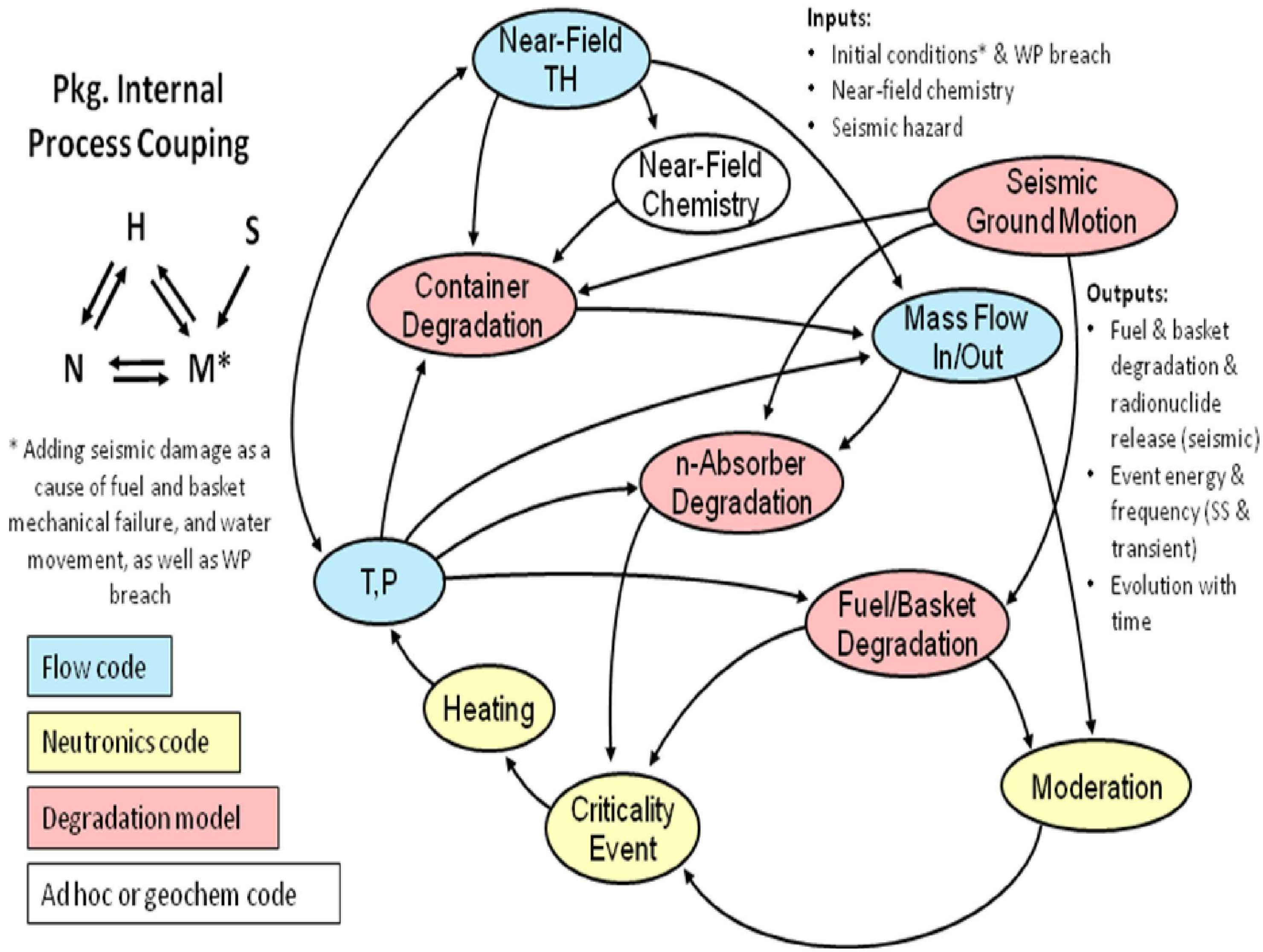

Figure 5. Diagram for neutronic-thermal-hydraulic-mechanical coupling with chemical/seismic degradation of fuel, basket and waste package containment (multi-code external).

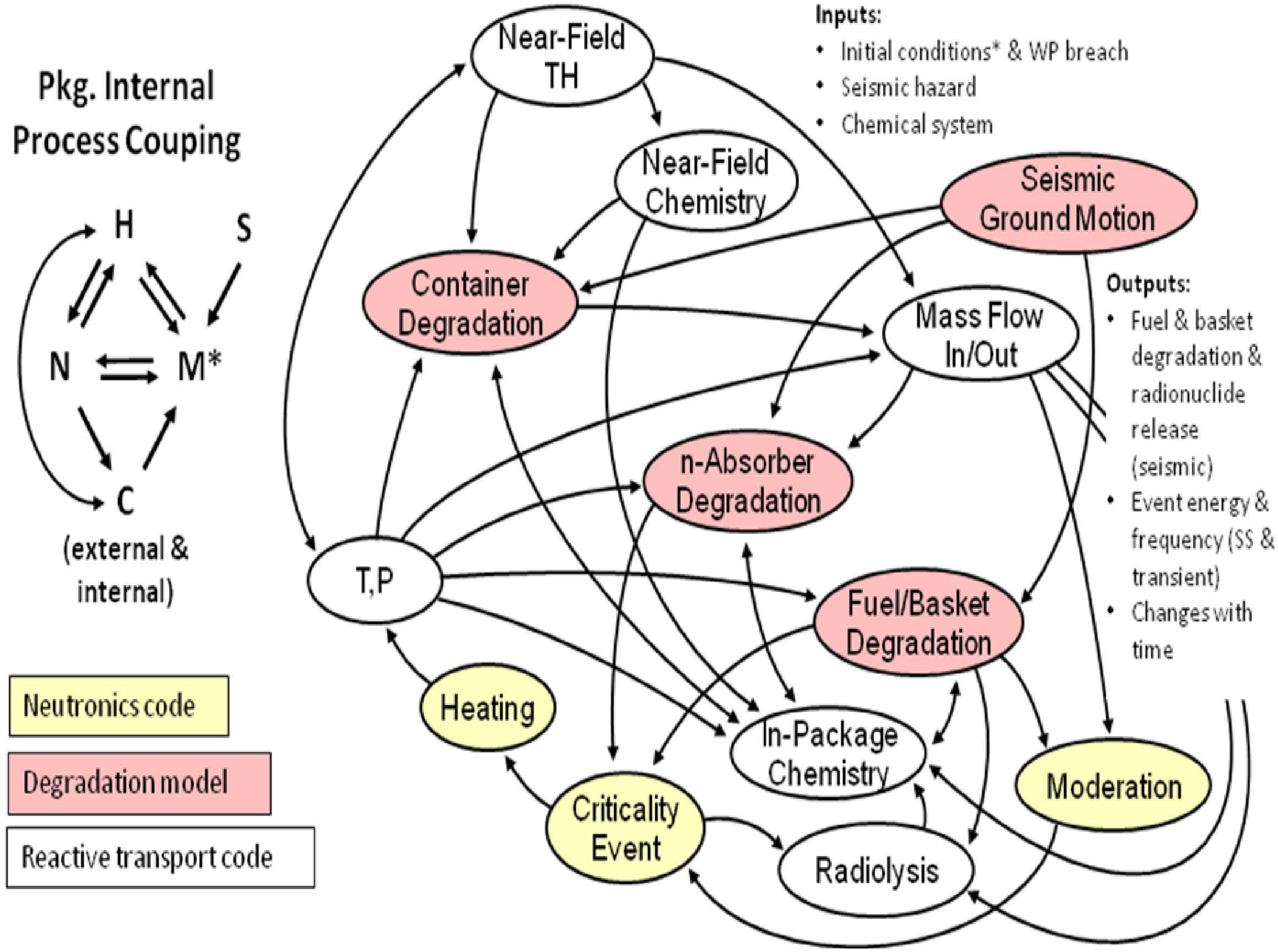

Figure 6. Diagram for neutronic-thermal-hydraulic-mechanical-chemical coupling (multi-code external).

Process Metrics

The various models discussed here will interface at physical boundaries or process boundaries (e.g., fluxes, or state variables such as temperature). A coupling scheme will require careful definition and close control of the variables that are shared between codes or handed off to effect external coupling. The following is an initial list of such quantities that could also be analyzed as simulation output. It is presented as a strawman to emphasize the need for controls.

- Heat generation rate and duration (specify subdomain, power and duration)
  - Radiogenic decay (localized to fuel and its degradation products).
  - Criticality events (localized to fuel, and distributed as neutron and gamma radiation).
- Heat transfer (specify temperature or heat flux distributions)
  - Within fuel assemblies
  - Within basket cells
  - In/out of WP breaches (enthalpies)
  - Interaction with the near field
- Water/gas movement (specify pressure or flow-rate distributions)
  - Within fuel assemblies
  - Within basket cells
  - In/out of WP breaches
  - Interaction with the near field
- CSNF waste form (WF) degradation (integrated over all fuel, or contoured for detailed study)
  - Extent of failed cladding (e.g., Miner's rule metric)
  - Radionuclide releases (especially rapid release fractions)
  - Radiolytic environment (measures of localized energy absorption)
- Basket degradation representation vs. time (integrated over basket, or contoured for detailed study)
  - Fraction of each neutron absorber plate degraded (e.g., Miner's rule metric)
  - Basket collapse (e.g., draw configuration or contours of void fraction)
  - Corrosion product accumulation (draw configuration, or contours of material and density)
- WP envelope degradation vs. time
  - # of breaches and breach areas (corrosion from outside)
  - # of breaches and breach areas (corrosion of inside surfaces and components)
  - Composite breach transmissibility (integrated through all layers and pathways)
- Radionuclide transport to near-field
  - Average or spatially variable concentrations of rapid release, total dissolved, and colloidal inventories by isotope at the damaged fuel assemblies

- Transport rates from externally driven advection, Fickian diffusion, and advective pumping from criticality (define diffusive flux, e.g., using zero ex-container concentration)

- Response to seismic ground motion
  - Above degradation indicators before/after seismic events.
  - Generated movies of co-seismic deformations.

8. Combined Approach to Criticality Process Modeling

This section summarizes the approaches to be used for developing N-TH-M and C-M-TH models in FY19. Baselined work products are listed in Table 2.

Table 2. FY19 Deliverables for multi-physics model development work packages.

Deliverable	Title	Due	Responsible
M5SF-18SN010305071	Scoping calculations and coupling strategy	9/24/18	SNL
M4SF-18OR0103050120	Prepare BWR data evaluation report	12/28/2018	ORNL
M3SF-18OR0103050112	Neutronic and thermal hydraulic coupling for waste package	3/29/2019	ORNL
M3SF-18OR010305018	Update of DPC direct disposal criticality analysis report	4/19/2019	ORNL
M3SF-18OR0103050113	Structural performance analysis of waste package for various criticality scenarios	4/30/2019	ORNL
M3SF-18OR0103050110	Multiphysics criticality consequence analysis capability development status report	5/31/2019	ORNL
M3SF-19SN010305071	DPC Criticality Simulation Preliminary Phase	9/18/2019	SNL

8.1 Neutronic – Thermal-Hydraulic – Mechanical

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:

- **Neutronic** – Determination of the power, heat deposition, particle fluence, and nuclide number densities resulting from subcritical and critical fission inside the fuel assemblies;
- **Thermal-hydraulic** – Determination of the temperature, pressure, and density of the water inside the DPC.
- **Mechanical** – Determination of stress and strain on the WP 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 WP. 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 (Hamilton et al. 2016a). 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 WP at a given point in time.

The thermal-hydraulic component 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 (Hamilton et al. 2016b). The coupling approach employed is illustrated in Figure 7.

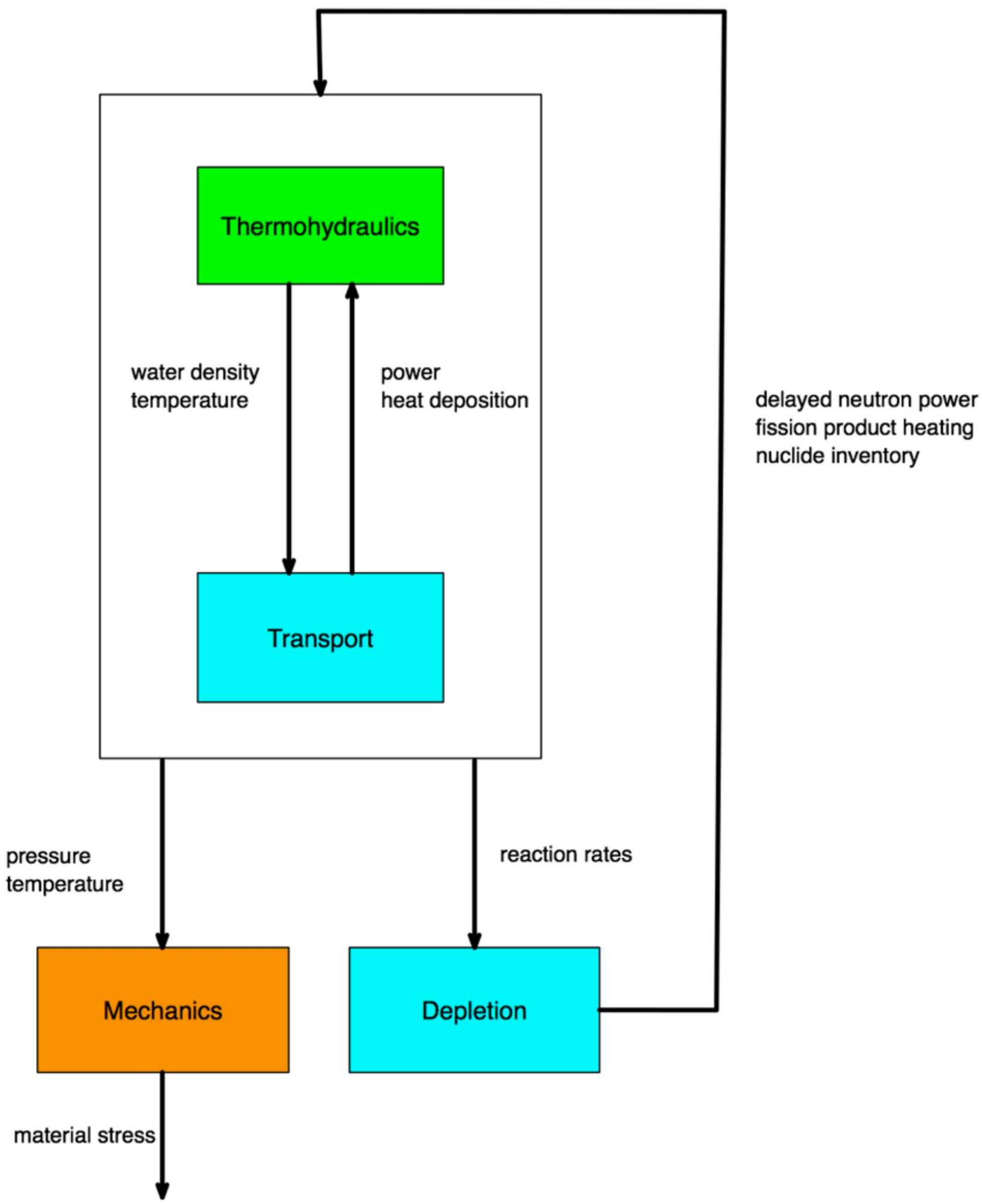

Figure 7. Coupling between neutronics (blue), thermohydraulics (green), and mechanics (orange) (from Evans et al. 2018).

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 7.

Modeling and Simulation Tools

Several current, highly optimized, parallelized simulation tools are planned to be used for this work at ORNL. Details of the codes and how they will be used are discussed by Evans et al. (2018) and the reader is referred there (and to their references) for details. The following codes are included in the approach:

Shift – *Shift* is a high-performance, massively parallel Monte Carlo neutronics code featuring both continuous-energy and multigroup physics. *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. *Shift* has previously been used for used nuclear fuel cask dose analysis.

COBRA-SFS – *COBRA-SFS* is a program for steady-state and transient simulation of the thermal-hydraulic behavior of spent nuclear fuel systems. Similar to other codes in the *COBRA* family, such as *COBRA-TF, 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.

Diablo – *Diablo* is a three-dimensional, Lagrangian, nonlinear structural-thermal-mechanics code. It is part of the DOE 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*, 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.

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 uncertainty quantification (UQ) for nonlinear, coupled problems is 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 from SNL 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.

Validation Approach

The objective is to leverage coupled thermal-hydraulics-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 validation problems, and there are additional coupled benchmark problems in the literature. Other validation cases that apply to this problem will also be investigated. Finally, other high-fidelity coupled thermal-hydraulic-neutronic simulations are underway or available for natural circulating reactor cores in the *ExaSMR* project. These simulations will provide an additional benchmark for the calculations proposed here.

This roadmap describes a multi-physics modeling approach that will be used to support consequence screening by building a more mechanistic understanding of postclosure criticality events in a repository. The approach will incorporate 2-way coupling between neutronics and thermal-hydraulics and one-way coupling with a mechanics. The *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 the *Diablo* 3D finite-element code. The initial phase of this work will consider a criticality event internal to a DPC. This workplan will be refined in the future as needed.

8.2 Fuel and Basket Degradation Modeling (C-M-TH)

This parallel effort will simulate certain effects from criticality on the repository (e.g., corrosion of nuclear fuel and WP internals, and heating in addition to decay heat) but not the criticality process itself. The work will develop a framework to investigate processes including:

- Corrosion of the fuel rods, fuel assembly hardware, and the basket structure
- Temperature dependence of corrosion and other degradation processes
- Radiolysis (α or γ emitted by the fuel) which can modify the corrosion environment
- Gravitational deformation (e.g., creep) of the fuel and basket
- Settling of corrosion products and debris from degradation
- Additional mechanical damage from seismic shaking
- Thermal and pressure loading of the WP shell
- Radionuclide release from damaged fuel (related to the extent of cladding damage)
- Mobility of release radionuclides (e.g., solubility, colloid partitioning)
- Aqueous chemical transport of radionuclides out of the WP
- Thermal-hydrologic-mechanical (THM) processes external to the WP

These processes and their interaction will be investigated separately from neutron propagation. Effects from criticality on degradation processes will be approximated using heat sources and temperature dependent corrosion rate functions. Results will represent long-term changes in the configuration of SNF, fuel assemblies, and fuel baskets, which can be handed off for neutron propagation simulations to evaluate the potential for criticality. Degraded configurations will be evaluated leading to two types of criticality events:

- **Steady-state** – Degraded configurations that develop gradually will be presented as "snapshots" that evolve slowly with time. Such configurations will be generated for successive states until the duration of likely criticality is exceeded because of radioactive decay (e.g., 50 kyr; see Wagner and Parks 2003) or degradation reaches a point where criticality is no longer possible.
- **Transient** – Seismic shaking or faulting will be used to generate transient changes in configuration. Transient effects may include rapid displacement of degraded neutron absorber material, or changes in fuel rod geometry.

For both types of criticality events there may be an eventual need for full coupling of neutron propagation, thermal hydraulics, and the degradation processes found to be significant from this effort. However, that is deferred to a later phase and is not included here.

Technical Approach

The approach to degradation modeling will be incremental, starting with relatively simple degradation models focused on different scales within a DPC-based WP. Modeling will start with individual fuel cells within a basket, each containing one assembly, then proceed to an entire DPC fuel basket, then to the breach behavior of the WP layers (i.e., DPC shell and one or more layers comprising the disposal overpack). Ultimately, it is intended that degradation models will be coupled with the PFLOTRAN code to represent flow of water and transport of released radionuclides.

Fuel Assembly Cell Model

The model of degradation within a fuel assembly cell will analyze the behavior of neutron absorbers, fuel rods, fuel assembly hardware, and the basket around the cell, caused by moisture that reaches these components after WP breach. Geometry and properties will be selected for a representative PWR fuel assembly oriented horizontally in a representative basket cell. The recent generation of fuel baskets using aluminum-based material for both structural and neutron absorbing components, is potentially the simplest type to model at this stage. The weight of overlying cells and fuel will be applied. The model will be 3-D but limited in the third dimension at first, to control computational effort. Key processes will be corrosion at metal-water interfaces, with temperature dependence, displacement of corrosion products within the cell, weakening of fuel rods and structural components, and deformation under gravitational loading. Changing temperature fields will be approximated and their effect on degradation and deformation of the components will be accounted for. The model will be capable of representing gross deformation (failure) associated with bending and buckling of structural components. Compositions of all materials and phases present in the model (and potentially altered and displaced) will be tracked for mass balance. Seismic ground motion will be added to the problem to investigate transient configuration changes. Note that conductive heat transport will be included, but flow processes and convective heat transport within the WP will not (deferred to a later modeling effort).

Basket Degradation Model

This model will simulate structural failure and disaggregation of basket structural elements, and configuration as they fall under gravity within the canister. A model of structural collapse for a representative DPC fuel basket will be developed using submodels (e.g., corrosion) and other insights gained from the fuel assembly model. Fuel assemblies and basket structural components (plates, spacer disks, guide tubes, etc.) will be represented as coarsely discretized blocks (rigid or deformable). The rates and variability of processes leading to basket collapse will be based on results from modeling at the fuel assembly cell scale. These processes will include seismic ground motion.

Waste Package Breach Model

This model will evaluate whether heat (and pressure) from a criticality event could affect the geometry and transmissivity of a breach that which admitted ground water in the first place. Inflow to and outflow from the package is important because it impacts the intensity, duration, and repetition rate of criticality events. The question to be answered is whether pressure in the package could increase to the point where breach transmissivity increases, either temporarily or permanently. Criticality events will be represented in the model by thermal pulses with varying assumed power and duration, and the consequent increases in water pressure in a closed vessel, either saturated or unsaturated. Breaches will be represented by longitudinally oriented cracks (investigation of other crack geometries is deferred to future work). Seismic ground motion will not be considered for this model.

Software Tools

This work will involve coupling of multiple simulation codes, and other solutions or functions, that represent processes within and outside of the WP. These tools must be flexible and inter-operable so they can be readily coupled, with scripting capabilities for adding constitutive behavior that is not already included in code libraries. The codes will be commercial off-the-shelf software with scripting capability for problem-specific user input.

For problems involving disaggregation and collapse, the distinct element method (DEM, also called the discrete element method) is the best approach for simulating configuration changes. Using the DEM components of the fuel and basket will be discretized into arbitrarily small polygonal bodies with uniform properties, that initially cohere to form fuel rods, basket plates, etc., but change properties and connectivity as degradation proceeds. With degradation the bodies can change properties, disaggregate, and fall interacting with other bodies until they come to rest. The numerical approach is based on Newton's 2nd Law, so seismic shaking can be readily introduced as a time-dependent body force. The DEM was originally developed for fractured continua, and has also been used for powders and larger aggregates, suspensions, etc. Mechanical interactions within a fluid such as water, add buoyancy and viscous forces directly related to velocities. The DEM can be coupled with continuum codes in subdomains where distinct elements are not needed, for example, where disaggregation will never occur and fractures are not important to deformation.

The codes *3DEC* and *FLAC3D* are selected for this effort because they meet these requirements and are commercially available. Previous work for geologic disposal R&D using these codes and closely similar ones (*UDEC*, *FLAC*, *PFC*) has demonstrated excellent functionality, inter-operability, scripting capability, and documentation. The codes will be these versions (or backward-compatible):

- *FLAC3D* 6.0 (options: dynamic, C++ plug-in, creep, and thermal)
- *3DEC* 5.2 (options: dynamic, C++ plug-in, structure, and thermal)

Metal corrosion, corrosion product accumulation, property changes with temperature, etc., will be implemented using the *FISH* scripting language within the *3DEC* and *FLAC3D* codes.

Work products will consist of four technical reports, comprising one initial scoping report and three model development reports documenting the incremental approach described above.

9. Model Integration and Future Outlook

At this point in the workplan the reader is likely to ask how the N-TH-M model and the C-M-TH degradation model described in Section 8 will be integrated, and how they will be integrated with probabilistic consequence screening. The answer is that some computationally intensive calculations will be done to demonstrate understanding of the degradation and criticality event processes, and that integration with performance assessment depends on the needs of probabilistic consequence screening, which will be developed in the consequence screening work packages (SF-18SN01030506 and SF-19SN01030506) in FY18-19.

Demonstration calculations foreseen for FY19 include handing off a sequence of degraded states from the C-M-TH model for N-TH analysis. Additional calculations with the N-TH-M model will evaluate how changes in WP breach transmissibility affect criticality events, particularly transient events for which the ejection of water is a key uncertainty that affects the energy and damage produced. Substantial model development is needed before these demonstrations can be achieved, and further planning of integrated calculations is deferred pending the outcome of that development.

The ORNL roadmap document (Evans et al. 2018) describes run-time coupling of N-TH-M simulations with PA, which is very likely not necessary because criticality consequence screening can use bounding effects to evaluate significance. The previous PA work (Mohanty et al. 2004) showed that the incidence of criticality in a repository (especially the number of events and their timing) could be more important than specific details of the event consequences, which can be bounded. This strategy will be evaluated in upcoming deliverable M3SF-18SN01030506: *Probabilistic Postclosure DPC Criticality Consequence Analysis – Scoping* (22Jan2019).

Ultimately, coupling of in-package flow and radionuclide transport, with reactive chemical transport (Figure 6) is the goal of multi-physics simulation. This will be achieved incrementally, guided by further work planning in revisions to workplans such as this one.

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