DPC Direct Disposal Feasibility Assessment Status

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Agenda

- Background/current approach to support DPC direct disposal assessment
- Criticality analysis status
- DPC filling assessment status
- Flow simulation of filler materials within DPC
- Planned future work
Direct disposal of already loaded dual-purpose canisters (DPCs) is feasible but requires some work to make reality.

### Background
- As of 5/1/2018 there are 2,761 dry storage systems in use in the US containing 115,709 spent fuel assemblies
- ~200 new DPCs loaded per year
- DPCs were not designed, licensed, or loaded with consideration of geologic disposal conditions and requirements
- Addressing criticality over disposal time periods (e.g., 10,000+ years) is necessary to support a repository performance assessment

### Options
- More detailed modeling to recover uncredited margins
- Add filler to displace moderator from being between fuel rods
- Evaluate consequences of criticality on repository PA

### As-loaded analyses
- As-loaded analyses is being performed through UNF-ST&DARDS to evaluate available margins
  - Based on current modeling approaches, some DPCs don’t have enough excess margin so other options are needed (e.g., moderator displacement)

### Work
- Work has started looking into being able to add filler materials through existing vent and drain ports
- New work to start (FY18) will look at development of an integrated PA that can account for criticality
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Substantial progress has been made to address the criticality aspect of direct disposal of DPCs over the past years.

- **As-loaded canister-specific criticality analysis**
  - Analysis completed for 616 loaded DPCs at 28 sites
  - New update to GC-859 data collection should make more loading maps usable

- **Criticality analysis methodology developed for BWRs**

- **Evaluated ground water elements that could provide credit (e.g., Cl) in different repository media**

- **Misload analysis methodology developed**

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**Criticality Analysis Roadmap**

<table>
<thead>
<tr>
<th>Feasibility Assessment</th>
<th>Licensing Determination</th>
</tr>
</thead>
<tbody>
<tr>
<td>Perform DPC model development to establish baseline</td>
<td>Criticality validation (e.g., experiments with Cl in solution, relevant configurations)</td>
</tr>
<tr>
<td>Develop and apply misload analysis methodology</td>
<td>Justify and incorporate site-specific parameter distributions</td>
</tr>
<tr>
<td>Assess loads required for significant impact to in-package chemistry</td>
<td>Justify use of non-bounding assumptions</td>
</tr>
<tr>
<td>Groundwater analyses for different geologies</td>
<td>Validate site-specific geochemistry models</td>
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</tbody>
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UNF-ST&DARDS is a unique tool being applied to analyze each loaded DPC for suitability for direct disposal

- Performs as-loaded criticality analysis of each loaded DPC
  - Full burnup credit
  - Component credit
  - Other credit based on design specifics

- FY18 Summary to date:
  - Two new DPC models (templates) have been developed
  - 60 DPCs from five sites (2 shutdown, 3 operating) were added to library

- As-loaded criticality analysis has shown that a fraction of the analyzed DPCs still have criticality potential (host media that is not salt) based on current modeling and material degradation assumptions

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76% of the analyzed 616 DPCs are below the representative subcritical limit with as-loaded analysis with fresh water

- A representative subcriticality limit of $k_{eff} = 0.98$ is being used for this assessment

<table>
<thead>
<tr>
<th>Description (Analysis year: 12000)</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Total DPCs analyzed</td>
<td>616</td>
</tr>
<tr>
<td>Total DPCs below subcritical limit with loss of neutron absorber (design-basis loading)</td>
<td>0 (0%)</td>
</tr>
<tr>
<td>Total DPCs below subcritical limit with loss of neutron absorber (as-loaded)</td>
<td>473 (~76%)</td>
</tr>
<tr>
<td>Total DPCs below subcritical limit with loss of neutron absorber and carbon steel structures (as-loaded)</td>
<td>420 (~68%)</td>
</tr>
<tr>
<td>Total DPCs below subcritical limit with loss of neutron absorber and carbon steel structures (as-loaded) considering misload*</td>
<td>397 (~64%)</td>
</tr>
</tbody>
</table>

* Misload includes assemblies are placed in wrong location within canister
Preconditioning DPCs with filler material is being considered as an option to prevent post-closure criticality

- Currently two classes of filler materials are being investigated
  - Cement slurry materials
  - Low temperature metals and alloys

- A Multiphysics simulation capability is being developed to support and assess DPC filling process
  - Stage 1 - Single physics with validation experiments (unit testing)
    - Flow simulation (under development) to determine injectibility, void filling, filling time, filling method (pump vs. gravity)
    - Thermodynamic simulation (not started) to understand solidification behavior
    - Heat transfer (first phase completed) to understand temperature distribution, waste package temperature
  - Stage 2: Multiphysics with validation experiments (scaled DPC testing)
    - Multiphysics coupling (flow + thermodynamic + heat transfer) to develop a predictive tool

- The Multiphysics simulation capability will be used to narrow down candidate materials
- The Multiphysics simulation capability will be used to design external heating equipment (if needed)
- Additional simulations such as structural to determine the structural load and experiments such as radiation hardening as described in the work plan will be needed
- Need to develop instrumentations for various data recording during filling to certify the filling process with certain confidence level
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Filler evaluation approach integrates lab testing, technical analysis, numerical simulation, and bench-scale testing

<table>
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<th>Phase 1</th>
<th>Phase 2</th>
<th>Phase 3</th>
<th>Phase 4</th>
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<tr>
<td>6.1 Testing for Cement Materials</td>
<td>6.2 Testing and Analysis for Molten Metal/Metal Alloy and Glass Materials</td>
<td>6.3 Testing and Analysis for Dry Particulate Filler Materials</td>
<td></td>
</tr>
<tr>
<td>Injectability</td>
<td>Injectability (continued)</td>
<td>Gas Generation</td>
<td></td>
</tr>
<tr>
<td>Durability (leaching)</td>
<td>Durability (leaching irradiated samples)</td>
<td>Postclosure Performance</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Retrievalability/Recoverability</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

7.1.1 Supporting Analysis for Cement Fillers
- Thermochemical Analysis of Cement Composition and Cure
- Postclosure Leaching Analysis
- Natural Analogues
- DPC Shell Pressure Rating
- Fate of Hydrogen Gas in Sealed Canisters

7.1.2 Supporting Analysis for Metal/Metal Alloy and Glass Fillers
- Literature Review and Technology Survey

7.2.1 Phase 1 Numerical Simulation
- Criticality
- Thermal
- Flow
- Filler Dose Analysis

7.2.2 Phase 2 Numerical Simulation
- Coupled Thermal-Flow
- Radiolysis
- Pre-Test Predictions

7.2.3 Phase 3 Numerical Simulation
- Coupled Thermal-Flow
- Coupled Thermal-Flow-Mechanical
- Pre-Test Predictions
- Postclosure PA

7.2.4 Phase 4 Numerical Simulation
- Pre-Test Predictions
- Final Project Documentation

7.3.1 Phase 1 Physical Model Studies
- Molten Metal/Metal Alloy Filler Phase 1 Activities

7.3.2 Phase 2 Physical Model Studies
- Cement Filler Unit-Cell Testing
- Molten Metal/Metal Alloy Filler Unit-Cell Testing
- Dry Particulate Filler Self-Leveling Flow Test

7.3.3 Phase 3 Physical Model Studies
- Cement Filler Separate Effects Tests
- Molten Metal/Metal Alloy Filler Separate Effects Tests

7.3.4 Phase 4 Scaled Demonstration
- Final Project Documentation

Notes: A Many Phase 1 activities can be supported in FY18 with currently available resources.
Laboratory testing will be performed to demonstrate the proposed filling operation at a limited scale to validate the CFD simulations.

A scaled canister (10.38”Ø) will be built to test the filling performance with identified fillers, such as glycerin.

Suitable instrumentation will be used for monitoring the process (viscosity, flow rate, level measurements, void detection, etc.)
DPC Filling Simulations
Simulations Objectives;
Design of a Spent Fuel Cask Mockup for filling analyses;
Numerical Method and Computational Approach;
Filler Materials;
Path forward to complete the analyses;
Simulation Results;
- Drain pipe preliminary simulations;
- Problem sizing and compute time evaluation;
- Modeling and filling the mouse hole region;
Simulation Objectives

- To numerically evaluate the filling process, initially on ideal surfaces (equal advancing and receding contact angles);
- Experiment with different liquid metals and surrogates;
- Explore filling options based on existing or new cask features;
- Aid the experiment design by scaling the major quantities;
- Build a basis for further model validation;
- Identify potential caveats that may compromise the filling;
- Surface wettability of ‘high energy’, rough surfaces, and characterization (heterogeneous vs homogeneous);
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Mockup Geometry Design

- Lower 16% (height 74cm, Ø26 cm) of the real canister including mouse holes, assembly stands, first (support) grid and the first spacer grid;
- 5x5 real rod array used as design concept (based on DNB testing rationale);
- Five assemblies total, full length, enclosed in a circular container;
- To minimize the computational mesh, the spacer grid is simplified by removing the vanes;
- The geometry is idealized to avoid proprietary concerns;
- Major components have nominal dimensions as in: Final Safety Analysis Report for the HI-STORM 100 Cask System (HI-2002444), Holtec International to allow for filling assessment;
- Some reduction of feature complexity is applied for flow modeling simplification, when appropriate;
Employ 3D CFD methods for two-phase two-component fluid systems;

Isothermal Segregated Flows of liquid and gas;

Volume of Flow mixture model suggested as first candidate;
  - Fastest option for separate two phase flows;
  - Volume fraction of each phase is computed by the following transport equation:

\[
\frac{\partial}{\partial t} \int_V \alpha_i dV + \oint_A \alpha_i \mathbf{v} \cdot d\mathbf{a} = \int_V \left( S_{\alpha_i} - \frac{\alpha_i D\rho_i}{\rho_i} \right) dV - \int_V \frac{1}{\rho_i} \nabla \cdot (\alpha_i \rho_i \mathbf{v}_{dr,i}) dV + \oint_A \frac{\mu_i}{\sigma_i \rho} \nabla \alpha_i \cdot d\mathbf{a}
\]
  - High resolution level tracking scheme combined with viscous laminar solution;

Code selection: STARCCM+ based on availability of ORNL site licenses and large experience with the code;
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## Filler Materials

- Two types of materials: for real application, focused on filling with liquid metals, and for lab testing (surrogates);
- Density and dynamic viscosity regarded as properties affecting the filling process;
- Scope to be extended with more metals or other materials depending on program direction;

<table>
<thead>
<tr>
<th>Material</th>
<th>Melting Temp (°C)</th>
<th>Density (g/cm³)</th>
<th>Viscosity (Pa.s)</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Glycerin (C_{3}H_{8}O_{3})</td>
<td>liquid</td>
<td>1.26@RT</td>
<td>0.95@RT</td>
<td><a href="http://www.MatWeb.com">www.MatWeb.com</a></td>
</tr>
<tr>
<td>Silicone Oil</td>
<td>liquid</td>
<td>0.96@25C</td>
<td>0.33@25C</td>
<td><a href="http://www.sigmaaldrich.com">www.sigmaaldrich.com</a></td>
</tr>
<tr>
<td>Lead</td>
<td>327 (600K)</td>
<td>10.70@600K</td>
<td>0.0026@600K</td>
<td>V. Sobolev (2007)</td>
</tr>
<tr>
<td>Lead-Bismuth</td>
<td>124 (398K)</td>
<td>10.53@398K</td>
<td>0.0032@398K</td>
<td>B. Alchagirov (2003)</td>
</tr>
<tr>
<td>Mercury</td>
<td>liquid</td>
<td>13.53@RT</td>
<td>0.0015@RT</td>
<td>Thermal Fluids Central</td>
</tr>
<tr>
<td>Water</td>
<td>liquid</td>
<td>0.97@RT</td>
<td>0.00088@RT</td>
<td>Web (for comparison)</td>
</tr>
</tbody>
</table>

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Implement data mapping algorithms;
Consider the following canister domains/regions;
  - Mouse hole – calculations completed, show no issues with filling rate of 1.26 cc/sec and the following fillers: Glycerin, Lead-Bismuth and Mercury;
  - Lower assembly support grid region;
  - Single spacer grid region;
  - Top of canister space (yet to be modeled);
The problem is a good candidate for HPC. No available allocation of time on Summit. It may require around (for 6M elements and < 1000 el/core) 6000 cores for scale ~6 times smaller that the original;
No issues found after filling up the mouse holes on macroscale;
Filling through the drain pipe will require separate analysis;
Model validation on lab scale test to confirm proper viscous shear;
Look at microscale of surface wettabiliy effects, contact angles, surface tension of liquids, etc.
Filling through the Drain pipe

- A cylindrical volume of 6m³ was modeled with real size drain pipe (14’, Ø 0.625”);
- 100 ml/sec filling rate providing total filling time of 6e4 sec, or about 17 hours;
- The flow assumed constant, as of a PD pump;
- Filling liquid – Mercury (high density) causes high hydrostatic pressure;
  - Results demonstrate stability issues with the current model (see plots) and may require different numerics to resolve pressure propagation;
  - Decision taken to treat the drain fill simulation separate from the canister filling problem;
Problem setup and Filling rate

- The entire geometry was ported into Starccm for meshing. One half (symmetry) of it was modeled and meshed successfully;
- Trim mesh was used that resulted in ~6 million elements;
- Total volume: 11.46 litres
- Calculation of the filling rate based on 6m³ and 100ml/s
  rate = $6.10^4$ sec filling time ~ 17 hours;
- Real height of cask – 14’ (4.27 m)
  model height – 0.673 m, axial scale - 6.34
- Model filling rate calculation:
  \[
  \frac{(11.46e-3 \times 6.34)}{6e4} = 1.21 \text{ cc/sec}
  \]
- Drain flow area
  180 mm² = 180e-6 m²,
  inlet velocity = $1.21/180 = 0.007$m/s
Simulation Results:
- Runs on 32 cores with timestep of 5ms: 24.5 hours of compute time for 9.56 sec of transient e.g. more than a year for one hour. Some numerical diffusion is seen to appear at 50th sec. Runs stopped.
- Model transitioned to a larger cluster and run on 640 cores:
  - Run with timestep of 2ms: the run completes but numerical diffusion appears at ~60th sec.
  - Run with timestep of 1ms: 29 hours for ~39 sec physical time (9.5s to 48.5s) – first 39 sec computed successfully. Same run continued and crashes at 79th sec due to numerical diffusion: 0.7 hours/second, e.g. ~100 days for an hour of transient;
  - Run with increased filling rate (10 times). Timestep and speed as above. Diffusion occurs at ~74th sec., e.g. the higher filling rate does not stabilize the solution, BUT the filling seems to proceed normally. Therefore higher filling rates could possibly be employed assuming lower rates would work even better (see plots).

Computing strategy has to change: faster filling rate and/or in only part of the geometry

Model of the lower 70mm (includes the mouse holes). Meshed with a coarse poly mesh: 45,000 elements only;
Filling of lower canister: mouse holes

- Stable solution with a max timestep of 5ms, 0.12 hours/sec on 32 cores (45k elements). About 1000sec of physical time to be computed translating to 120 hours (4-6 days);

- Mouse hole region successfully filled with Glycerin, Pb-Bi and Hg;
  - The first calculation showed uneven level after the mouse hole are filled;
  - The section was capped with an extra volume to equalize pressure and runs were completed. Capping helps and level propagates evenly. 1290 cc total volume is filled for 1040 sec (1290/1.26=1024sec, with about 1.5% time error). Plots cross section: Plots entire volume:

- A computing approach based on domain decomposition and interface data mapping seems promising:
  - Problem is suitable to such approach because the key phenomena is attributed to the moving liquid front. The rest of the domain is less important and computing quantities on it has little merit, but consume resources;
  - The approach allows for simulation of only one of the several parallel regions which reduces the domain several times;
  - It would require developing transitioning (data mapping) algorithms, which is possible but is not a routine operation;

- Initial modeling of the following segment has started. The 310mm section including the lower grid + spacer was meshed with ~500k elements. The lower grid holes produce many elements and will need to be modeled separately;

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Future effort includes criticality consequence analysis of a repository

- Micro-level analysis to determine changes in isotopic inventory, temperature, pressure in case of a criticality event in a DPC given certain boundary conditions (e.g., water flow rate inside a DPC)
  - Multiphysics (neutronics and thermal hydraulic) analysis to determine change in isotopic inventory, pressure, and temperature
  - Structural analysis coupled with neutronics and thermal hydraulics to determine any potential damages to the DPC, waste package, and surrounding

- Macro level analysis including PRA to determine the potential criticality impact on the repository performance

- Continue developing a fully validated Multiphysics filler simulation model that can be used to support the DPC filling process

- Continue development of criticality models to support as-loaded criticality analysis

- Continue data collection to support quantification of the uncertainties in the as-loaded criticality analysis

- Leverage data in UNF-ST&DARDS to incorporate spatial detail on thermal and dose attributes into PA
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Backup
New work to start in FY18 allows acceleration of working through the different aspects of the overall DPC criticality analysis approach.

- Define assumptions and boundary conditions
- Scoping analyses to establish baseline
  - Establish baseline set of representative configurations for analysis
  - Discretize configurations by site and DPC design
  - Perform detailed criticality analysis for DPCs and base configurations
- Envelope analysis
  - Perform parametric evaluations to establish “envelope” within which there is potential for criticality
  - Establish conditions, parameter ranges, distributions, values that can produce parameter envelope conducive to criticality
- Probability analysis
  - Evaluate probability of occurrence of parameter envelope integrated over repository
  - Is probability screening criterion satisfied?
- Risk assessment (consequences)
  - Perform consequence analyses on DPCs that achieve criticality
  - Establish impact to nominal PA parameter ranges and distributions
  - Is change within PA parameter uncertainty distribution?
  - DPC direct disposal conditionally not feasible
  - DPC direct disposal conditionally feasible

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UNF-ST&DARDS is a comprehensive data and analysis system for the safe, secure and sustainable management of SNF

- **Characterizes spent fuel / systems that the nation will be managing for decades**
  - Best available information to inform decision making and address emerging issues
  - Integrated data and analysis capability enables automated characterization of all SNF assemblies (e.g., radioactivity, decay heat, and isotopic compositions) and casks (e.g., criticality, dose rates, containment, and temperatures) in the domestic inventory

- **A comprehensive system for analysis of the SNF from the time it is discharged from the reactor to the time it is disposed of in a geologic repository**

- **Provides the Unified Database**
  - Controlled source of technical data for the entire waste management system
  - An important DOE Office of Nuclear Energy resource for SNF management and disposition
Criticality analysis of 60 DPCs at five sites has been completed in FY-18

- Two new DPC models (templates) have been developed
- Five sites including two shutdown and three operating sites have been analyzed using the two new DPC models
- Two degradation scenarios were considered
  - Loss of neutron absorber panels (all five sites)
  - Loss of carbon steel components and neutron absorber panels (one site)
- 60 DPCs were also analyzed for misload scenarios
- A filler material (non neutron absorbing) scoping calculation has been performed to determine the minimum filler height

<table>
<thead>
<tr>
<th>axial fuel zone</th>
<th>Filler height (cm)</th>
<th>$k_{ef}$</th>
<th>sigma</th>
</tr>
</thead>
<tbody>
<tr>
<td>14</td>
<td>307.0225</td>
<td>1.02292</td>
<td>0.00036</td>
</tr>
<tr>
<td>15</td>
<td>327.3425</td>
<td>1.02065</td>
<td>0.00028</td>
</tr>
<tr>
<td>16</td>
<td>347.6625</td>
<td>1.01169</td>
<td>0.00027</td>
</tr>
<tr>
<td>17</td>
<td>367.9825</td>
<td>0.96016</td>
<td>0.00028</td>
</tr>
<tr>
<td>18</td>
<td>388.3025</td>
<td>0.83271</td>
<td>0.00024</td>
</tr>
</tbody>
</table>