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Modeling transport of corrosion products in Multi-Purpose Canisters using *PFC3D*

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This is a technical paper that does not take into account contractual limitations or obligations under the Standard Contract for Disposal of Spent Nuclear Fuel and/or High-Level Radioactive Waste (10 CFR Part 961). For example, under the provisions of the Standard Contract, spent fuel in multi-assembly canisters is not an acceptable waste form, absent a mutually agreed to contract amendment. To the extent discussions or recommendations in this paper conflict with the provisions of the Standard Contract, the Standard Contract governs the obligations of the parties, and this paper in no manner supersedes, overrides, or amends the Standard Contract. This paper reflects technical work which could support future decision making by the U.S. Department of Energy (DOE). No inferences should be drawn from this paper regarding future actions by DOE, which are limited both by the terms of the Standard Contract and a lack of Congressional appropriations for the Department to fulfill its obligations under the Nuclear Waste Policy Act including licensing and construction of a spent nuclear fuel repository.

1 INTRODUCTION

Dual purpose canisters (DPCs) are widely used for dry storage, and for transportation (where certified) of commercial spent nuclear fuel (SNF) assemblies. The U.S. Department of Energy, Office of Spent Fuel and Waste Science & Technology is investigating the technical feasibility of direct geological disposal of SNF in loaded DPCs. Because DPCs, and in particular the neutron absorbing components, were not designed for geologic disposal, post closure criticality control is an important aspect of this investigation. Over geological timescales, it is probable that the canister and its disposal overpack would eventually be breached by initial cracks (fractures) due to stress corrosion cracking or other corrosion processes. A breach in the canister could allow ground water to fill the void space around the fuel, in repository settings that are either unsaturated or saturated (above or below the water table). If the canister internals including neutron absorber components are sufficiently degraded by exposure to ground water, a criticality event could occur. Such an event would create transient elevated temperature and pressure conditions within the DPC and overpack.

This paper analyzes the degradation of SNF DPCs presently used for storage and transportation, if they were used for disposal as well. The type of DPC analyzed consists of a cylindrical shell of stainless steel, containing a rectilinear "egg-crate" style basket made from aluminum-based material to hold the fuel assemblies. Aluminum is used in many basket designs as part of metal-matrix composite materials that absorb thermal neutrons for reactivity control, help to dissipate radiogenic heat, and serve as the structural framework that holds the fuel assemblies. If the canister is used for disposal, and it is breached after it has been in a geologic repository for thousands of years, and subsequently flooded by ground water, the aluminum-based basket plate material is likely to degrade. Degradation of the structural and neutron absorbing performance of the fuel basket could lead to a criticality event under certain conditions. This paper presents numerical modeling of the corrosion of basket plates and movement of corrosion products, for geometry representing a 17×17 pressurized water reactor fuel assembly.

2 DESIGN AND ANALYSIS

Itasca's distinct element modeling framework *PFC3D* (Itasca 2019) is used to represent the transport and deposition of corrosion product material. A pseudo-3D model is developed representing a thick slice of the cross-section perpendicular to the axis of the canister, with periodic boundaries along the axis of the canister, i.e., material leaving from one face re-enters the model from the other face. This is done to account for proper packing in 3D. To study the effect of different orientations of the canister, the direction of gravity can be changed. However, it is assumed that the axis of the canister stays horizontal. The fuel rods and basket components are fixed in this model and are represented by rigid boundaries. The loose corrosion products are simulated by generating clumps adjacent to the walls that represent the plates. The clumps are then allowed to move and settle, and in the process, to interact with fuel rods, plates and other clumps that represent already settled material. Clumps are used because they have a rolling resistance due to their shape. Currently, a clump shape made up of two glued balls is used.

The fuel assembly cell is assumed to be filled with water. Buoyancy forces act on the clumps as they settle through the model. A velocity-proportional drag force based on Stoke's law is also applied to each particle. Based on an average particle size of about 50 microns, the terminal velocity of the particles is estimated in the range of 0.1 m/s to 0.01 m/s (depending on the temperature and viscosity of water). This implies the corrosion products will settle to the bottom in a time frame of a few seconds to a few minutes. Given the slow rate of corrosion, there will not be many particles settling at the same time. A settling particle will likely interact with fuels rods, plates, and other already settled particles only—and not with other settling particles. Using this assumption, the computation time is reduced by having multiple particles settling at the same time provided they do not interact with each other. Based on the model size, the number of particles that can be generated at the same time without interacting with each other is determined. These particles are generated randomly along the length of the plates, settled, and brought to equilibrium. The "real" time is then incremented by a value equal to the time during which the mass of corrosion products equal to the mass of these particles would have been generated. This process is then repeated until the desired duration of "simulated" time is reached. The logarithmic law for corrosion process is used. The model output is a cartesian grid with the concentrations of the individual corrosion products and neutron absorber materials.

After the specified duration of corrosion has been simulated, a seismic analysis is carried out. It is assumed that the canister is embedded in ground at least partially so that the ground motion is transferred directly to the canister and the basket structure is intact so that there is no relative motion between the basket and canister. To model the seismic shaking, one horizontal and the vertical components of the ground motion (both normal to the axis of the canister) are applied as velocities of the basket and fuel rods. The third component (horizontal) cannot be used for this case due to the periodic boundary condition in out-of-plane direction.

3 RESULTS AND DISCUSSION

Figure 1 shows distribution of corrosion products after same duration of time for two different orientations of the fuel assembly, with tilt angle of 0° and 30°. For the 0° case, the larger concentration on the sides is because all particles generated on the side walls end up in that region. For 30° case, higher concentration is observed in the lowest corner as expected. Figure 2 shows results at different times during and at the end of shaking for 0° case. Redistribution of corrosion products due to the shaking can be observed.

4 CONCLUSIONS

A *PFC3D* model to simulate transport of corrosion products is presented along with results for different orientation of the canister. A possible improvement is to model the plates as bonded assemblies of balls that represent the aluminum matrix mixed with boron carbide particles. As part of the corrosion process, the bonds in this assembly would then be allowed to break as dictated by decreasing strengths and contact forces caused by plate stresses (representing the corrosion product). That will more realistically model the corrosion process in terms of size of particle released and timing as a function of location, i.e., particles in the roof may fall at a faster rate than those on the sides and they may have a different size distribution, cohesion, and other properties as well.

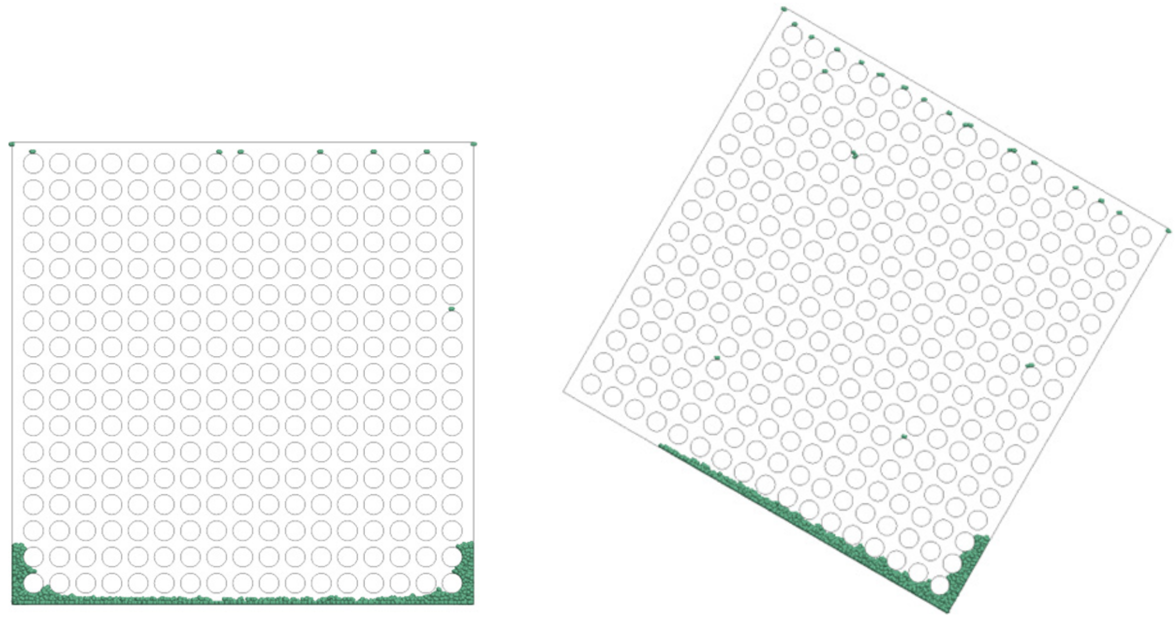

Figure 1. Distribution of corrosion products after a specified amount of time for 0° (left) and 30° (right) tilt angles.

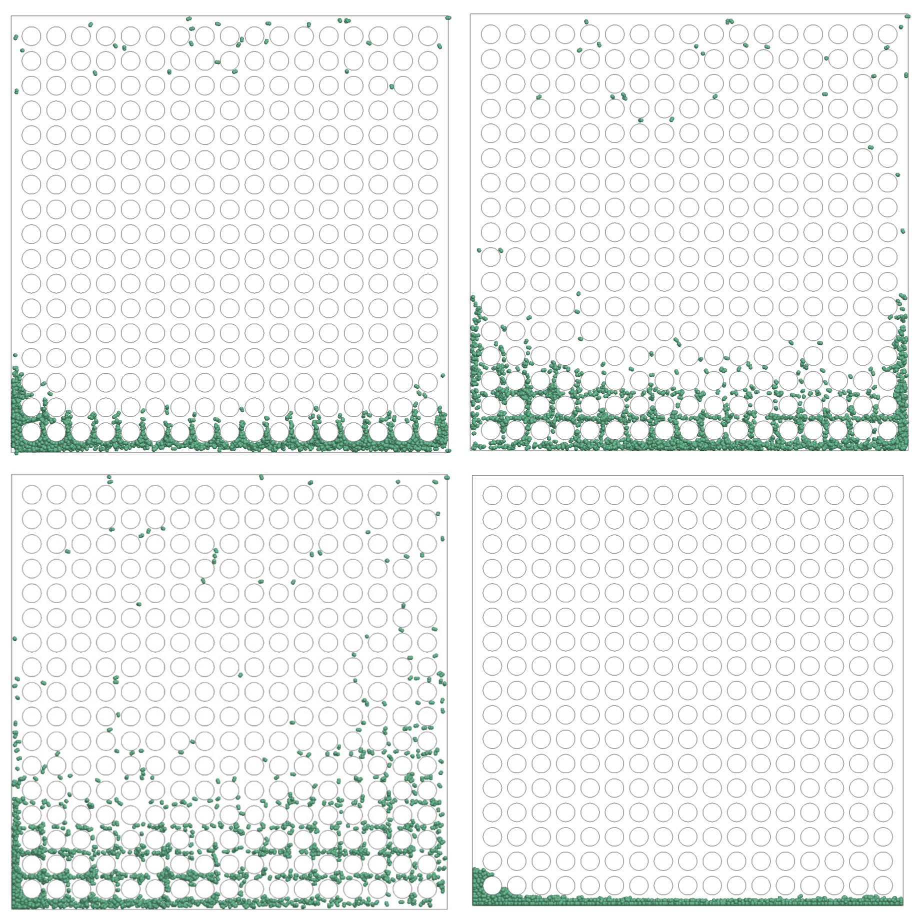

Figure 2. Model configuration at (top left) 1 second, (top right) 2 seconds, (bottom left) 5 seconds, and (bottom right) equilibrium after the end of shaking for 0° inclination case.

REFERENCES

2019 Itasca Consulting Group, Inc. (2019) *PFC3D – Particle Flow Code in 3-Dimensions, Version 6*. Minneapolis: Itasca.

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