Center for Performance and Design of Nuclear Waste Forms and Containers (WastePD)
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Mission Statement*: to understand the fundamental mechanisms of waste form performance and apply that understanding to design new waste forms with improved performance.*

The report of a 2015 DOE workshop on Basic Research Needs for Environmental Management described the need for “new materials for long-term storage of nuclear waste, including waste forms.” The main performance criterion for waste forms, and the primary consideration for the design of new ones, is their ability to isolate and immobilize the radionuclides by withstanding corrosion in a repository environment over geologic time scales. WastePD is focused on this topic, specifically the environmental degradation mechanisms and the science underlying the design and performance prediction of new corrosion-resistant waste forms and canister materials.

Nuclear waste will eventually be placed in a mined repository in different forms, including three classes of solid matter: glasses, crystalline ceramics, and metals, and all three can degrade during exposure to the environment. WastePD consists of three thrusts focused on glass, ceramic, and metal corrosion, as shown in the figure. The thrusts are tied together by synergistic activities, intersectional topics of study, and an aligning framework.

Glasses and crystalline ceramics are often considered to be nonreactive and corrosion resistant, but they do degrade. When exposed to water, glass reacts to form a thin alteration layer on its surface that protects the glass and slows the rate of attack. In some environments, however, this protective layer becomes unstable and the glass exhibits an accelerated rate of attack. The details of the exact nature and stability of the protective layer are not known, so the transition to a non-protective condition cannot be predicted. As a result, current repository performance models take a conservative approach by assuming that glass will corrode at an accelerated rate rather than the slow passive rate. A better understanding of the glass corrosion process could lead to improved glass waste forms, support more robust repository models, and influence the repository design.

Crystalline ceramic waste forms can also release the incorporated radionuclides during interaction with the environment through matrix dissolution, selective leaching, radionuclide diffusion and surface reaction. An alteration phase may also form on the surface of ceramic waste forms to protect against further corrosion. Furthermore, many ceramic hosts under consideration for nuclear waste are semi-conductive and therefore can undergo transformative electrochemical reactions in aggressive environments. The environmental degradation of ceramic waste forms has not been studied in detail and little is known about the phenomena involved.

By their nature, metals are often susceptible to environmental degradation by electrochemical processes, although extremely corrosion resistant alloys (CRAs) like stainless steels (SS) have been developed by the judicious combination of alloying elements and prescribed processing. Like glass and ceramics, CRAs are protected by the spontaneous formation of a very thin surface oxide layer. However, such nm-thick films can break down and lead to accelerated forms of corrosion. The design of CRAs has in the past been based on empirical knowledge, which is not useful when considering new classes of alloys such as High Entropy

Alloys (HEAs). New approaches shown to be successful for computational design of materials have not been extended to corrosion resistance. Thus, it is clear that there are unifying concepts in the corrosion of the three materials classes of waste forms.

The design and long-term performance prediction of all materials, including glass, ceramics and metals, is currently empirical, based on correlations, experience, and intuition. The main goal of WastePD is to develop the Science of Environmental Degradation of Materials (SEDMat), with applicability to all three materials classes. SEDMat will enable a transition from empiricism to design based on calculable parameters, and ultimately to multiscale, multiphysics models that describe and predict the sub-processes of the overall corrosion phenomenon.

SEDMat will require enhanced fundamental understanding. For nuclear waste glass corrosion, it is critical to attain physical insights into the structure of the glass/solution interface and the behavior of reactive and inactive species present at that interface. Focus is on the formation of an amorphous, hydrated, porous, alumino-silicate layer on the glass and ceramic surfaces, and the roles of composition, structure and near-field environment. The corrosion of crystalline ceramics, in addition to short-range structural effects similar to glass, is also influenced by grain size and grain boundary structures. Different model ceramic systems, including apatite, hollandite, and perovskite are investigated as promising forms for incorporating I, Sr, and Cl fission products. The focus is on the interfacial behaviors across solid-solid and solid-liquid boundaries that can be closely linked with the ceramic waste form corrosion and stability under near field conditions. Metal HEAs, like multicomponent waste glasses, have almost limitless possible composition variations that enable fundamental material design concepts to be tested and validated.

WastePD is the first center ever created to address the corrosion of glass, crystalline ceramics and metals in a comprehensive and coordinated manner. The interactions between experts in the different materials create new approaches and understanding that would not have been possible otherwise. An example is how WastePD provides a unique synergistic platform for studying the interaction of corrosion behaviors between material classes. Glass or ceramic waste forms in a repository will be exposed to environments resulting from the corrosion of SS canisters. Studies of glass and ceramic wasteforms corroding in contact with SS are providing new insight into how SS corrosion products affect glass and ceramic corrosion and how the glass and ceramic corrosion products in turn influence SS corrosion.

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