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Cementitious Barriers Modeling for Performance Assessments of Shallow Land Burial of Low Level Radioactive Waste - 9243

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ABSTRACT

The Cementitious Barriers Partnership (CBP) was created to develop predictive capabilities for the aging of cementitious barriers over long timeframes. The CBP is a multi-agency, multi-national consortium working under a U.S. Department of Energy (DOE) Environmental Management (EM-21) funded Cooperative Research and Development Agreement (CRADA) with the Savannah River National Laboratory (SRNL) as the lead laboratory. Members of the CBP are SRNL, Vanderbilt University, the U.S. Nuclear Regulatory Commission (USNRC), National Institute of Standards and Technology (NIST), SIMCO Technologies, Inc. (Canada), and the Energy Research Centre of the Netherlands (ECN). A first step in developing advanced tools is to determine the current state-of-the-art. A review has been undertaken to assess the treatment of cementitious barriers in Performance Assessments (PA).

Representatives of US DOE sites which have PAs for their low level waste disposal facilities were contacted. These sites are the Idaho National Laboratory, Oak Ridge National Laboratory, Los Alamos National Laboratory, Nevada Test Site, and Hanford. Several of the more arid sites did not employ cementitious barriers. Of those sites which do employ cementitious barriers, a wide range of treatment of the barriers in a PA was present. Some sites used conservative, simplistic models that even though conservative still showed compliance with disposal limits. Other sites used much more detailed models to demonstrate compliance. These more detailed models tend to be correlation-based rather than mechanistically-based. With the US DOE's Low Level Waste Disposal Federal Review Group (LFRG) moving towards embracing a risk-based, best estimate with an uncertainties type of analysis, the conservative treatment of the cementitious barriers seems to be obviated. The CBP is creating a tool that adheres to the LFRG chairman's paradigm of continuous improvement.

INTRODUCTION

The Cementitious Barriers Partnership's (CBP) genesis was a recommendation from the Cementitious Materials for Waste Treatment, Disposal, Remediation, and Decommissioning Workshop held in December 2006 [4]. The purpose of the workshop was to facilitate technical exchange among subject matter experts across the DOE complex, additional national and international experts, and representatives from local advisory groups and state and federal agencies with roles at DOE sites. The workshop

was attended by 110 people with an additional 250 participating via the workshop webcast. The CBP was formed to implement a coherent program for implementing the Workshop's recommendation.

The CBP is a multi-agency, multi-national consortium working under a U.S. DOE EM-21 funded CRADA with the Savannah River National Laboratory (SRNL) as the lead laboratory. Members of the CBP are SRNL, Vanderbilt University, USNRC, NIST, SIMCO Technologies, Inc. (Canada), and ECN. The aim of the CBP is "The Development of Next Generation Simulation Tools to Evaluate Cementitious Barriers and Materials Used in Nuclear Applications." To accomplish this aim, the CBP is in the processing of developing an integrated computational and experimental program (see Figure 1).

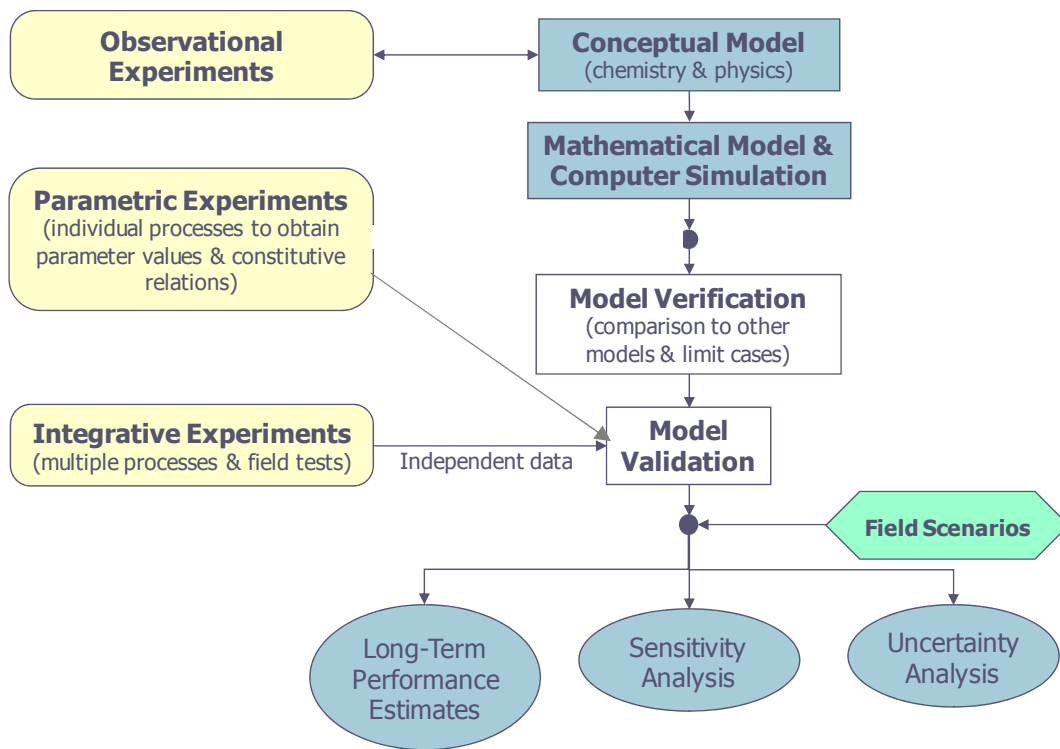


Figure 1 Process- and Mechanism based Modeling and Experimentation

This next generation computational tool will be applicable to any cementitious barrier use. Its initial customer is seen as the DOE's low level waste performance assessment community.

Figure 2 shows examples of applications of cementitious barriers within the DOE complex. These applications involve the disposal of low-level radioactive waste. A requirement for this type of disposal is that the public and environment be protected for, depending under which regulatory framework the disposal falls, 1,000 to 10,000 years. The analyses that are used to calculate behavior out to such distant future times inherently

contain uncertainties. The CBP's mission, in developing its next generation tool, is to improve the calculations by addressing these inherent uncertainties.

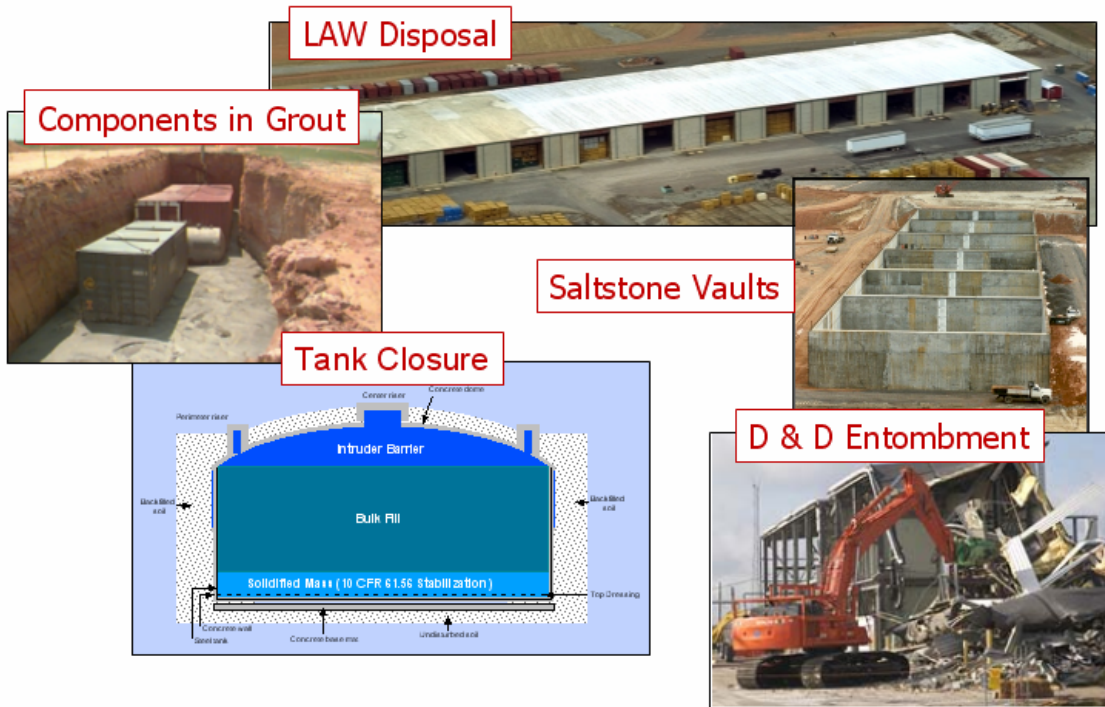


Figure 2 Example DOE Applications of Cementitious Barriers

Examples of the commercial nuclear industry's application of cementitious barriers are shown in Figure 3. The commercial nuclear industry is interested in not only the disposal (or storage) of low-level nuclear waste, but also in the behavior of the barriers in operating nuclear facilities. The nuclear renaissance supplies an added impetus to developing the next generation of analytical tools to assess the behavior and assist in the design of the new facilities. The tools developed by the CBP will decrease the uncertainty in the design of structures meant for the protection of the public and environment. The CBP tools can also be applied to those structures to provide a better estimate of their expected behavior.

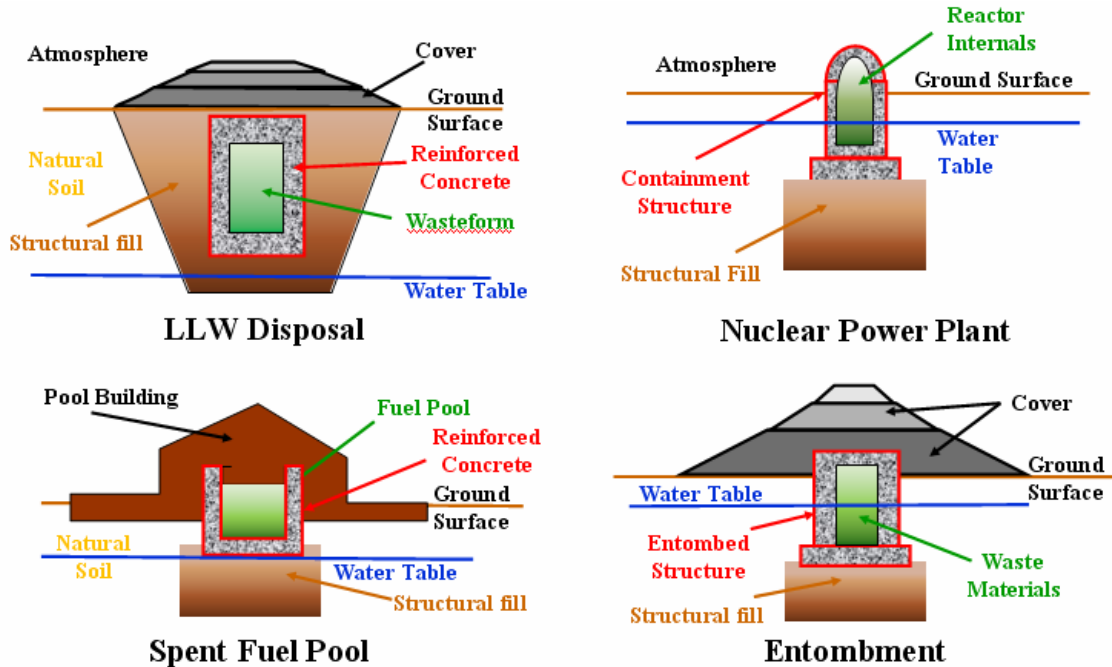


Figure 3 Example Commercial Uses of Cementitious Barriers

CURRENT APPROACHES

A first step in developing the CBP's advanced tools is to determine the current state of cementitious barriers in extant Performance Assessments. A review was conducted of DOE PAs as these are seen as the tools' initial customer base. The review looked at how cementitious barriers were modeled in the PAs from both the flow and transport point of view. In PAs that contained cementitious barriers, the barriers serve to isolate the low-level radioactive waste by excluding water from the waste and/or by the chemical interaction of the waste with the barrier.

A review was made of the PAs from the following DOE sites. Sites or disposal units that did not consider cementitious barriers do not have references indicated.

- Savannah River Site [8,9]
- Oak Ridge National Laboratory [5]
- Hanford [1,6]
- Nevada Test Site (NTS)
- Los Alamos National Laboratory (LANL)
- Idaho National Laboratory [2,3]

The NTS and LANL low-level waste depositories are in such arid environments that water is not of concern and cementitious barriers are either not used or no credit is taken for them in the PAs. The treatment of the cementitious barriers in PAs for the other sites will be discussed below in general terms.

Flow Aspects

The hydraulic aspects of the behavior of cementitious barriers refer to their ability to prevent groundwater flow through the barrier. This includes both intact and degraded conditions. The flow through intact barriers is determined using some adaptation of van Genuchten analysis as the conceptual approach. It has been stated that the van Genuchten analysis is not strictly applicable to cementitious media, but there is, at the moment, no better way to address this flow. Another issue is that there are known issues with the van Genuchten analysis near saturation [9] and several of the sites have essentially saturated cementitious media.

The aforementioned van Genuchten analysis implies that the cementitious media are treated as porous media and that a potential flow type analysis is applicable. The opportunity for the CBP is to assess these assumptions and determine if they are adequate for determining the rate at which water penetrates the cementitious media. If it is shown there are phenomena other than potential flow that control the passage of water through the media, then the CBP is in position to develop a new flow model.

Degraded behavior refers to both the existence of cracks in the cementitious media and degradation of the media's matrix. The matrix degradation is usually dealt with by assuming an increase in hydraulic conductivity. There is no apparent mechanistic treatment of the increasing hydraulic conductivity, just various assumptions as to what the shape of its moisture retention-hydraulic conductivity curve should be. This is not usually accompanied by appropriate potential curves, i. e., only one set of head curves is used for the entire degradation process. Cracking tends to be treated by assuming a single equivalent crack, either by adjusting the bulk media hydraulic conductivity or by the addition of an equivalent crack flow path. Either of these methods has implications on the mass transport that are not typically addressed. There are no uncertainties applied to either modeling assumptions.

Transport Aspects

Transport aspects fall into two broad categories: analyses that use a diffusion based mechanism and those that use an advection based mechanism. Regardless of which method is used, the equations show that the parameter controlling the release of a contaminant into a flow field is always a distribution coefficient, typically referred to as K_d . K_d is an experimentally derived bulk material property. As such, the treatment of cracking, mentioned in the preceding section, should have some affect on the K_d but that effect is not considered. It is interesting to note that the USNRC sees the treatment of cracking as an area of high concern [10].

A recent development in the transport aspects of contaminants appeared in the Savannah river Site's (SRS) F-Tank Farm PA [8]. The cementitious media were seen as evolving in time from a reducing to an oxidizing state. Values of K_d were obtained for several sub-

states within either reducing or oxidizing regimes. Detailed computational chemistry analyses were performed to determine transition points, based on pH and eH, as a function of pore flush volumes. The PA was then able to take credit for the reducing environment that was generally favorable with regard to contaminant transport. This is also an excellent example of the LFRG chairman's application of the continuous improvement paradigm.

Unfortunately, this recent development also points out one of the failings of the current analyses, the independence of the transport and flow calculation with regard to chemical changes within the cementitious material. The flow parameters are adjusted according to one set of assumptions while the transport parameters are adjusted by another set. The coupling of these phenomena in a mechanistic way while remaining computationally efficient is a CBP goal.

Next Generation Computational Tool

A brief description of the next generation CBP computational tool follows. The description is written in a manner in which it is recognized that the information supplied by the tool is a part of a larger analysis.

The fundamental concept consists of three distinct classes of computational models:

1. *Detailed computer codes* designed to represent selected phenomena at a detailed level. In general, these are codes that will be supplied by the CBP members.
2. *Abstracted models* based on the detailed codes. These are higher level approximations to the detailed codes designed to capture aspects of the parametric sensitivity that is important to the overall response.
3. An *integrating function or model* that assimilates the calculated results from the contributing codes into a form of a material transport equation that can accommodate inputs for all of the represented phenomena and reduces the result to effective parameters and properties to be used by the external calling function – such as a PA.

Abstracted models based on the detailed codes are used for a rapid evaluation of parameter sensitivities, while detailed codes are applied in the principal region of interest to provide greater accuracy for final results. A common integration model is used to couple abstracted or detailed codes, control time and space discretization, and compute appropriately averaged results consistent with the requirements of the external calling program. Initial applications will provide parametric input to PAs, but the integrated model will be generally applicable to structures incorporating cementitious materials.

The integrated modeling concept incorporates the coupled performance of the various codes with an uncertainty evaluation to calculate effective physical parameters for external applications. The sources of uncertainty thought to be important are:

1. Uncertainties in the measurement of physical properties or behaviors.
2. Approximations in defining mathematical relationships to describe physical phenomena.
3. Discrete solutions to the mathematical models, including operator splitting techniques and convergence issues in both space and time.
4. Interactions amongst parameters and convergence of those interactions.

CONCLUSION

A review of the treatment of cementitious barriers in current DOE PAs shows that there are many opportunities for improvement. The evolution of the state of the cementitious media is approximated by assumptions and independent phenomena. In addition, the uncertainties associated with the current approaches are generally not well quantified. The CBP's goal of providing a next generation computational tool that integrates these phenomena will aid in the reduction of risk associated with shallow land disposal of low-level radioactive waste.

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