













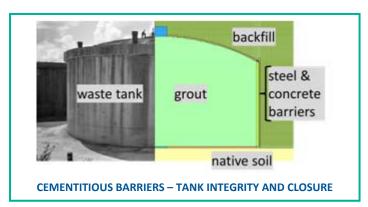


Cementitious Barriers Partnership Software Toolbox

http://cementbarriers.org

CBP Software Toolbox, Version 2.0 Release

This version is an update to Version 1.0 released in November 2012 and includes three additional software modules. This toolbox is enabling users (e.g., DOE, NRC licensees, and other interested stakeholders) to more easily evaluate the performance of cementitious barriers and waste forms over the long term (i.e., up to and > 1000 years).



The CBP Software Toolbox is a suite of software modeling tools for simulating reactive transport and long-term degradation of cementitious materials used for disposal of wastes. Several software packages are integrated into the Toolbox, each one having a specialized purpose, while interfacing with a GoldSim platform for probabilistic analysis. LeachXS™/ORCHESTRA (LXO) component embodies an extensive material property measurements database and integrated chemical evolution and leaching assessment models with emphasis on cementitious materials (CM) used in DOE facilities, such as Saltstone (Savannah River), Cast Stone (Hanford), tank closure grouts, and barrier concretes. STADIUM® predicts the degradation of unsaturated concrete structures exposed to chemically aggressive environments. THAMES, being developed by NIST for a future Toolbox release, simulates evolving microstructure and mineralogy in cementitious materials.

Impact

This innovative software toolbox provides a mechanism to meet DOE high priority needs by improving long-term performance predictions of cementitious barriers by:

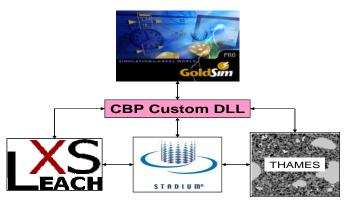
- Reducing and quantifying uncertainty in Performance Assessment (PA) predictions.
- Providing model model verification for validation of performance predictions.
- Simulating important degradation and leaching mechanisms.
- Providing an extensive material property database with cementitious materials used in DOE facilities.

Contact

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New CBP Software Tools for Understanding CM Performance



Three new CBP software modules have been added to the CBP Toolbox - Version 2.0 to enhance evaluation of the performance of cementitious materials and barriers:

- Dual-Regime Modeling transport in fractured and non-fractured CM using LXO
- Tank/Vault Carbonation Significant update of Version 1.0 carbonation module using LXO
- Chloride Attack Modeling degradation using **STADIUM** ENERGY

Office of **Environmental Management**



Collaboration to Improve Performance Predictions

Filling a Need - Collaborative Concurrent Modeling and Experimental **Validation to Improve Performance Predictions**

The DOE Environmental Management program actively supports the CBP collaborative modeling and experimental program to expand and improve long-term performance predictions of cement barriers. This Toolbox is an important step in filling the need identified by the international technical community for a defensible method for modeling cementitious materials degradation over the long-term. This Toolbox Version 2.0 provides methods to model three important cement chemical degradation mechanisms: carbonation, chloride and sulfate attack. In addition the CBP now includes a module to evaluate leaching and transport through fractured media. In the future, the CBP plans to expand Toolbox modeling to include other physical and chemical degradation mechanisms including understanding variable saturation on flow and transport through fractured media.

CBP Goal

Develop a reasonable and credible set of tools to predict the structural, hydraulic and chemical performance of cement barriers used in nuclear applications over extended time frames (e.g., up to or >100 years for operating facilities and > 1000 years for waste management)

Example Uses and Reference Cases

- Cementitious waste form in concrete disposal vault with cap (← Landfills Partnership)
- Grouted high-level waste (HLW) tank closure
- Spent nuclear fuel pool integrity
- Nuclear processing facilities closure / D&D
- Grouted vadose zone to immobilize contamination
- Materials surrogate low-activity waste (LAW) cementitious waste form, reducing grout, reinforced concrete (historical) and reinforced concrete (future)

CBP Software Toolbox, Version 2.0

Sulfate attack Carbonation Chloride attack **Dual regime**

CBP Basic Elements

Mechanistic / Phenomenological Basis

Parameter Estimation and Measurement

Boundary Conditions (physical, chemical interfaces)

Uncertainty Characterization

Foundation

CBP Coordinated Experimental and Computational Program

- Develop and improve conceptual models and partner codes
- Define test methods and estimate important parameters
- Calibrate and validate models and perform probabilistic analyses

The CBP Software Toolbox Development Team

- Federal Agencies: U.S. DOE Office of Environmental Management; National Institute of Standards and Technology (NIST); U.S. Nuclear Regulatory Commission (NRC)
- National Laboratory: Savannah River National Laboratory (SRNL)
- University: Vanderbilt University
- International Agencies: SIMCO Technologies; Energy Research Centre of the Netherlands (ECN), Nuclear Research Group (NRG), Hans van der Sloot Consultancy
- Other: Consortium for Risk Evaluation with Stakeholder Participation (CRESP)

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