Cementitious Barriers Partnership Software Toolbox
## http://cementbarriers.org

CBP Software Toolbox, Version 1.0 Release

The CBP has developed a one-of-a-kind software package, referred to as the CBP Software Toolbox. This toolbox will enable 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).

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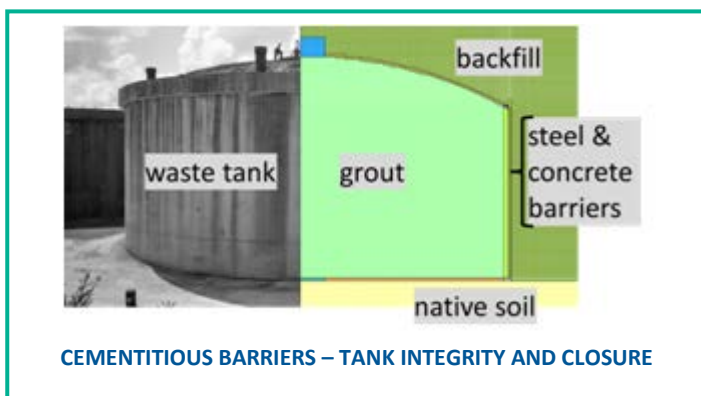
The CBP Software Toolbox is a suite of software modeling tools for simulating reactive transport and long-term degradation of cementitious materials used for disposal of wastes. Several software packages are integrated into the Toolbox, each one having a specialized purpose, while interfacing with a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

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.

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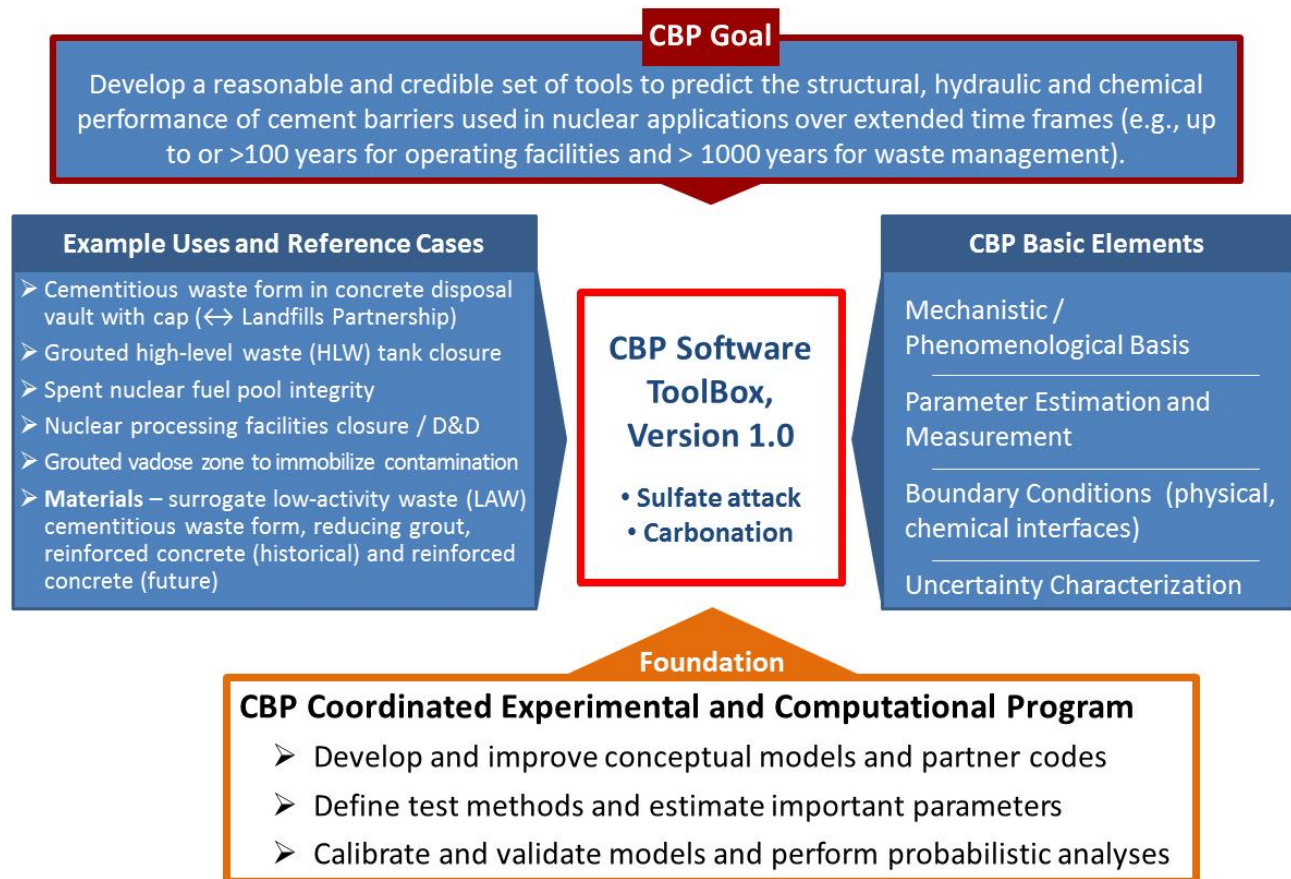## Demonstration and User Workshops
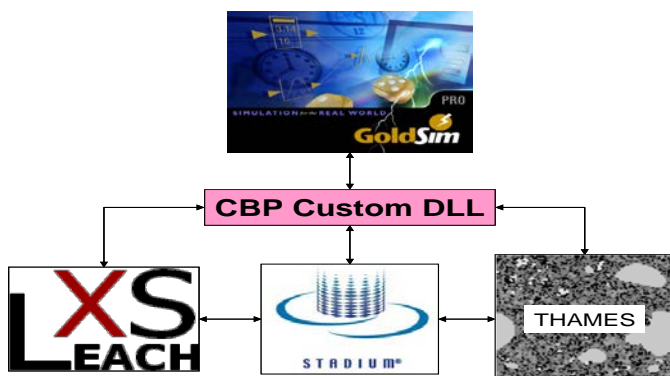
Three two-day workshops were conducted in Washington, DC, the Savannah River Site, and Hanford in 2012 to introduce participants to each software component through presentation materials, hands-on tutorial exercises, and consulting on user-selected scenarios. Following the workshops, participants will be given access to the CBP Software Toolbox components for their use.

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 the first step in filling the need identified by the international technical community for a defensible method for modeling cementitious materials degradation over the long-term. Two important cement chemical degradation mechanisms are carbonation and sulfate attack and this Toolbox provides a method to model those. In the future, the CBP plans to expand Toolbox modeling to other physical and chemical degradation mechanisms including 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 ($\leftrightarrow$ 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)

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- **Sulfate attack**
- **Carbonation**

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

Partners in Success

- 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)
- Other: Consortium for Risk Evaluation with Stakeholder Participation (CRESP)

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