Cementitious Barriers Partnership: Demonstration of Coupling and Code Integration

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Linking Prototype Cases to Performance Models through System Abstraction and Validated by Laboratory and Field Testing
Sulfate Attack as a “Proof of Principle” for Coupling of Phenomena
THAMES (NIST)

Virtual “micro-probe” of microstructure
- Constructs time-dependent 3-D virtual microstructures of a cementitious binder during hydration or degradation
- Computes important engineering properties of a concrete made from a binder at prescribed times

Planned model improvements
- Embed geochemical modeling code (GEMS) into microstructure module
- Improve hydration microstructure growth rules
- Parallelize THAMES code
- Incorporate microstructure impact on GEMS boundary conditions
- Incorporate degradation reactions and effects on microstructure
- Improve predictions for more complex systems
THAMES Overview

Start
- Input w/c, PSD, particle shape distribution, phase fractions

GENMIC
- 3-D lattice μ-structure

EVOLVER
- Speciation, hydration product fractions, enthalpy change
  - 3-D lattice μ-structure

Output?
- NO
  - GEMS
- YES
  - Output Binder Microstructure and Data

CONCROPS
- Output Concrete Effective Properties

Output Binder Microstructure and Data
- Dissolved components
STADIUM® (SIMCO Technologies)

- **Simulates ionic transport in saturated/unsaturated, isothermal/non-isothermal cementitious materials**
  - Simulates contaminant ingress, ionic leaching in pore solution, and modifications to microstructure of cementitious material
  - Accounts for electrical coupling between ions and activity gradients and dissolution/precipitation due to the high paste reactivity
  - Main components: ionic transport, electrodiffusion potential conservation, moisture transport, and energy conservation
  - Test results and methods available that relate directly to model predictions and validation

- **Planned model improvements**
  - Model damage due to sulfate exposure
  - Model effect of pore solution viscosity
  - Model effect of pore solution density of highly concentrated solutions
  - Model carbonation and acid exposure and resulting secondary species
STADIUM Overview

STADIUM Graphical User Interface

Input parameters: material properties, exposure conditions

Output analysis: chloride ingress rate, corrosion initiation

Mass and energy transport equations

Chemical equilibrium equations

STADIUM Calculation Engine

No - time stepping

Yes - end of calculation?
LeachXS™/ORCHESTRA (ECN)

LeachXS is a database/expert decision support system for characterization and environmental impact assessment

- Includes leaching results for 600+ materials (cements, concretes, stabilized wastes, soils), scenarios, and regulations
- Assists evaluation and lab guidance, data management /evaluation, source term description, impact evaluation, and decision analysis
- Geochemical speciation and chemical reaction/transport modeling integrated into LeachXS using ORCHESTRA model

Planned model improvements

- Parallelize LeachXS/ORCHESTRA equilibrium module calculations
- Incorporate radionuclides and decay in LeachXS/ORCHESTRA
- Evaluate chemical model performance by comparing with pH dependent solubility and diffusion data
- Account for chemical model uncertainty on transport predictions
- Account for impact of variable saturation and intermittent wetting
- Account for effects of physical and chemical heterogeneity
LeachXS/ORCHESTRA Overview

- Materials (Leaching data, Composition, Physical characteristics)
- Scenarios (e.g., fill characteristics, geometry, infiltration, hydrology)
- Regulatory (Regulatory thresholds and criteria from different jurisdictions)

LeachXS
(Materials and Scenarios Evaluation)

Orchestra
(Geochemical Speciation and Reactive Transport Simulator)

Excel Spreadsheets
(Data, Figures)

Reports
(Figures, Tables, Scenario and Material Descriptions)

Other Models
(Source Term and Parameters for Fate, Transport, and Risk Models)

Materials Leaching Database
Scenario Database
Regulatory Database
Thermo-dynamic Databases
Integrated Model Description

CBP Custom DLL

LEACH

THAMES

LS

STADIUM

GoldSim
Integrated Model General Design Principles

- **Model development proceeding in phases**
  - Weakest appropriate coupling amongst models

- **Parallel improvement of partner codes and coupling**
  - Influence, but stay within, CBP partners' main code development paths
  - Accept reasonable extant duplication of functionality (e.g., bulk chemistry), but require consistency

- **Data and I/O considerations**
  - Common repository (database) for common data
  - Common data formats, so an output can be an input
  - Common graphics format
  - Consistent mesh/node generation
Coupling Decisions and Software Integration

- Exposure scenarios
- Coupled processes
- Mathematical formulation (equation set / variables)
- Software implementation

Improved CBP partner codes vs. Coupled CBP partner codes

- Define roles of CBP partner codes
- Parameters exchanged
- Exchange frequency
- New I/O file capability
- File format (e.g. XML)
- Design CBP front-end (GoldSim and more)
Integrated Model Development

Phase I: Use existing CBP partner codes "as is"
  • Minimal coupling

Phase II: Coupling through functions
  • Modest coupling where appropriate
  • Enhanced I/O needed in partner codes
  • Use "system call" DLLs using instructions file (at run time)

Phase III: Selected coupling at each timestep
  • Strongest coupling / synchronization
  • Call partner codes as DLL subroutines (object code level)
Cementitious Barriers Partnership (CBP) DLL Link to STADIUM® and LeachXS™ Codes

The Cementitious Barriers Partnership (CBP) Project is a multi-disciplinary, multi-institutional collaboration supported by the US Department of Energy (DOE) Office of Waste Processing. The objective of the CBP project is to develop a set of tools to improve understanding and prediction of the long-term structural, hydraulic, and chemical performance of cementitious barriers used in nuclear applications.

A Dashboard is a user interface employed in GoldSim to control a simulation. Click on ‘+’ to open Container. Double-click links in GoldSim to activate.

cementbarriers.org
CBP DLL Subroutine

Avoid need for low-level programming by user

- Put generic executable content in pre-compiled subroutine (DLL)
- Put application content in “instructions file” read at run-time
- Primary instructions: PUT (create input), EXE (execute file), GET (retrieve input), and LOG (record)

Provide flexible, user-friendly access to partner code input and output files via instructions file

- Row selection by number, label, value
- Field selection by number

Used to couple STADIUM and LeachXS/ORCHESTRA to GoldSim model
Uncertainty Analysis

**Sources of uncertainty**
- Inherent variability
- Data uncertainty
- Model uncertainty

**Approaches to uncertainty management**
- GoldSim has sensitivity and uncertainty analysis capabilities
- More advanced capabilities will be used to evaluate model uncertainty impacts
Summary of Uncertainty Analysis

- Uncertainties due to physical variability, data uncertainty, and model uncertainty must be considered.

- Several methods available for uncertainty propagation through computational models.

- Methods for model uncertainty and error quantification currently under study.

- Bayesian framework appears attractive for managing various uncertainties.

- Methods for epistemic uncertainty under investigation.

- Application to large problems (time-dependent, complicated multi-physics) needs investigation (accuracy, computational effort, uncertainty quantification, confidence assessment).