CBP
Cementitious Barriers Partnership

Webinar

Performance Assessment Community of Practice and Cementitious Barriers Partnership (CBP)

Tools and Capabilities of the Cementitious Barriers Partnership Toolbox, Version 2.0

Wednesday, February 5, 2014

For additional information on the Cementitious Barriers Partnership and Toolbox presentations, please contact:

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http://cementbarriers.org/

Webinar

Performance Assessment Community of Practice and

Cementitious Barriers Partnership (CBP)

Tools and Capabilities of the Cementitious Barriers Partnership Toolbox, Version 2.0

Wednesday, February 5, 2014,

1:00 – 3:00 pm CENTRAL Standard Time

Webinar Link: **See next page**

Agenda

1:00 pm	**Introduction to Cementitious Barriers Partnership** **Overview of Scope, Tools and Processes Considered** David Kosson, Vanderbilt University
1:20 pm	**Opportunities for Use of CBP information and Tools in Performance Assessments and Related Processes** Greg Flach, Savannah River National Laboratory
1:40 pm	**Use of LeachXS/Orchestra for Evaluating Leaching Source Terms for Wasteforms, Tank Closures, Contaminated Soils and Other Applications** Hans van der Sloot, Energy Research Centre of The Netherlands and Hans van der Sloot Consultancy and Kevin Brown, Vanderbilt University
2:00 pm	**Use of STADIUM for Evaluating Structural Durability and Performance of Concrete and Cement Materials** Eric Samson, SIMCO Inc.
2:20 pm	**Use of GoldSim in Conjunction with CBP Tools for Uncertainty Assessment and Integration with Performance Assessments** Kevin Brown, Vanderbilt University and Greg Flach, Savannah River National Laboratory
2:40 pm	**Feedback from Webinar Participants**
3:00 pm	**Adjourn**

Cementitious Barriers Partnership
Project Overview and User Needs Input

David S. Kosson
Vanderbilt University and CRESP
Cementitious Barriers Partnership

CBP P & RA CoP
February 5, 2014

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Project Need

- Cementitious materials used broadly by DOE-EM to accomplish its mission.
  - Low-Activity Waste (LAW) forms (i.e., Saltstone at SRS)
  - High-Level Waste (HLW) Tank Integrity (i.e., GAO report) and Tank Closure requirements
  - Secondary waste treatment (i.e., Cast Stone at ORP-WTP)
  - Nuclear power plant concrete structures (e.g., Seabrook NPP)
  - Used nuclear fuel storage – fuel pools and dry casks (e.g., TMI-2)
  - Facility Decommissioning & Decontamination (D&D) and entombment (P-Reactor at SRS)
  - Alternative waste forms for near surface disposal (i.e., grouted waste forms)
  - Grouting for vadose zone remediation
- Considerable technical debate over physical/chemical performance and service life of cement materials in nuclear applications because of absence of modern, phenomenologically-based models and experimental methods that are mutually agreed upon by technical and regulatory communities.

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Project 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 and >100 years for operating facilities and >1000 years for waste management).

- Mechanistic / Phenomenological Basis
- Parameter Estimation and Measurement
- Boundary Conditions (physical, chemical interfaces)
- Uncertainty Characterization

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Project Team Members

Vanderbilt University & CRESP
D. Kosson*, K. Brown*, S. Mahadevan, J. Arnold, F. Sanchez

Savannah River National Laboratory (SRNL)
C. Langton*, G. Flach*, H. Burns*, R. Seitz, S. Marra

Energy Research Centre of The Netherlands (ECN) & CRESP
H. van der Sloot (HvdS Consultancy), J.C.L. Meeussen (NRG), P. Seignette

National Institute of Standards and Technology (NIST)
E. Garboczi, K. Snyder, J. Bullard, P. Stutzman

Nuclear Regulatory Commission (NRC)
D. Esh, M. Furman, J. Phillip

SIMCO Technologies, Inc. (Canada)
E. Samson, J. Marchand

*Project Leadership Team

DOE-EM Project Manager: Pramod Mallick

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Technical Strategy / Approach

- **Reference Cases** – provide basis for comparison and demonstration of CBP tools
  - Cementitious waste form in concrete disposal vault with cap
  - Grouted high-level waste (HLW) tank closure
  - Used nuclear fuel pool, dray cask storage (future)
  - Nuclear processing facilities closure / D&D (e.g., canyons)
  - Grouted vadose zone contamination
  - Materials – surrogate low-activity waste (LAW) cementitious waste form, reducing grout, reinforced concrete (historical), reinforced concrete (future)
- **Extension/enhancement of existing tools** – CEMHYD3D/THAMES, STADIUM, LeachXS/ORCHESTRA, GoldSim Performance Assessment (PA) framework
- **Coordinated experimental and computational program**
  - Conceptual model improvement
  - Define test methods and parameter measurements
  - Model validation

→ **CBP Software ToolBox Version 2.0 Release (January 2014)**

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Key Aging Phenomena

Key Phenomena Addressed

- Chloride ingress and corrosion
- Leaching
- Sulfate attack (2011)
- Carbonation (2012)
- Oxidation (2012-2014)
- Cracking (2013-2014)
- Pore structure relationships with mass transfer and hydraulic properties (future)
- Alkali-silica reaction (ASR) (future)

Integration with Conceptual Models

- Coupled phenomena
- Saturated, unsaturated and variable saturation
- Liquid, vapor mass transfer
- System geometry and boundary conditions

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CBP Partner Codes and Integration

- **Partner Codes provide for scenario development, design evaluation and model parameterization**
  - ✓ STADIUM – Physical & Hydraulic Performance
  - ✓ LeachXS/ORCHESTRA – Chemical Performance & Constituent Release, also coupled with physical properties/damage evolution
  - ✓ THAMES – Microstructure Evolution & Properties*
- **GoldSim Software ToolBox (CBP Custom DLL) with STADIUM and LeachXS/ORCHESTRA**
  - ✓ User scenarios developed in Partner Codes
  - ✓ Monte Carlo simulations
  - ✓ Integration with GoldSim Performance Assessment Models

*Further development on hold, pending available funding.

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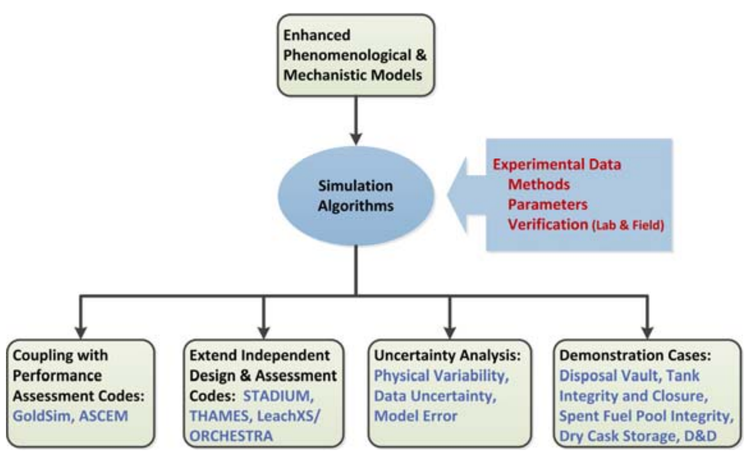
CBP Software ToolBox Development



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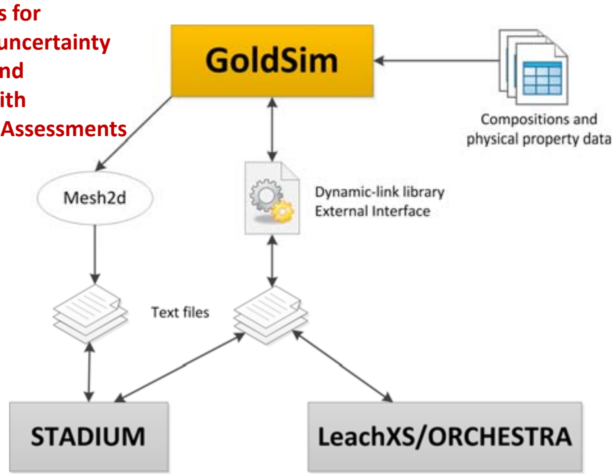
CBP Software ToolBox—Phase I

Provides tools for Monte Carlo uncertainty assessment and integration with Performance Assessments



L E A F

Leaching Environmental Assessment Framework

A Decision Support System for Beneficial Use and Disposal Decisions in the United States and Internationally…

- Four leaching test methods
- Data management tools
- Geochemical speciation and mass transfer modeling
- Quality assurance/quality control for materials production
- Integrated leaching assessment approaches

… designed to identify characteristic leaching behaviors for a wide range of materials and scenarios.

More information at http://www.vanderbilt.edu/leaching

L E A F

LEAF Leaching Methods*

Method 1313 – Liquid-Solid Partitioning as a Function of Eluate pH using a Parallel Batch Procedure

Method 1314 – Liquid-Solid Partitioning as a Function of Liquid-Solid Ratio (L/S) using an Up-flow Percolation Column Procedure

Method 1315 – Mass Transfer Rates in Monolithic and Compacted Granular Materials using a Semi-dynamic Tank Leaching Procedure

Method 1316 – Liquid-Solid Partitioning as a Function of Liquid-Solid Ratio using a Parallel Batch Procedure

**Posting to SW-846 as “New Methods” completed August 2013*

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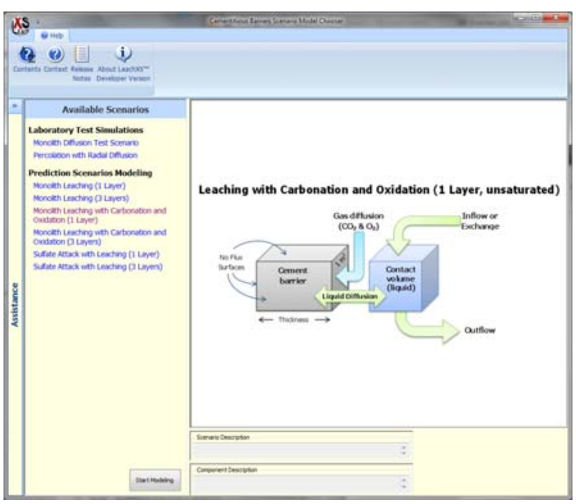
Multiple, Flexible Base Models Available in LeachXS/ORCHESTRA



- Select general field or laboratory scenario to model
- Select from existing CBP reference materials or customize materials
- Select interface conditions (e.g., fixed volume, continuous flow or intermittent flow/ exchange & solutions (e.g., “Hanford infiltration” or “saltstone pore water”)
- Resulting model transferable to GoldSIM simulations

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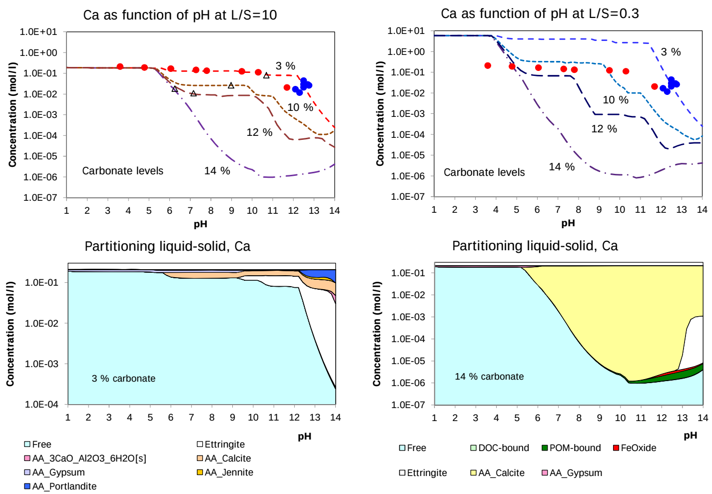
Geochemical Speciation Modeling

Progressive Carbonation of Stabilized Waste



Allows evaluation of conditions not readily reproduced in the Lab (e.g., redox changes, aging processes)

Chemical Speciation Fingerprint (CSF) developed based on Method 1313 and other information sources

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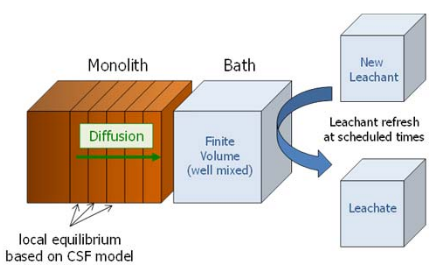
Monolith Diffusion



- Laboratory and field simulations
- Variable water contacting sequence, chemistry
- Saturated or unsaturated
- Carbonation, oxidation ingress
- Sulfate attack with leaching

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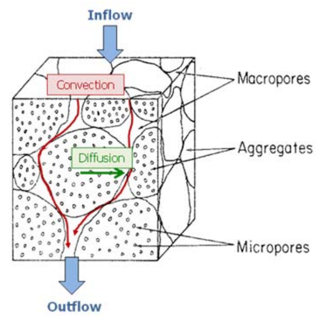
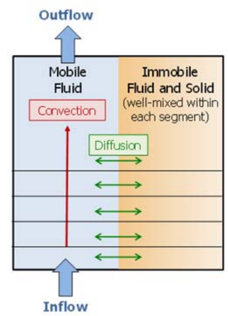
Percolation with Mobile-Immobile Zones





- Laboratory and field simulations
- Variable water flow rate, chemistry
- Effects of preferential flow (e.g., grouted materials, contaminated soils)

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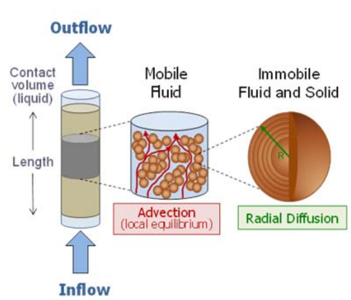
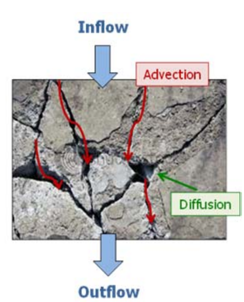
Percolation with Radial Diffusion





- Laboratory and field simulations
- Cracked materials or packed beds (e.g., wasteforms, tank closure)
- Effects of preferential flow
- Variable water flow rate, chemistry

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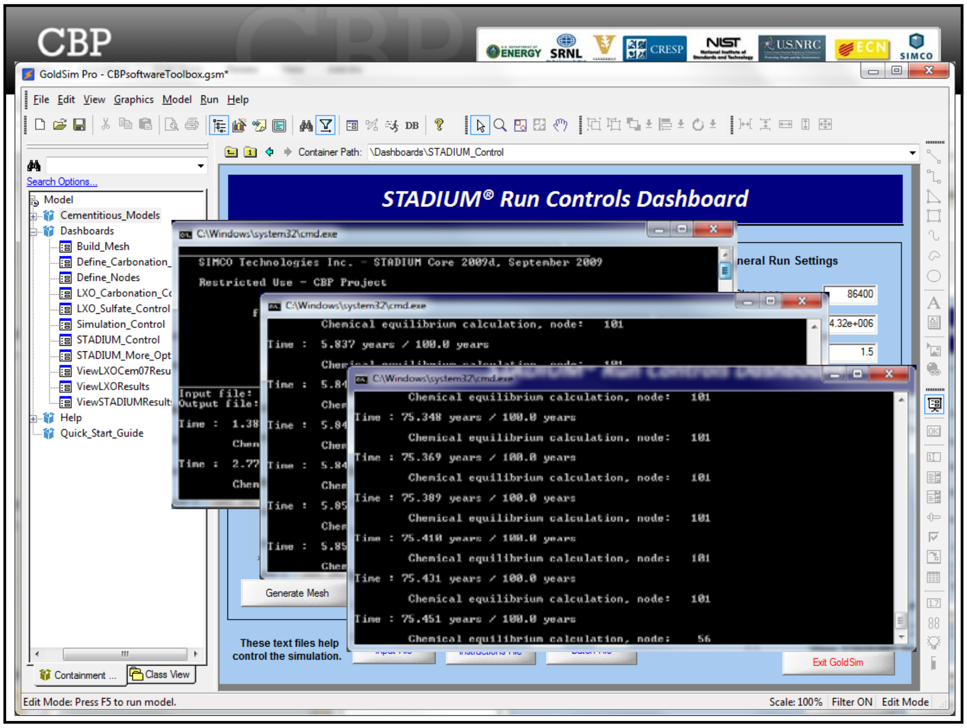
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GoldSim Pro - CBPsoftwareToolbox.gsm*
File Edit View Graphics Model Run Help
Container Path: \Dashboards\STADIUM_Control
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Model
Cementitious_Models
Dashboards
Build_Mesh
Define_Nodes
Simulation_Control
STADIUM_Control
ViewLXOResults
Help
Quick_Start_Guide
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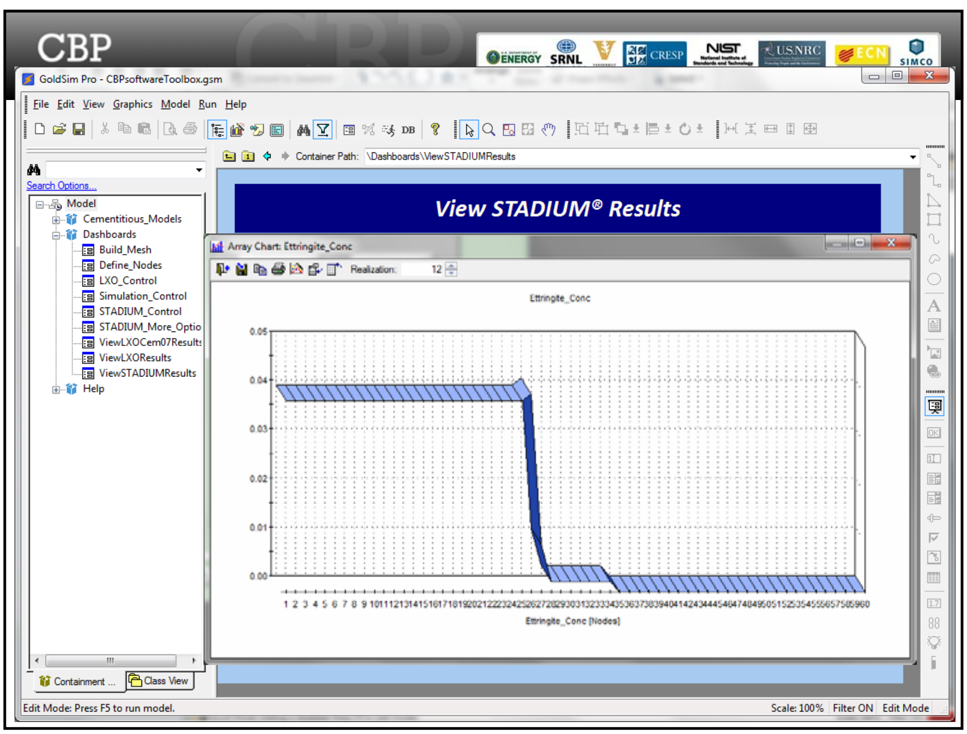
SIMCO Technologies Inc. - STADIUM Core 2009d, September 2009
Restricted Use - CBP Project
Chemical equilibrium calculation, node: 101
Time : 75.348 years / 100.0 years
Generate Mesh
These text files help control the simulation.
Exit GoldSim
Edit Mode: Press F5 to run model.
Scale: 100% Filter ON Edit Mode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GoldSim Pro - CBPsoftwareToolbox.gsm
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View STADIUM® Results
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Primary Near-term Applications

- Hanford
  - Single shell tank integrity
  - C-Tank Farm – HLW tank closure assessment
  - Integrated Disposal Area PA
  - Source term from Cast Stone (secondary waste, LAW supplemental treatment)
  - In-situ grouting performance
- Savannah River
  - Saltstone Performance
  - Disposal vaults and other concrete facilities
- Nuclear Energy
  - Dry cask storage performance
  - License extensions

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Key Questions

- Waste Forms and Disposal Systems
  - What is the rate of release for radionuclides and contaminants under a range of scenarios?
  - What is the evolution of system pH?
  - What are the effects of cracking?
  - What is the rate and impact of aging processes (oxidation (Tc-99), carbonation, leaching)?
- Structural Systems Performance
  - What is the service life?
  - What are the impacts of ingress of aggressive species (chloride, sulfate)?

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Additional Needs

- Training and supporting instructional materials
- Working with end-users to address specific cases and questions.

We want your input!

Please send comments to:
David.Kosson@Vanderbilt.edu

Opportunities for Use of CBP Information and Tools in Performance Assessments and Related Processes

Greg Flach
Savannah River National Laboratory

PA Community of Practice / CBP Webinar
February 5, 2014

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SRNL-STI-2014-00047

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CBP Products and PA Process

Higher fidelity models for simulating transport and degradation phenomena in cementitious materials

- Primary, secondary, and trace species transport
- External Sulfate Attack
- Carbonation

Experimental data

- Property measurements
- Validation data

Probabilistic framework

- Integration with GoldSim (www.goldsim.com)

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Savannah River Saltstone PA Example

Material degradation

– External sulfate attack

– Carbonation

Material characterization

– Hydraulic

– Chemical

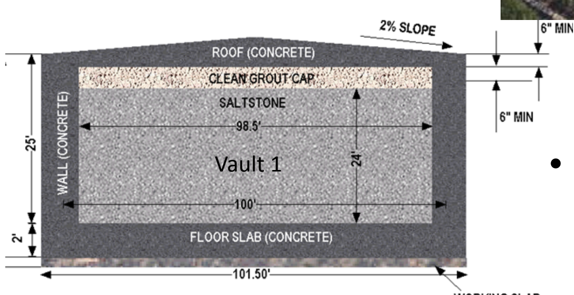
Conceptual model validation

– Unsaturated hydraulic properties for fractured grout

Saltstone Disposal Facility

Saltstone Facility:

- **Salt waste mixed with dry grout to form "Saltstone"**
- **~0.1 mol/L SO_4^{2-} in feedwater**



- **Sulfate attack identified as primary concrete degradation mechanism**

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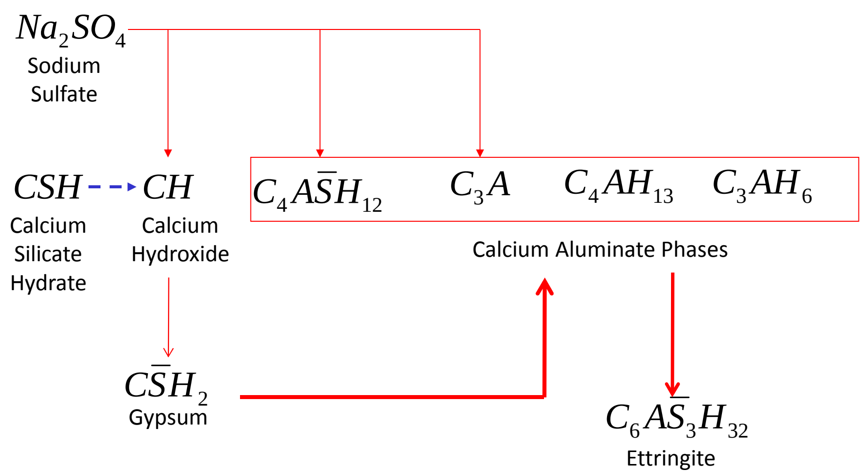
Example Chemical Reactions



Effects : expansion, cracking and strength loss

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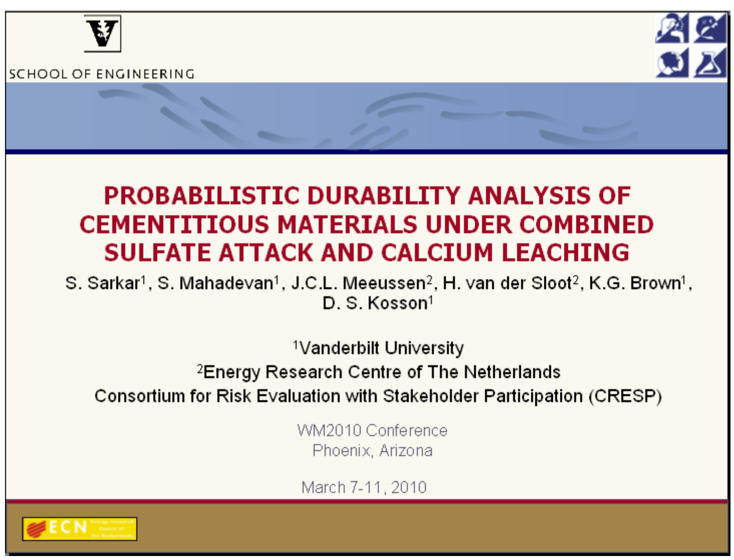
External Sulfate Attack

WM2010



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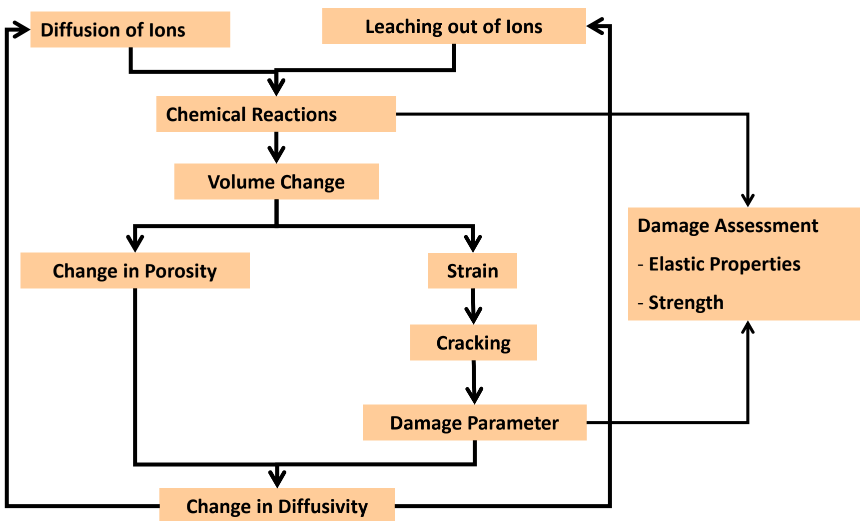
Numerical Model Framework



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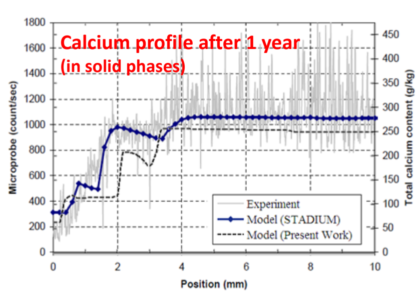
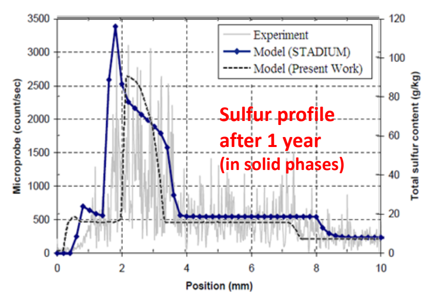
Model Validation

Model calibrated with experimental results after 3 months and validated against experimental results after 1 year (experimental data from Samson and Marchand, 2007)





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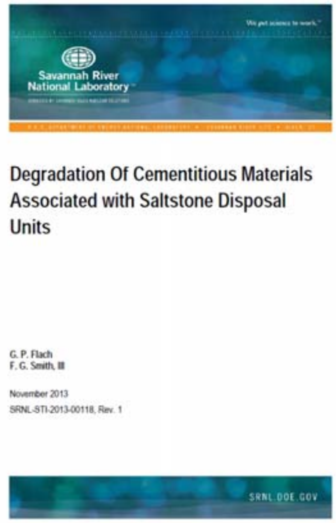
FY13 Saltstone Special Analysis

CBP Software Toolbox Version 1.0


We put science to work.
Savannah River National Laboratory

Degradation Of Cementitious Materials Associated with Saltstone Disposal Units

G. P. Flach
F. G. Smith, III

November 2013
SRNL-STI-2013-00118, Rev. 1

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Material Properties and Conditions

Saltstone Disposal Unit Concrete

Table 9 – Initial solid phases in the concrete mixtures

Properties	Concretes Vault 1/4	Vault 2
Hydration (%)		
Cement	80	75
Slag	75	65
Fly Ash	[illegible]	[illegible]
Silica Fum[illegible]	[illegible]	[illegible]
Mineral phases (g[illegible]		
C-S-H	[illegible]	[illegible]
Portlandite	[illegible]	[illegible]
Monosulfo[illegible] (AFm)	[illegible]	[illegible]
C_4FH_{13}	[illegible]	[illegible]

Table 11 - Chemical analyses of pore fluids extracted after 28 days of curing

Species	Vault 1/4 (mmol/L)	Vault 2
OH^-	244.4	113.9
Na^+	[illegible]	[illegible]
K^+	[illegible]	[illegible]
SO_4^{2-}	[illegible]	[illegible]
Ca^{2+}	[illegible]	[illegible]
Cl^-	[illegible]	[illegible]

Table 13 - Diffusion properties estimated from migration test analyses

Properties	Vault 1/4	Vault 2
OH diffusion coeff. (E-11 m^2/s)		
28 days	4.29	2.80
97 days	3.69	0.41
Cl diffusion coeff. (E-11 m^2/s)		
28 days	1.65	1.08
97 days	1.42	0.16
Tortuosity (-)		
28 days	0.0081	0.0053
97 days	0.0070	0.0008

SIMCO Technologies inc.

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Equivalent Continuum Model (ECM)

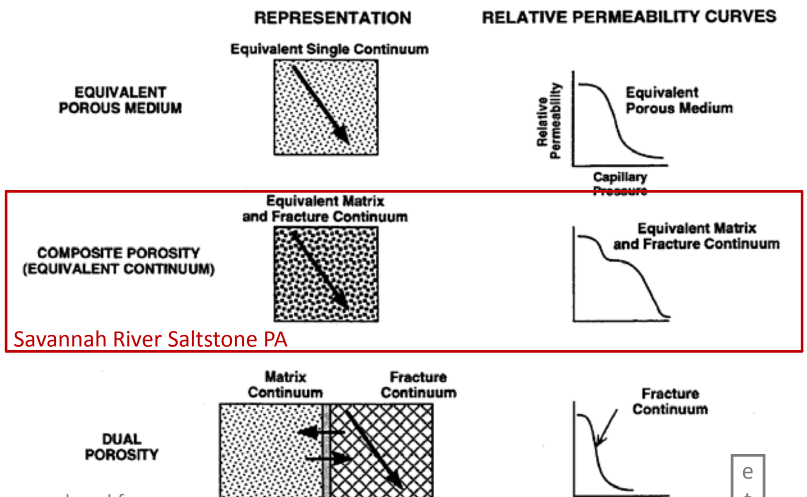

Figure reproduced from:
S. J. Altman, B. W. Arnold, R. W. Barnard, G. E. Barr, C. K. Ho, S. A. McKenna, R. R. Eaton

SAND96–0819 • UC–814
Unlimited Release
Printed September 1996

etc

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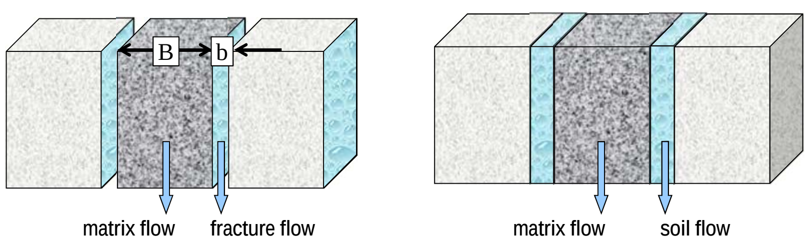
Soil – Fracture Analogy

- **Assume a seam of coarse-grained porous material behaves similar to a fracture**



- **Define soil fraction (f) by equating saturated hydraulic conductivities**

$$\frac{B}{B+b}K_{matrix} + \frac{b}{B+b}K_{fracture} = K_{blend} = (1-f)\cdot K_{matrix} + f\cdot K_{soil}$$

$$f = \frac{K_{blend} - K_{matrix}}{K_{soil} - K_{matrix}}$$

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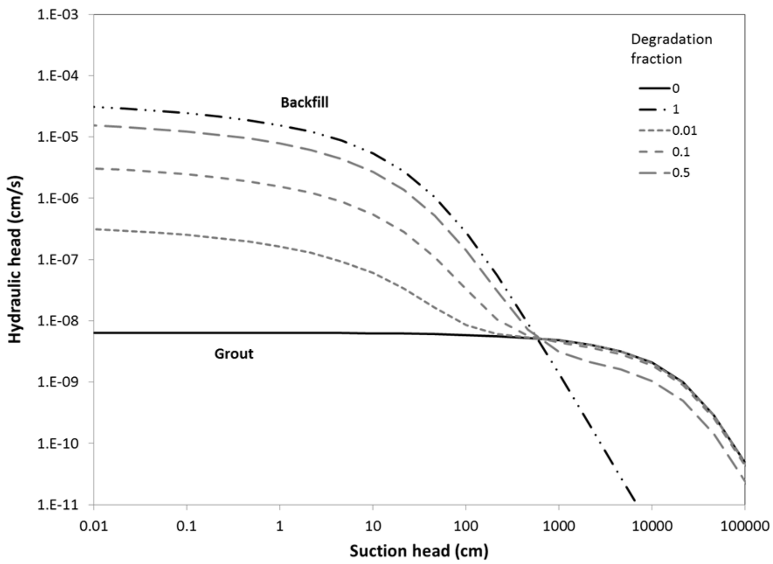
Backfill Soil + Intact Waste Grout



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Multi-Step Outflow Extraction

Dixon, K. L. and R. L. Nichols, *Method Development for Determining the Hydraulic Conductivity of Fractured Porous Media*, SRNL-STI-2013-00522, September 2013

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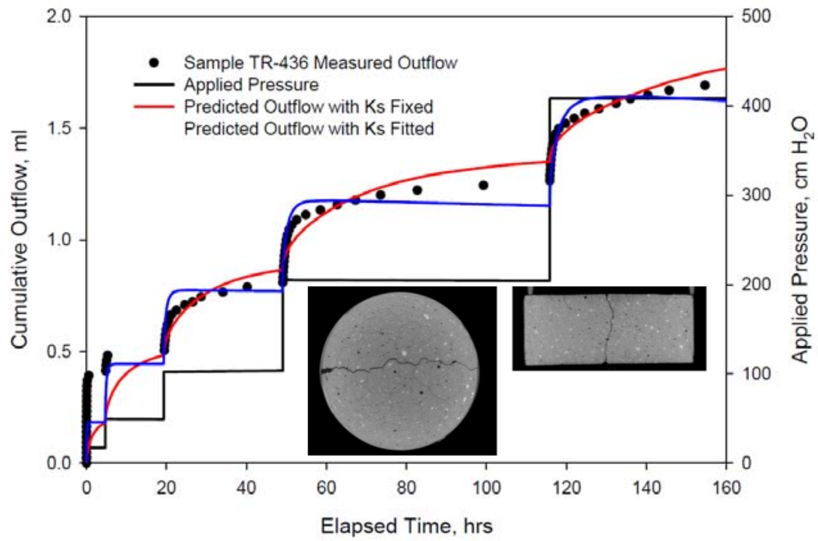
Example Outflow Data and Fit



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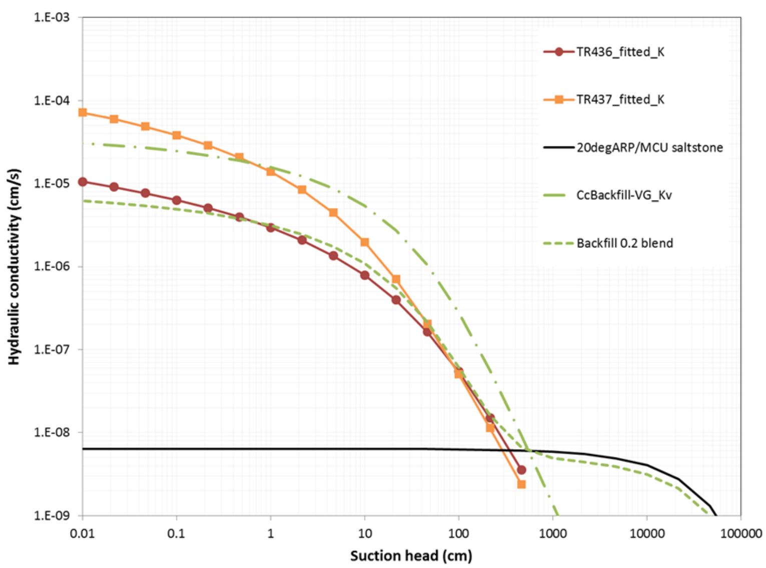
Conceptual Model Validation



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Summary

- **CBP software data and tools can engage the PA process in multiple ways**
  - **Provide higher fidelity models for particular phenomena**
  - **Support model abstraction**
  - **CBP tools are 'GoldSim-ready'**
  - **Material characterization**
- **CBP data and software have proven to be useful in the Savannah River Site Saltstone PA**
  - **Cementitious material degradation**
  - **Material characterization**
  - **Conceptual model validation**

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Use of LeachXS/Orchestra for Evaluating Leaching Source Terms for Waste Forms, Tank Closures, Contaminated Soils and Other Applications

Hans van der Sloot[1], David Kosson[2] ,
Kevin Brown[2] , Hans Meeussen[3] , Paul Seigenette[4]

[1] HansvanderSloot Consultancy, Langedijk, The Netherlands
[2] Vanderbilt University, Nashville, TN
[3] NRG, Petten, The Netherlands
[4] ECN, Petten, The Netherlands

CBP Annual Meeting, Nashville, Tennessee
4-5 February 2014

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Status of Development

- Various models implemented into the LeachXS environment as part of CBP Software ToolBox Release (Phase II).

Laboratory test models
- pH dependence
- percolation
- monolith leach test

Prediction models
- Monolith 1D diffusion
- Carbonation/oxidation monolith 1D
- Sulfate attack monolith 1D
- Percolation dual porosity
- Percolation with radial diffusion

A LeachXS/ORCHESTRA user Guide is now available

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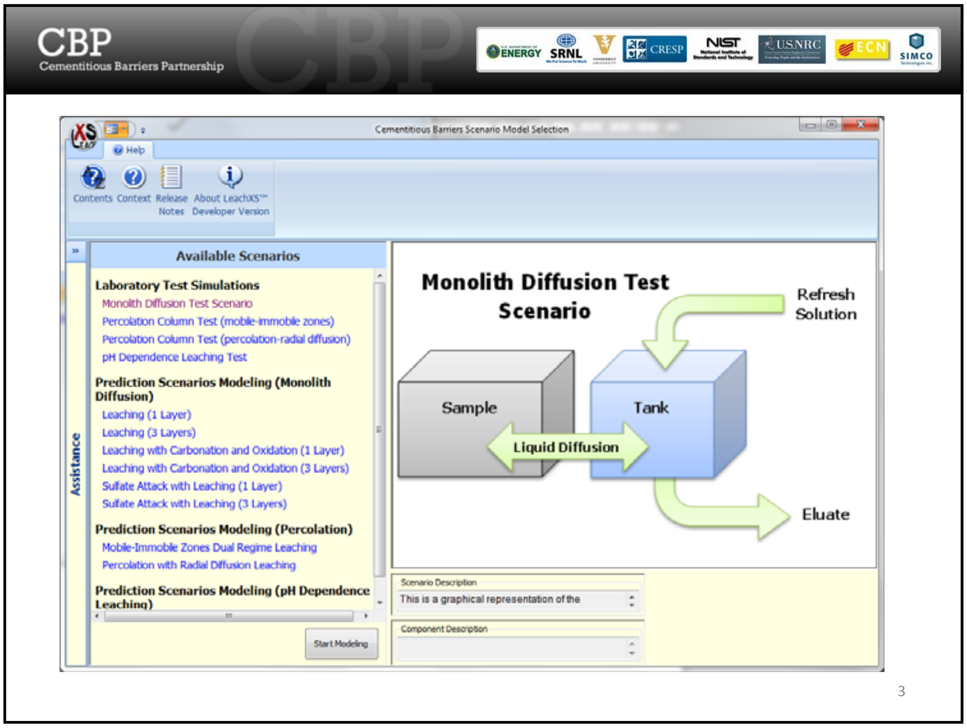
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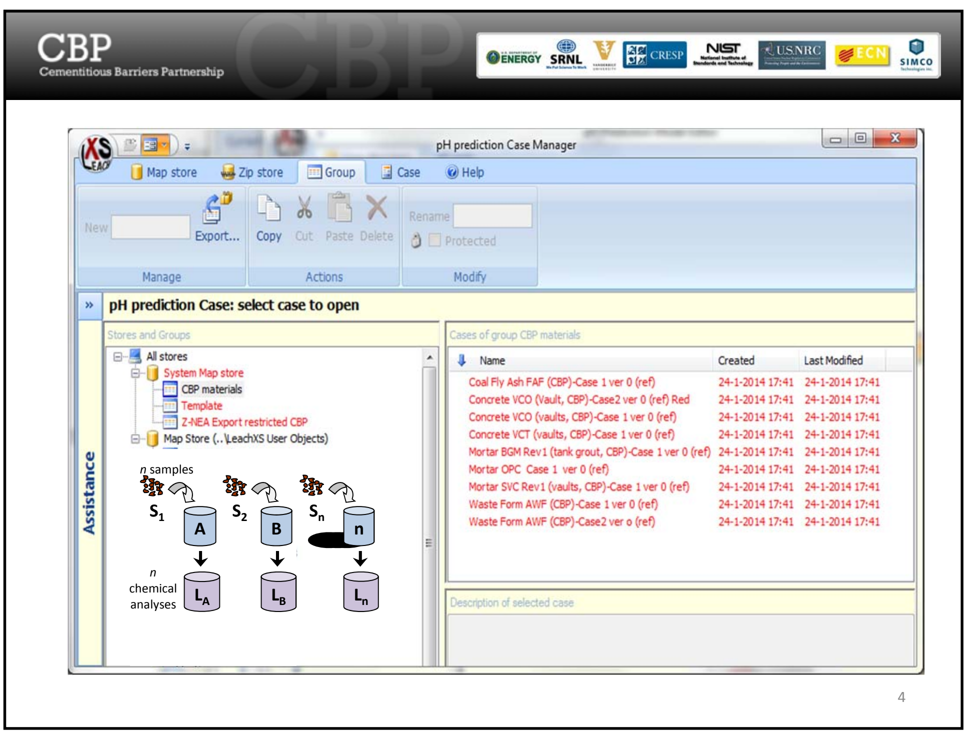
CRESP
NIST
U.S.NRC
ECN
SIMCO
Cementitious Barriers Scenario Model Selection
Help
Contents
Context
Release Notes
About LeachXS™ Developer Version
Available Scenarios
Laboratory Test Simulations
Monolith Diffusion Test Scenario
Percolation Column Test (mobile-immobile zones)
Percolation Column Test (percolation-radial diffusion)
pH Dependence Leaching Test
Prediction Scenarios Modeling (Monolith Diffusion)
Leaching (1 Layer)
Leaching (3 Layers)
Leaching with Carbonation and Oxidation (1 Layer)
Leaching with Carbonation and Oxidation (3 Layers)
Sulfate Attack with Leaching (1 Layer)
Sulfate Attack with Leaching (3 Layers)
Prediction Scenarios Modeling (Percolation)
Mobile-Immobile Zones Dual Regime Leaching
Percolation with Radial Diffusion Leaching
Prediction Scenarios Modeling (pH Dependence Leaching)
Start Modeling
Assistance
Monolith Diffusion Test Scenario
Refresh Solution
Sample
Tank
Liquid Diffusion
Eluate
Scenario Description
This is a graphical representation of the
Component Description
3


CBP
Cementitious Barriers Partnership
ENERGY
SRNL
CRESP
NIST
U.S.NRC
ECN
SIMCO
pH prediction Case Manager
Map store
Zip store
Group
Case
Help
New
Export...
Copy
Cut
Paste
Delete
Rename
Protected
Manage
Actions
Modify
pH prediction Case: select case to open
Stores and Groups
All stores
System Map store
CBP materials
Template
Z-NEA Export restricted CBP
Map Store (..\LeachXS User Objects)
n samples
S1
S2
Sn
A
B
n
n chemical analyses
LA
LB
Ln
Assistance
Cases of group CBP materials
Name
Created
Last Modified
Coal Fly Ash FAF (CBP)-Case 1 ver 0 (ref)
Concrete VCO (Vault, CBP)-Case2 ver 0 (ref) Red
Concrete VCO (vaults, CBP)-Case 1 ver 0 (ref)
Concrete VCT (vaults, CBP)-Case 1 ver 0 (ref)
Mortar BGM Rev1 (tank grout, CBP)-Case 1 ver 0 (ref)
Mortar OPC Case 1 ver 0 (ref)
Mortar SVC Rev1 (vaults, CBP)-Case 1 ver 0 (ref)
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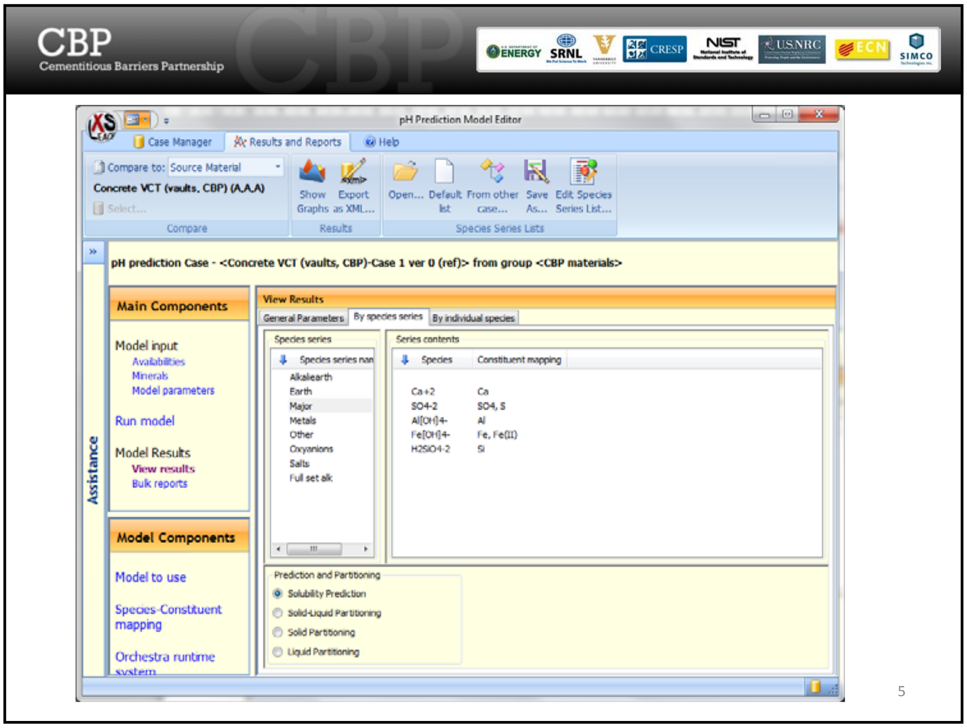
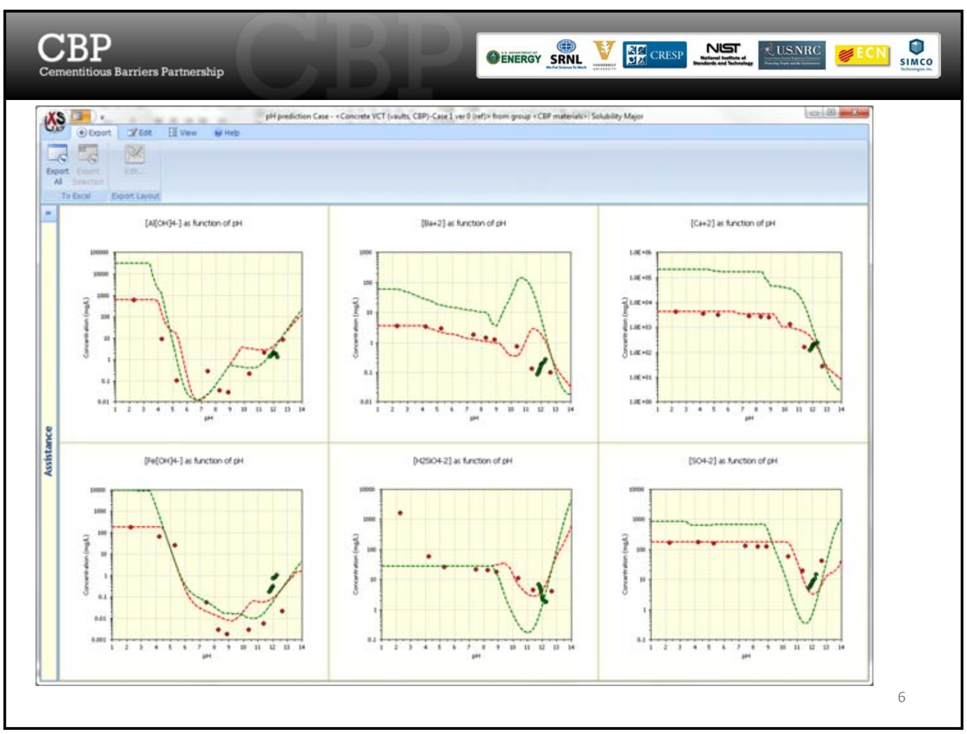
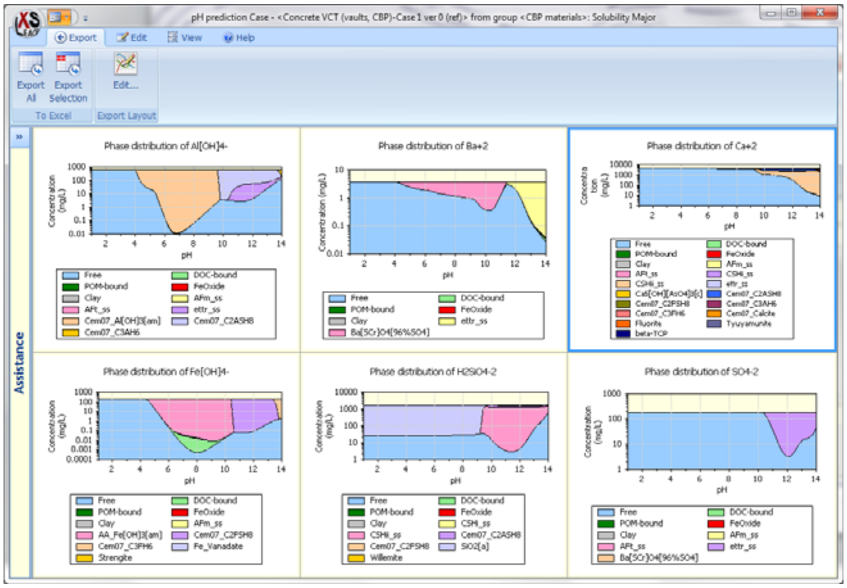
Waste Form AWF (CBP)-Case2 ver o (ref)
24-1-2014 17:41
Description of selected case
4


CBP
Cementitious Barriers Partnership
ENERGY
SRNL
CRESP
NIST
U.S.NRC
ECN
SIMCO
pH Prediction Model Editor
Case Manager
Results and Reports
Help
Compare to: Source Material
Concrete VCT (vaults, CBP) (A,A,A)
Select...
Compare
Show Graphs
Export as XML...
Results
Open...
Default list
From other case...
Save As...
Edit Species Series List...
Species Series Lists
pH prediction Case - <Concrete VCT (vaults, CBP)-Case 1 ver 0 (ref)> from group <CBP materials>
Assistance
Main Components
Model input
Availabilities
Minerals
Model parameters
Run model
Model Results
View results
Bulk reports
Model Components
Model to use
Species-Constituent mapping
Orchestra runtime system
View Results
General Parameters
By species series
By individual species
Species series
Species series nan
Alkaliearth
Earth
Major
Metals
Other
Oxyanions
Salts
Full set alk
Series contents
Species
Constituent mapping
Ca+2
Ca
SO4-2
SO4, S
Al[OH]4-
Al
Fe[OH]4-
Fe, Fe(II)
H2SiO4-2
Si
Prediction and Partitioning
Solubility Prediction
Solid-Liquid Partitioning
Solid Partitioning
Liquid Partitioning
5


CBP
Cementitious Barriers Partnership
ENERGY
SRNL
CRESP
NIST
U.S.NRC
ECN
SIMCO
Export
Edit
View
Help
Export All
To Excel
Export Layout
Assistance
[Al(OH)4-] as function of pH
[Ba+2] as function of pH
[Ca+2] as function of pH
[Fe(OH)4-] as function of pH
[H2SiO4-2] as function of pH
[SO4-2] as function of pH
6

CBP
Cementitious Barriers Partnership



7

CBP
Cementitious Barriers Partnership

Input (Chemical Speciation Fingerprint)

- Element availabilities (major, minor and trace elements from pH dependence test)
- Liquid to Solid ratio (L/S=10)
- Redox status of material/product pH+pe = 15 (oxidised) or other value when relevant
- Clay content (kg/kg)
- Reactive Hydrated Ironoxide surface (HFO in kg/kg)
- Reactive Solid Humic Acid (SHA in kg/kg)
- Reactive Dissolved Organic Carbon (DOC in kg/l from pH dependence test)
- Selection of potentially relevant minerals controlling solubility (Partly taken from a model run to determine saturation indices (SI) for all available minerals in the thermodynamic database) and expert knowledge

CBP
Cementitious Barriers Partnership

INPUT FOR CHEMICAL SPECIATION MODELLING: Caststone (1)

Name	Cement Stabilised RA waste								
Source material	Cast stone (A,P,A)								
Availabilities									
Species	Concentration mg/kg	Species	Concentration mg/kg	Species	Concentration mg/kg	Species	Concentration mg/kg		
Ag+	0.035	Cu+2	5.00	Li+	10.0	Sb[OH]6-	0.50		
Al+3	7.81E+03	F-	10.0	Mg+2	1.10E+04	SeO4-2	0.50		
Ba+2	10.0	Fe+3	3.90E+03	Mn+2	10.0	Sn+2	1.00		
Ca+2	1.72E+05	H2CO3	5.00E+03	MoO4-2	5.00	SO4-2	6.51E+03		
Cd+2	0.020	H3AsO4	10.0	Na+	8.01E+03	Sr+2	10.0		
Cl-	100.0	H3BO3	10.0	Ni+2	5.00	TcO4-	0.047		
Co+2	1.00	H4SiO4	1.60E+03	NO3-	3.49E+05	UO2+	1.00		
CrO4-2	2.72	I-	0.14	Pb+2	5.00	VO2+	5.00		
Cs+	2.00	K+	1.30E+03	PO4-3	115.1	Zn+2	10.0		

Model Parameters			Organic matter fractionation				
Name	Value	Unit	pH	Total DOC	Dissolv. Humic Acid	Total POM	Humic Acid in Solid
Sum of pH and pE	12.0			mg/L	mg/L	mg/kg	mg/kg
Liquid to Solid ratio	10.0	L/kg	12.9	28.0	5.59	20.5	144.1
Hydrous Ferric Oxide fraction	2.00E+03	mg/kg	11.7	3.54	0.71	264.6	192.9
Clay fraction	5.00E+03	mg/kg	10.1	2.72	0.54	272.8	194.6
Total Organic Carbon	300.0	mg/kg	8.69	3.27	0.65	267.3	193.5
			8.33	4.03	0.81	259.7	191.9
			7.03	4.13	0.83	258.7	191.7
			5.44	4.53	0.91	254.7	190.9
			3.64	5.32	1.06	246.8	189.4
			1.57	4.35	0.87	256.5	191.3

CBP
Cementitious Barriers Partnership

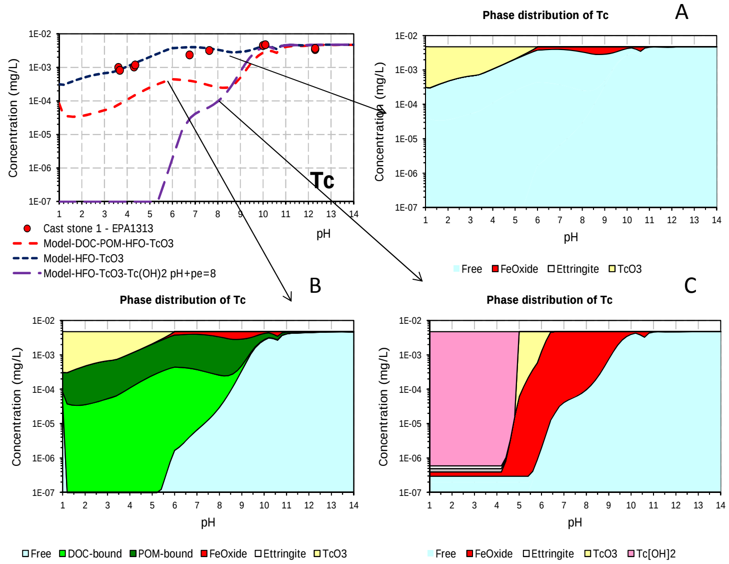
INPUT FOR CHEMICAL SPECIATION MODELLING: Cast stone (2)

Minerals	Log(K)	Reaction	Minerals	Log(K)	Reaction
AA_2CaO_Al2O3_SiO2_8H2O[s]	**-49.4**	**AA_2CaO_Al2O3_SiO2_8H2O[s] + 10 H+ -> 2 Al+3 + 2 Ca+2 + 11 H2O + 1 H4SiO4**	Goslarite	1.96	Goslarite -> 7 H2O + 1 SO4-2 + 1 Zn+2
AA_2CaO_Fe2O3_8H2O[s]	-53.3	AA_2CaO_Fe2O3_8H2O[s] + 10 H+ -> 2 Ca+2 + 2 Fe+3 + 13 H2O	Hydrocalumite-I	-65.0	Hydrocalumite-I + 12 H+ -> 2 Al+3 + 4 Ca+2 + 2 I-
AA_2CaO_Fe2O3_SiO2_8H2O[s]	**-42.3**	**AA_2CaO_Fe2O3_SiO2_8H2O[s] + 10 H+ -> 2 Ca+2 + 2 Fe+3 + 11 H2O + 1 H4SiO4**	I2	-18.2	I2 + 2 e- -> 2 I-
AA_3CaO_Al2O3_CaSO4_12H2O[s]	-74.3	AA_3CaO_Al2O3_CaSO4_12H2O[s] + 12 H+ -> 2 Al+3 + 4 Ca+2 + 18 H2O + 1 SO4-2	Iodyrite	16.1	Iodyrite -> 1 Ag+ + 1 I-
AA_3CaO_Fe2O3_6H2O[s]	**-72.4**	**AA_3CaO_Fe2O3_6H2O[s] + 12 H+ -> 3 Ca+2 + 2 Fe+3 + 12 H2O**	**Laumontite**	**-14.5**	**Laumontite + 8 H+ -> 2 Al+3 + 1 Ca+2 + 4 H4SiO4**
AA_3CaO_Fe2O3_CaCO3_11H2O[s]	-80.1	AA_3CaO_Fe2O3_CaCO3_11H2O[s] + 14 H+ -> 4 Ca+2 + 2 Fe+3 + 1 H2CO3 + 17 H2O	**Manganite**	**-25.3**	**Manganite + 3 H+ + 1 e- -> 2 H2O + 1 Mn+2**
AA_3CaO_Fe2O3_CaSO4_12H2O[s]	**-67.2**	**AA_3CaO_Fe2O3_CaSO4_12H2O[s] + 12 H+ -> 4 Ca+2 + 2 Fe+3 + 18 H2O + 1 SO4-2**	MgKPO4:6H2O[c]	10.6	MgKPO4:6H2O[c] -> 6 H2O + 1 K+ + 1 Mg+2 + 1 PO4-3
AA_Brucite	**-16.8**	**AA_Brucite + 2 H+ -> 2 H2O + 1 Mg+2**	Mn3[AsO4]2:8H2O	-12.5	Mn3[AsO4]2:8H2O + 6 H+ -> 8 H2O + 2 H3AsO4 + 3 Mn+2
AA_CO3-hydrotalcite	**-67.5**	**AA_CO3-hydrotalcite + 14 H+ -> 2 Al+3 + 1 H2CO3 + 14 H2O + 4 Mg+2**	Morenosite	2.36	Morenosite -> 7 H2O + 1 Ni+2 + 1 SO4-2
AA_CaO_Al2O3_10H2O[s]	-38.5	AA_CaO_Al2O3_10H2O[s] + 8 H+ -> 2 Al+3 + 1 Ca+2 + 14 H2O	**Ni[OH]2[s]**	**-10.8**	**Ni[OH]2[s] + 2 H+ -> 2 H2O + 1 Ni+2**
AA_Calcite	**-7.20**	**AA_Calcite + 2 H+ -> 1 Ca+2 + 1 H2CO3**	Pb2V2O7	0.95	Pb2V2O7 + 3 H+ -> 1.5 H2O + 1 Pb+2 + 1 VO2+
AA_Fe[OH]3[microcr]	**-3.00**	**AA_Fe[OH]3[microcr] + 3 H+ -> 1 Fe+3 + 3 H2O**	Pb3[VO4]2	-3.07	Pb3[VO4]2 + 4 H+ -> 2 H2O + 1.5 Pb+2 + 1 VO2+
AA_Gibbsite	-7.76	AA_Gibbsite + 3 H+ -> 1 Al+3 + 3 H2O	PbI2[s]	8.10	PbI2[s] -> 2 I- + 1 Pb+2
AA_Jennite	**-26.5**	**AA_Jennite + 3 H+ -> 1.5 Ca+2 + 2.1 H2O + 0.9 H4SiO4**	**PbMoO4[c]**	**15.8**	**PbMoO4[c] -> 1 MoO4-2 + 1 Pb+2**
AA_Magnesite	-7.32	AA_Magnesite + 2 H+ -> 1 H2CO3 + 1 Mg+2	**Pb[OH]2[C]**	**-8.15**	**Pb[OH]2[C] + 2 H+ -> 2 H2O + 1 Pb+2**
AA_Portlandite	**-22.8**	**AA_Portlandite + 2 H+ -> 1 Ca+2 + 2 H2O**	Pyrolusite	-41.4	Pyrolusite + 4 H+ + 2 e- -> 2 H2O + 1 Mn+2
AA_Tobermorite-I	-28.0	AA_Tobermorite-I + 4 H+ -> 2 Ca+2 + 1.2 H2O + 2.4 H4SiO4	**Schoepite**	**-8.19**	**Schoepite + 2 H+ + 1 e- -> 3 H2O + 1 UO2+**
AA_Tricarboaluminate	-110.7	AA_Tricarboaluminate + 18 H+ -> 2 Al+3 + 6 Ca+2 + 3 H2CO3 + 38 H2O	Tc2O7	-13.1	Tc2O7 + 1 H2O -> 2 H+ + 2 TcO4-
Ag3PO4	17.6	Ag3PO4 -> 3 Ag+ + 1 PO4-3	Tc2S7	8.09	Tc2S7 + 29 H2O -> 72 H+ + 7 SO4-2 + 2 TcO4- + 56 e-
B_UO2[OH]2	-8.33	B_UO2[OH]2 + 2 H+ + 1 e- -> 2 H2O + 1 UO2+	Tc3O4	220.7	Tc3O4 + 6.5 H2O -> 27 H+ + 3 TcO4- + 16 e-
BaSrSO4[50%Ba]	8.22	BaSrSO4[50%Ba] -> 0.5 Ba+2 + 1 SO4-2 + 0.5 Sr+2	Tc4O7	212.1	Tc4O7 + 7 H2O -> 29 H+ + 4 TcO4- + 16 e-
Ba[SCr]O4[77%SO4]	**10.1**	**Ba[SCr]O4[77%SO4] -> 1 Ba+2 + 0.23 CrO4-2 + 0.77 SO4-2**	TcO2:2H2O[am]	58.8	TcO2:2H2O[am] -> 6 H+ + 1 TcO4- + 4 e-
Ca2Cd[PO4]2	33.0	Ca2Cd[PO4]2 -> 2 Ca+2 + 1 Cd+2 + 2 PO4-3	**TcO3**	**77.4**	**TcO3 + 2.5 H2O -> 5 H+ + 1 TcO4- + 4 e-**
Ca3[AsO4]2:6H2O	-22.3	Ca3[AsO4]2:6H2O + 6 H+ -> 3 Ca+2 + 6 H2O + 2 H3AsO4	TcOH	99.6	TcOH + 3 H2O -> 11 H+ + 1 TcO4- + 8 e-
Ca4Cd[PO4]3OH	**39.2**	**Ca4Cd[PO4]3OH + 1 H+ -> 4 Ca+2 + 1 Cd+2 + 1 H2O + 3 PO4-3**	TcS2	187.9	TcS2 + 12 H2O -> 25 H+ + 2 SO4-2 + 1 TcO4- + 20 e-
CaMoO4[c]	7.94	CaMoO4[c] -> 1 Ca+2 + 1 MoO4-2	TcS3	274.7	TcS3 + 14.5 H2O -> 35 H+ + 3 SO4-2 + 1 TcO4- + 28 e-
Carnotite	-3.01	Carnotite + 4 H+ + 1 e- -> 2 H2O + 1 K+ + 1 UO2+ + 1 VO2+	Tc[OH]2	119.3	Tc[OH]2 + 2.5 H2O -> 11 H+ + 1 TcO4- + 8 e-
Cd[OH]2[A]	-13.7	Cd[OH]2[A] + 2 H+ -> 1 Cd+2 + 2 H2O	Tc[OH]3	47.7	Tc[OH]3 -> 7 H+ + 1 TcO4- + 4 e-
Cr[OH]3[A]	**68.1**	**Cr[OH]3[A] + 1 H2O -> 1 CrO4-2 + 5 H+ + 3 e-**	**Tyuyamunite**	**-4.82**	**Tyuyamunite + 4 H+ + 1 e- -> 0.5 Ca+2 + 2 H2O + 1 UO2+ + 1 VO2+**
Cu[OH]2[s]	**-8.64**	**Cu[OH]2[s] + 2 H+ -> 1 Cu+2 + 2 H2O**	**Uranophane**	**-23.1**	**Uranophane + 6 H+ + 2 e- -> 1 Ca+2 + 2 H4SiO4 + 2 UO2+**
Epsomite	2.14	Epsomite -> 7 H2O + 1 Mg+2 + 1 SO4-2	Willemite	-15.3	Willemite + 4 H+ -> 1 H4SiO4 + 2 Zn+2
Fe2[MoO4]3[1]	**38.8**	**Fe2[MoO4]3[1] -> 2 Fe+3 + 3 MoO4-2**	**ZnSiO3**	**-2.93**	**ZnSiO3 + 2 H+ + 1 H2O -> 1 H4SiO4 + 1 Zn+2**
Fe_Vanadate	**8.38**	**Fe_Vanadate + 2 H+ -> 0.5 Fe+3 + 1 H2O + 1 VO2+ + 0.5 e-**	**monosulfate_ECN**	**-72.6**	**monosulfate_ECN + 12 H+ -> 2 Al+3 + 4 Ca+2 + 12 H2O + 1 SO4-2**
Fluorite	11.0	Fluorite -> 1 Ca+2 + 2 F-			

Chemical reactions included to describe the multi-element interaction. In bold minerals identified as potentially most relevant

CBP Cementitious Barriers Partnership

Modeling of Tc Release from Cement Stabilised RA Waste under Different Exposure Conditions



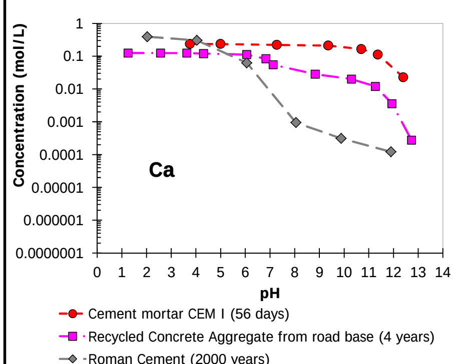
A – Modelling with sorption to HFO and mineral precipitation (pH+pe=15);

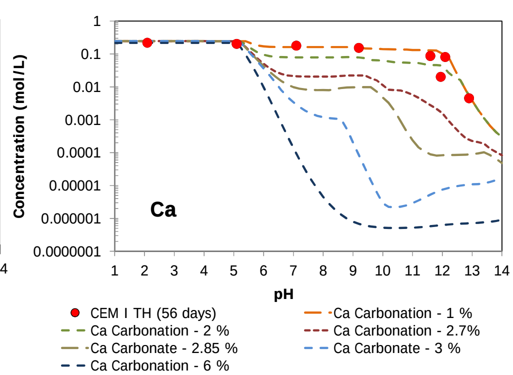
B – in addition to A assumed DOC and POM;

C - as A with imposed reducing conditions (pH+pe=8)

CBP Cementitious Barriers Partnership

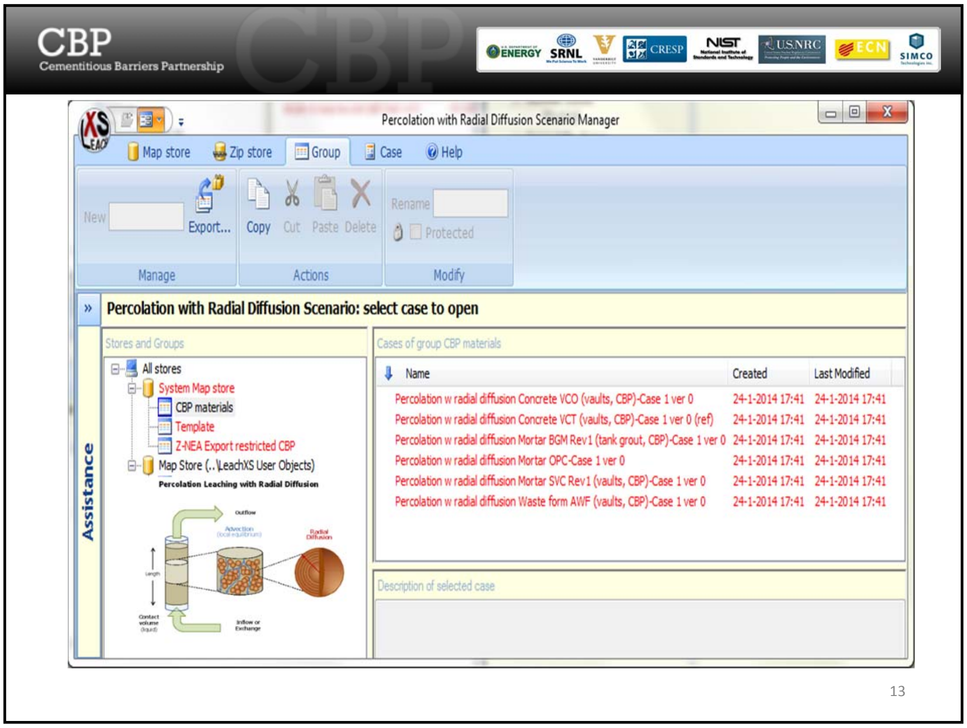
Comparison of carbonation in actual field materials with modelled Ca release based on different degrees of carbonation

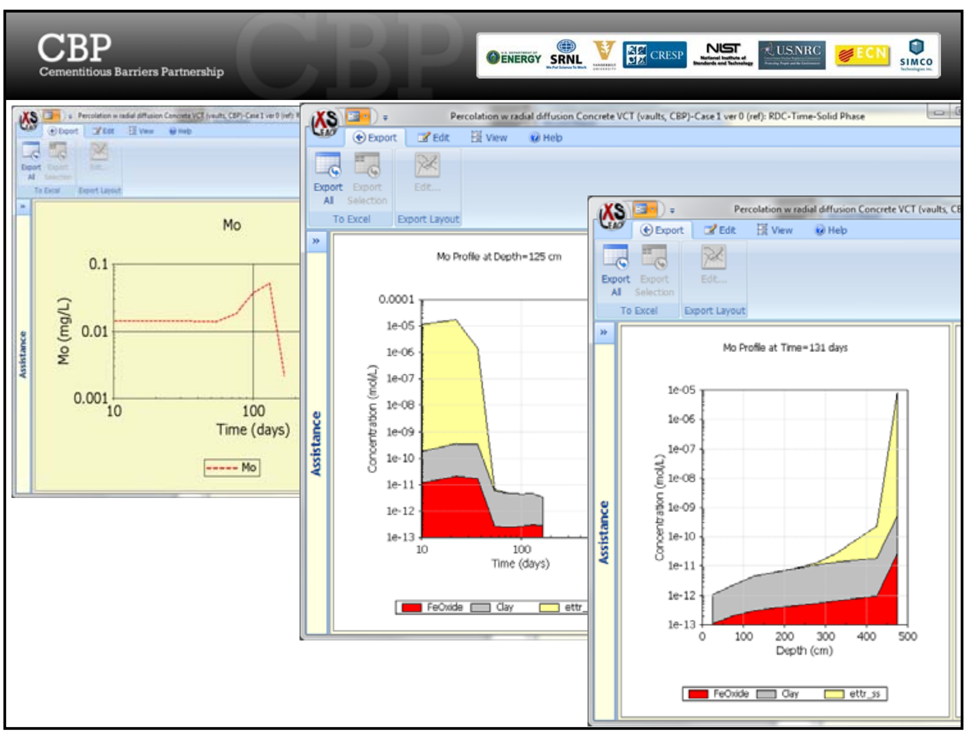




Roman cement carbonated to the core in 2000 years

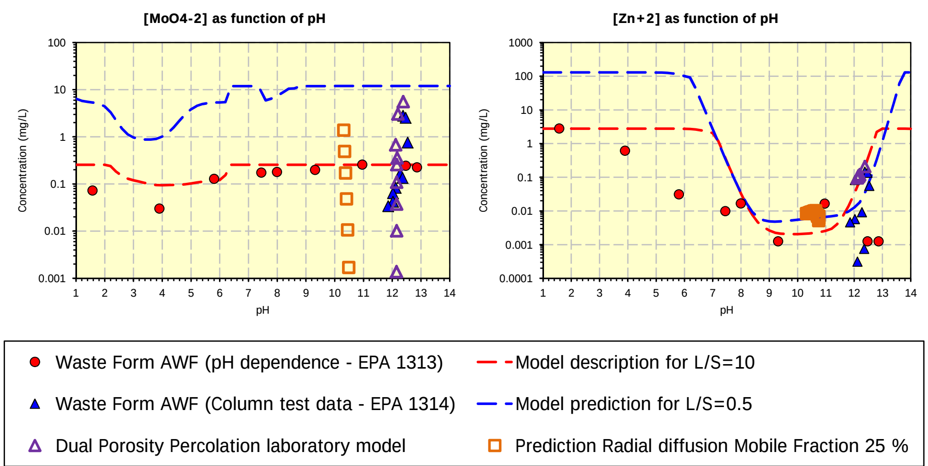
12


CBP
Cementitious Barriers Partnership
Percolation with Radial Diffusion Scenario Manager
Map store
Zip store
Group
Case
Help
New
Export...
Copy
Cut
Paste
Delete
Rename
Protected
Manage
Actions
Modify
Percolation with Radial Diffusion Scenario: select case to open
Stores and Groups
Cases of group CBP materials
All stores
System Map store
CBP materials
Template
Z-NEA Export restricted CBP
Map Store (..\LeachXS User Objects)
Percolation Leaching with Radial Diffusion
Name
Created
Last Modified
Percolation w radial diffusion Concrete VCO (vaults, CBP)-Case 1 ver 0 24-1-2014 17:41 24-1-2014 17:41
Percolation w radial diffusion Concrete VCT (vaults, CBP)-Case 1 ver 0 (ref) 24-1-2014 17:41 24-1-2014 17:41
Percolation w radial diffusion Mortar BGM Rev1 (tank grout, CBP)-Case 1 ver 0 24-1-2014 17:41 24-1-2014 17:41
Percolation w radial diffusion Mortar OPC-Case 1 ver 0 24-1-2014 17:41 24-1-2014 17:41
Percolation w radial diffusion Mortar SVC Rev1 (vaults, CBP)-Case 1 ver 0 24-1-2014 17:41 24-1-2014 17:41
Percolation w radial diffusion Waste form AWF (vaults, CBP)-Case 1 ver 0 24-1-2014 17:41 24-1-2014 17:41
Description of selected case
Assistance
13


CBP
Cementitious Barriers Partnership
Percolation w radial diffusion Concrete VCT (vaults, CBP)-Case 1 ver 0 (ref): RDC-Time-Solid Phase
Export
Edit
View
Help
Export All
Export Selection
Edit...
To Excel
Export Layout
Mo
Mo (mg/L)
Time (days)
Mo Profile at Depth=125 cm
Concentration (mol/L)
FeOxide
Clay
Mo Profile at Time=131 days
Depth (cm)
ettr_ss
Assistance

CBP Cementitious Barriers Partnership

Comparison of Laboratory test and prediction model results



Zn is solubility controlled (Willemite); Mo is washed out in pH range 8 -12

15

CBP Cementitious Barriers Partnership

Key Messages

- The LEAF methods provide a sound basis for evaluating release from cementitious materials and provide a sound basis for assessing impact in combination with geochemical modelling
- The chemical speciation fingerprint (CSF) derived from modeling release in the pH dependence test (LeachXS/ORCHESTRA) is suitable for subsequent chemical reaction/transport modelling in more complex scenarios
- Chemical speciation-based simulation of liquid-solid partitioning and reactive mass transport can be used to provide insights into mechanisms controlling leaching and conditions beyond testing
- Sensitivity evaluations can be used to evaluate the impacts of carbonation, redox changes, material composition and physical changes on liquid-solid partitioning

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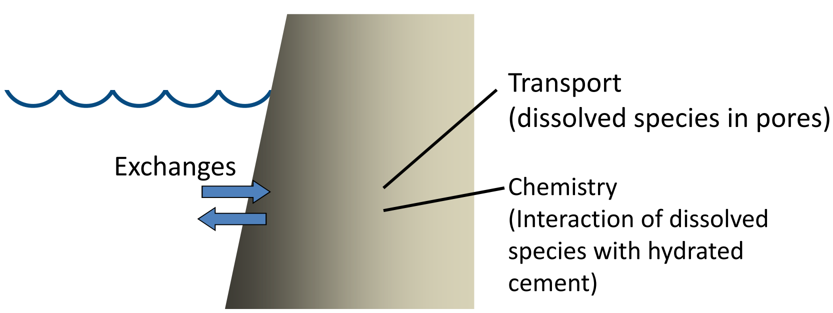
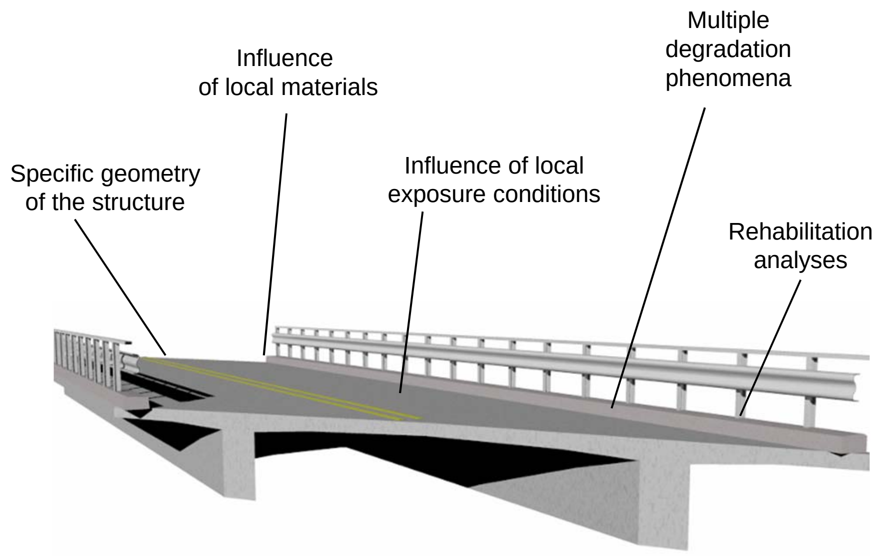
Main features

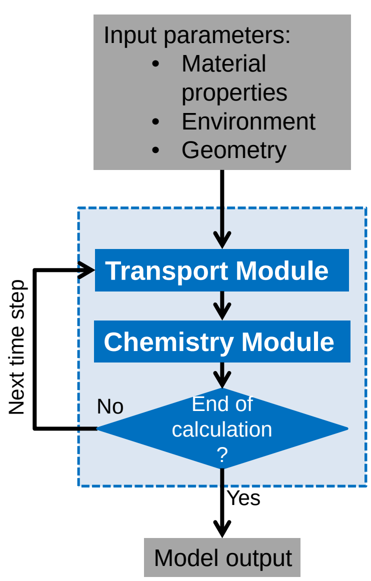
STADIUM® models the transport of chemical species in **cementitious materials** resulting from exchanges at the material/environment interface.



Main features



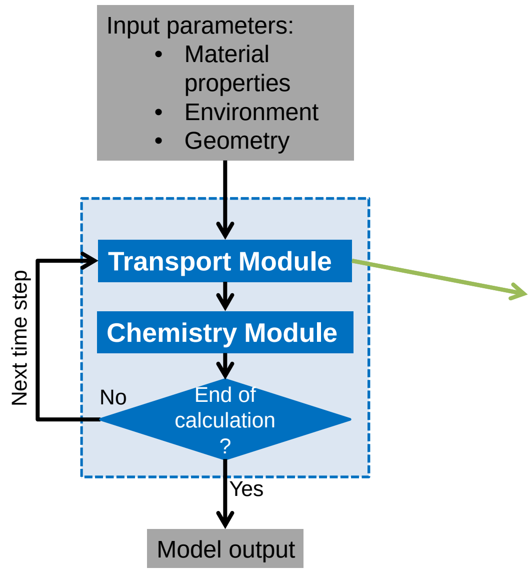
Main features



The model is divided in 2 main modules:

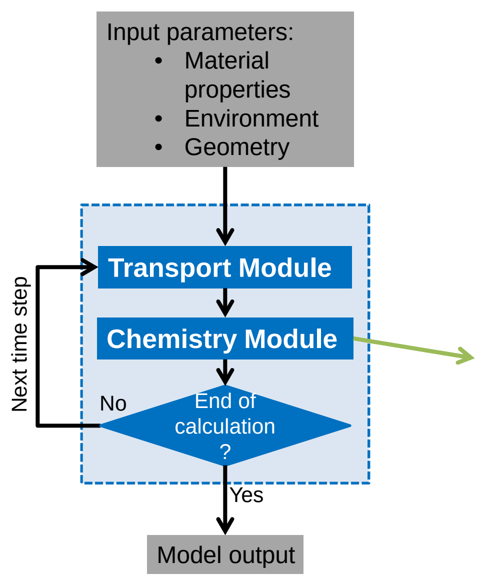
- The transport module makes the species move during one time step,
- The chemistry module simulates the reactions between species in the pores and the hydrated paste.

Main features



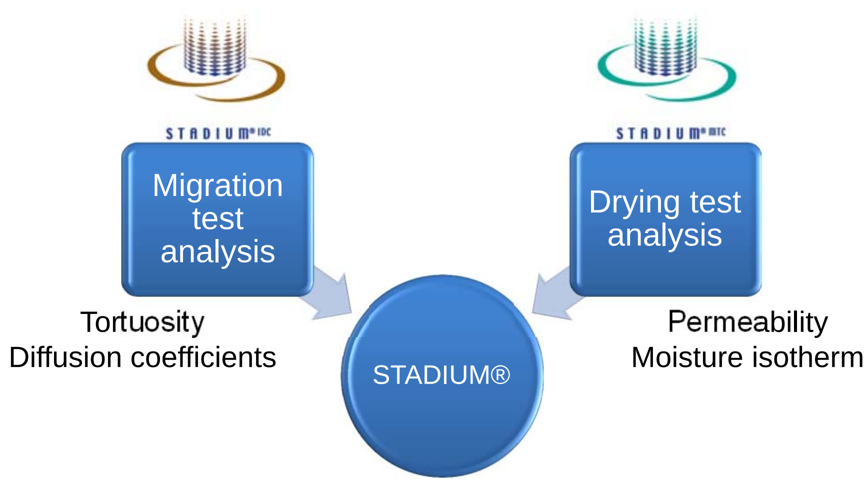
- Coupled species diffusion
- Moisture/Temperature coupling
- Transport of main species
- Feedback effect
- Time-dependent transport properties (hydration)
- Time-dependent B.C.

Main features



- Local Equilibrium Assumption
- Dissolution/precipitation
- Solid solutions
- Chemical/Pitzer database in separate text file
- Effect of temperature on chemistry

Input to transport module



Input to transport module

Test methods part of Unified Facilities Guide Specifications (UFGS) 03 31 29 (February 2010) test protocol

- US Navy (NAVFAC ESC)
- USACE
- USAF
- NASA

Specified by the US NAVY
UFGS-03 31 29

Performance specification protocol

Input to chemistry module

INPUT TO CHEMISTRY MODULE

- Mix composition
- Cement chemistry
- SCMs chemistry
- Chemistry database

→

CALCULATED PARAMETERS

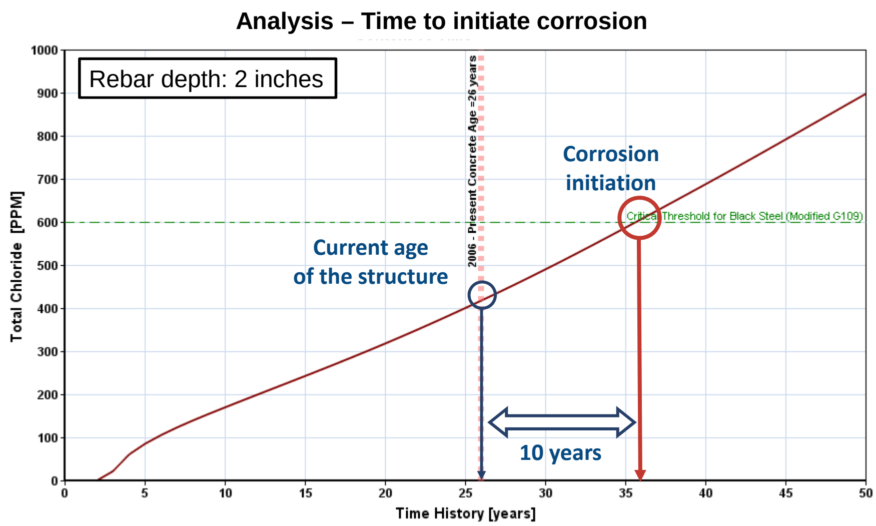
- Hydrated cement paste composition
- Pore solution composition

Model output

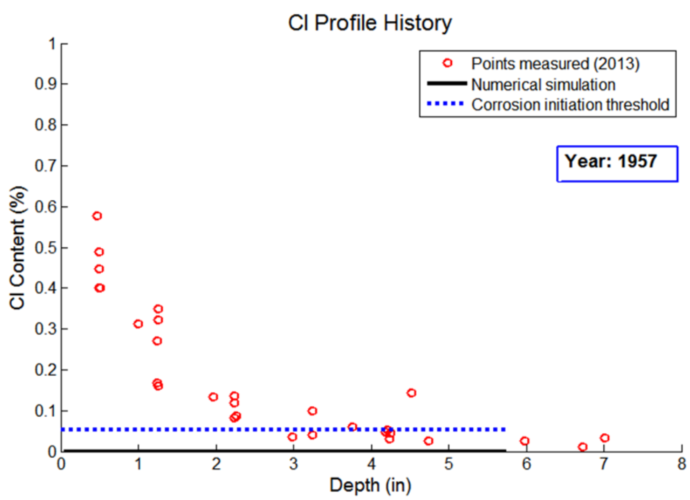
At the end of calculations, the model provides the following information:

- Space and time distribution of species concentrations,
- Space and time distribution of mineral contents,
- Space and time distribution of temperature and humidity,
- Analysis of the main variables to get: total calcium, sulfur and chloride content.
- Chloride content at specific depth to estimate the time to initiate corrosion for different rebar depths.

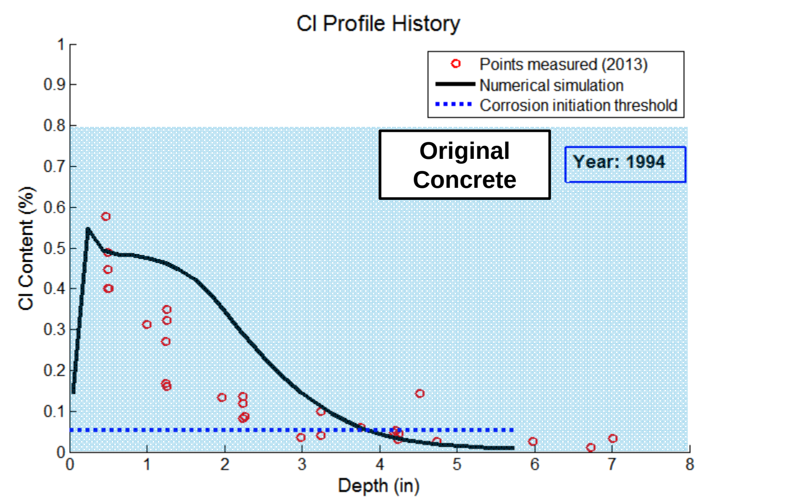
Typical application



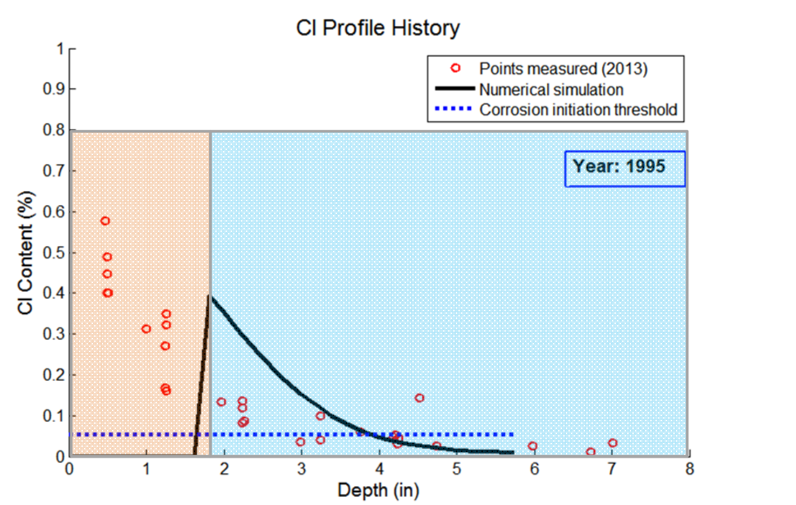
Advanced Application – Modeling Repairs



Advanced Application – Modeling Repairs



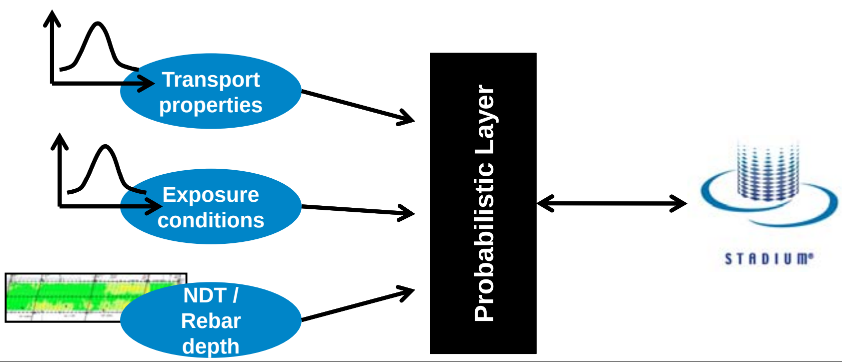
Advanced Application – Modeling Repairs



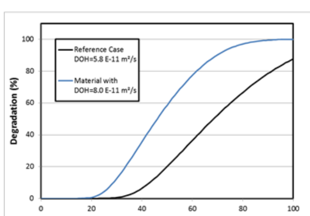
Probabilistic Approach – Risk of Corrosion

A probabilistic engine can handle calculations considering the distribution of key parameters:

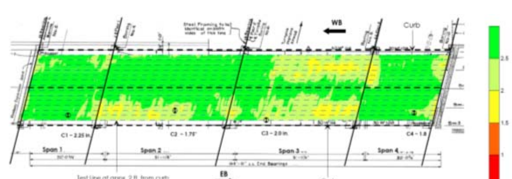
- Transport properties,
- Concrete cover,
- Exposure conditions,
- Corrosion threshold.



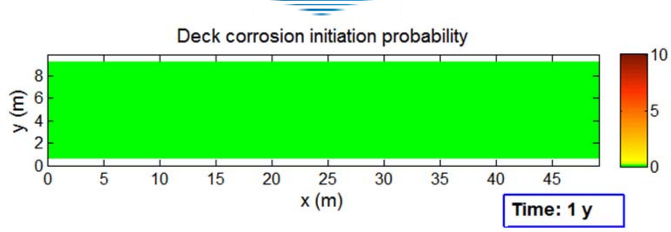
Probabilistic Approach – Risk of Corrosion



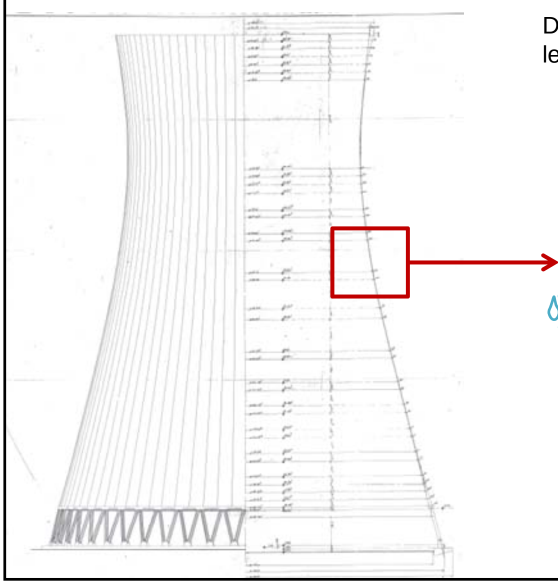
Degradation Curves



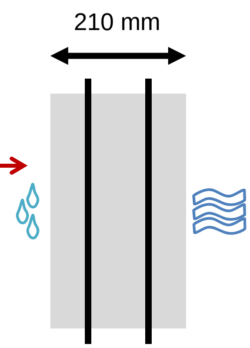
GPR mapping of rebar cover



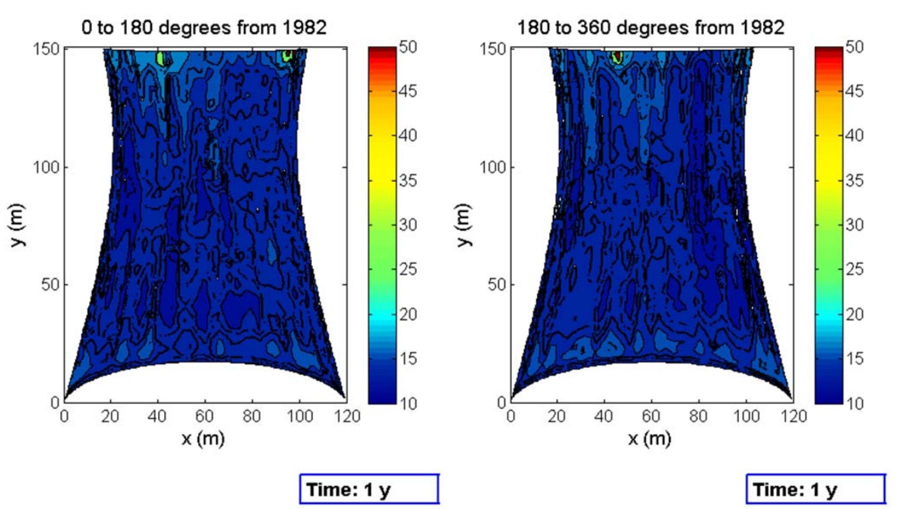
Application to cooling towers



Degradation due to long-term leaching

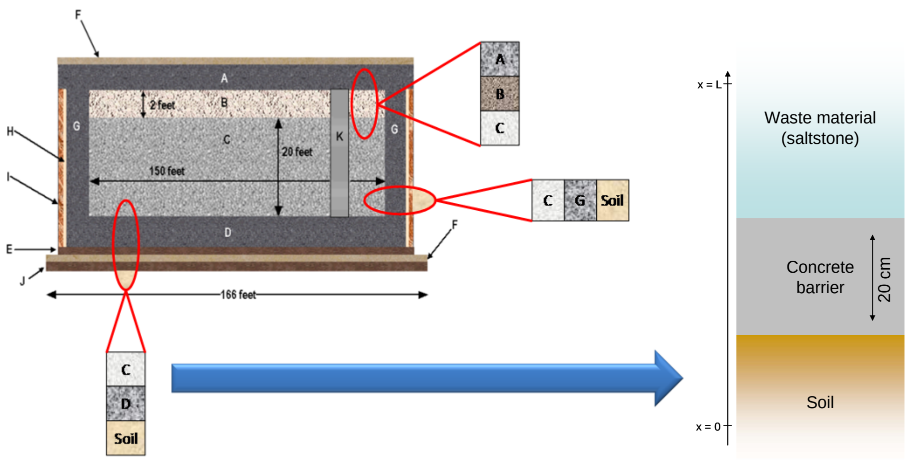


Application to cooling towers



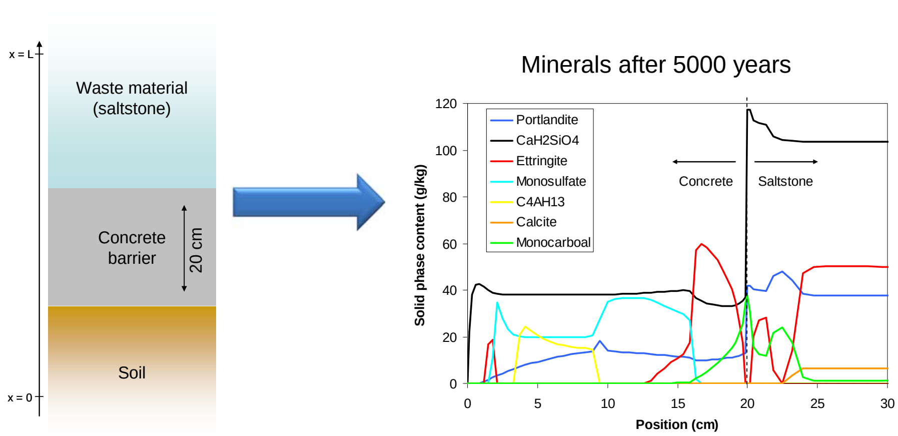
CBP test cases

Concrete in contact with saltstone



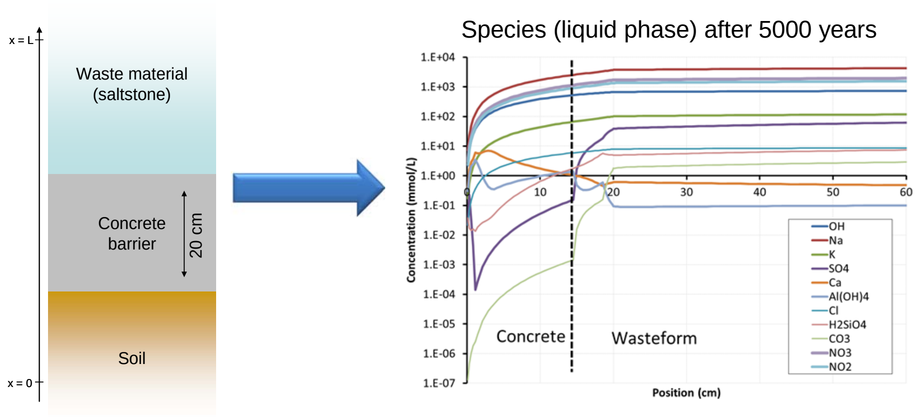
CBP test cases

Concrete in contact with saltstone



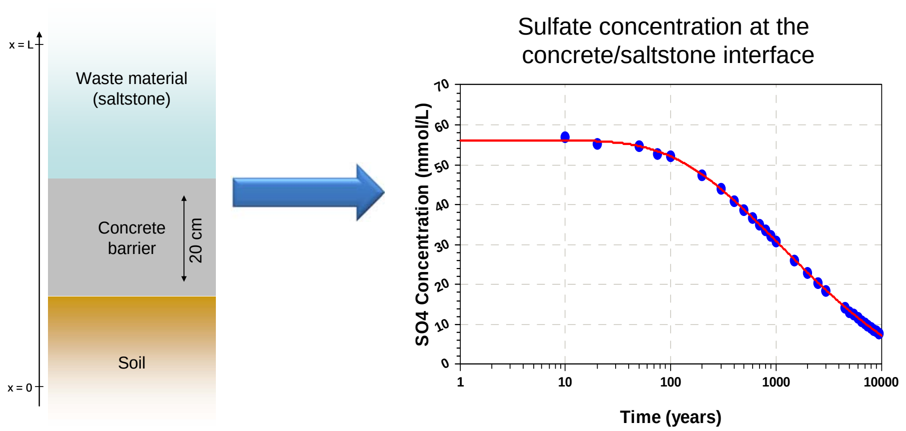
CBP test cases

Concrete in contact with saltstone



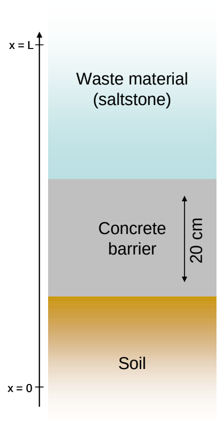
CBP test cases

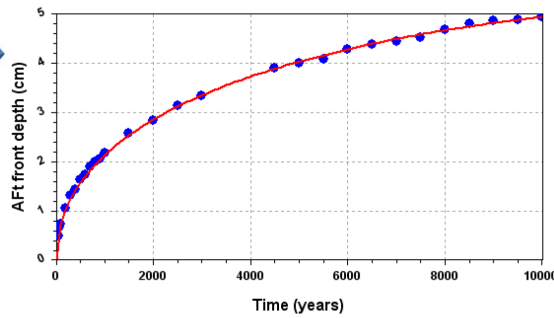
Concrete in contact with saltstone



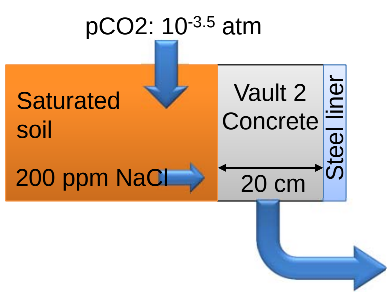
CBP test cases

Concrete in contact with saltstone

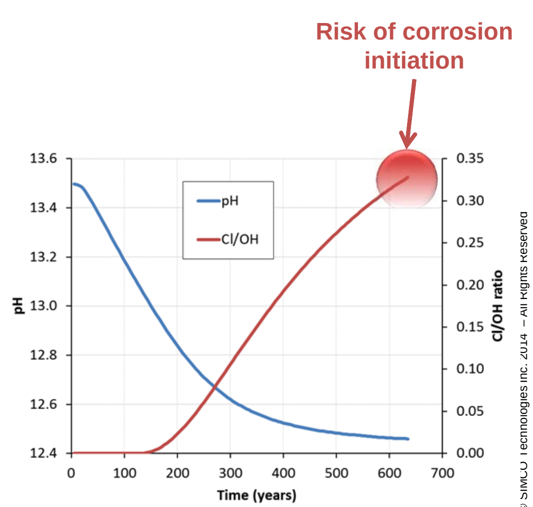




CBP test cases



Analysis: estimation of the risk of corrosion due to chloride and drop of pH at the concrete/liner interface




SIMCO
Thank you

Use of GoldSim in Conjunction with CBP Tools for Uncertainty Assessment and Integration with Performance Assessments

Kevin G. Brown
Vanderbilt University & CRESP

Greg Flach
Savannah River National Laboratory

Cementitious Barriers Partnership Meeting
Nashville, Tennessee
03-04 February 2014

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Summary

- The CBP Technical Approach and Strategy
  - Integration with Performance Assessments
  - Phased Approach to Integration
- CBP Software Toolbox Version 2.0
  - Improvements and additions
  - Briefly how the Software Toolbox is used
  - Important degradation mechanisms (sulfate ingress/attack, chloride attack, leaching and carbonation) for monolith and column scenarios
- Model parameter sensitivity and other studies
- Software Toolbox Strategy Moving Forward

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Technical Strategy / Approach

- **Reference Cases** – provide basis for comparison and demonstration of CBP tools
  - Cementitious waste form in concrete disposal vault with cap
  - Grouted high-level waste (HLW) tank closure
  - Spent/Used nuclear fuel pool / dry cask storage (future)
  - Nuclear processing facilities closure / D&D (e.g., canyons)
  - Grouted vadose zone contamination
  - Materials – surrogate low-activity waste (LAW) cementitious waste form, reducing grout, reinforced concrete (historical), reinforced concrete (future)
- **Extension/enhancement of existing tools** – CEMHYD3D→THAMES, STADIUM, LeachXS/ORCHESTRA, GoldSim Performance Assessment (PA) framework
- **Coordinated experimental and computational program**
  - Conceptual model and numerical solution improvements
  - Define test methods and parameter measurements
  - Model validation

→ **CBP Software Toolbox Version 2.0 Release**

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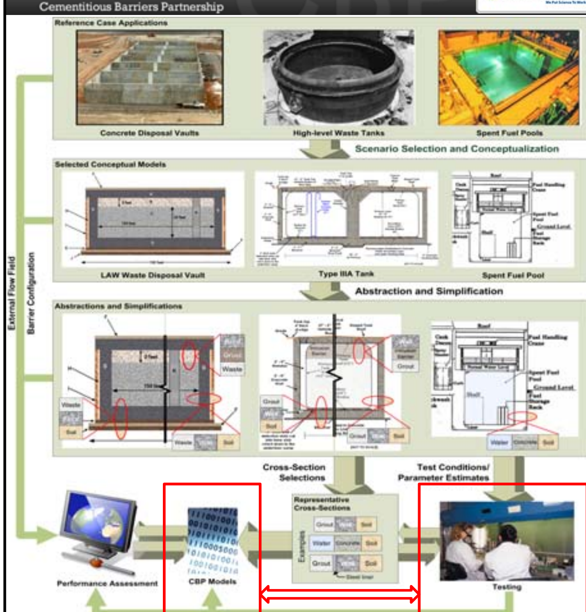

Linking Reference Cases to Performance Models through Abstraction with Models Validated by Lab and Field Testing

GoldSim Framework / DLL
- STADIUM®
- LeachXS™/ORCHESTRA
- THAMES (pending)

New USEPA Leach Methods (based on LEAF)
- USEPA Methods 1313 - 1316
- Included in USEPA SW-846

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Key Aging Phenomena

Key Phenomena

- ✓ Chloride ingress and corrosion
  - STADIUM model (2013)
- ✓ Constituent Leaching
- ✓ Sulfate attack and uncertainty analysis (2011)
- ✓ Carbonation (2012-2013)
- Oxidation (2012-2013)
- Cracking (2013)
- Pore structure relationships with mass transfer and hydraulic properties (future)
- Alkali-silica reaction (ASR) (future)

Integration with Conceptual Models

- Coupled phenomena
- Saturated, unsaturated and variable saturation
- Liquid, vapor mass transfer
- System geometry and boundary conditions

Phased CBP Toolbox Development

Phase I: Use CBP partner codes essentially "as is"

- No inter-code coupling between selected partner codes (LeachXS™/ORCHESTRA and STADIUM®)
- Uses CBP Custom Dynamic-link library (DLL) to link each partner code to GoldSim
- Focus on leaching, sulfate ingress and attack, chloride attack, and carbonation for monolith and column lab and field cases

Phase II: Couple the models for needed phenomena

- Modest coupling (including inter-code)
- Link **THAMES** partner code (“virtual microprobe”) to Toolbox
- Additional scenarios and degradation phenomena (e.g., cracking, alkali-silica reaction, pore filling) and model scenarios

CBP Toolbox Improvements (Version 2.0)

- Improved graphics capabilities using gnuplot
  - STADIUM and LeachXS/ORCHESTRA 2-D and 3-D graphs
- Improved error handing for the CBP Dynamic-link Library (DLL) used to connect Partner Codes to GoldSim probabilistic framework
- New STADIUM chloride attack model
- Improved LeachXS/ORCHESTRA (LXO) sulfate attack model
- Improved LXO carbonation model
  - Complete model revision including implementing a fully implicit finite difference (FD) scheme for transport
  - Models employing explicit and implicit solutions available
- New LXO percolation with radial diffusion model
  - New model added to evaluate leaching through a cracked cementitious material

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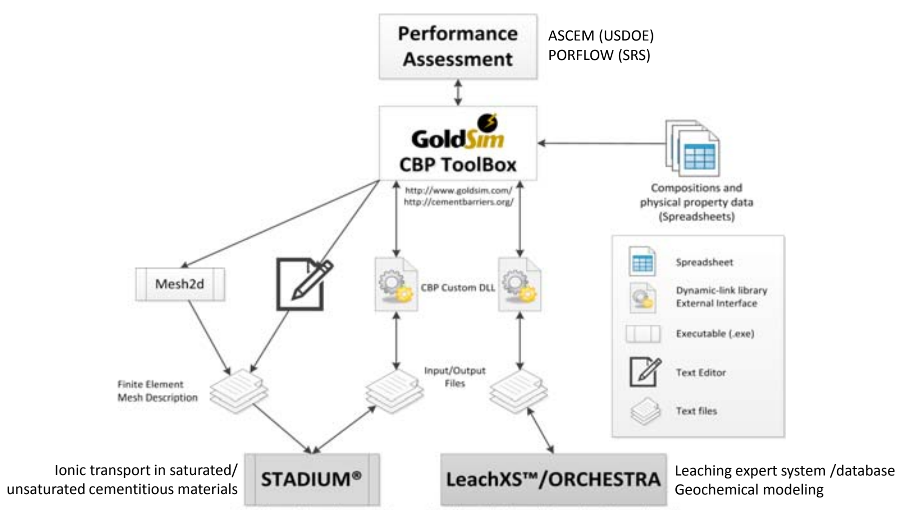
CBP Software Toolbox—Phase I



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Using the CBP Software Toolbox

1. Conceptualize problem scenario and determine appropriate model(s) and degree of coupling
   – Consider availability of needed data and impact of assumptions
2. Develop model in appropriate partner code for scenario
   – STADIUM® → SIMCO Technologies, Inc. (http://www.stadium-software.com/)
   – LeachXS™/ORCHESTRA (LXO) → ECN/VU/DHI/NRG (http://cementbarriers.org/partner-codes/leachxs-orchestra/)
3. Define parameters (GoldSim) and set up instructions and support file(s) needed to run simulation
   – Text Editor → Model and instruction files
   – Mesh2D Program → STADIUM® finite element mesh
4. Run simulation → Results to Performance Assessment

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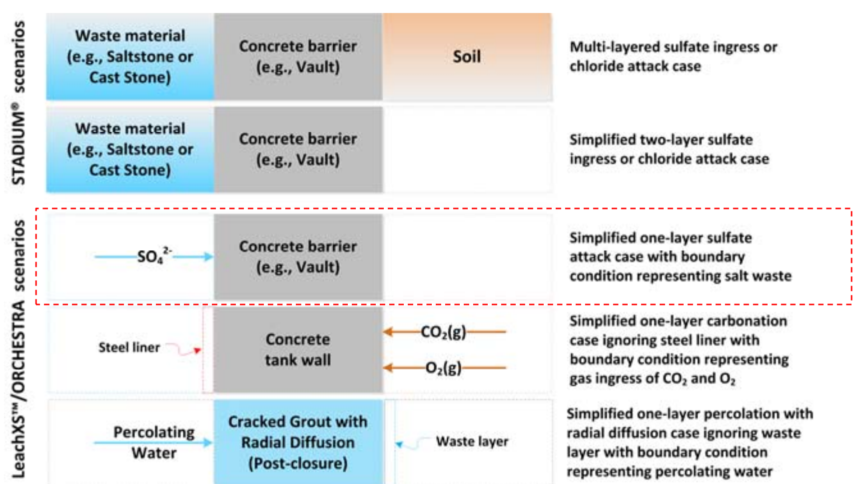
CBP Toolbox—Conceptualize Problem



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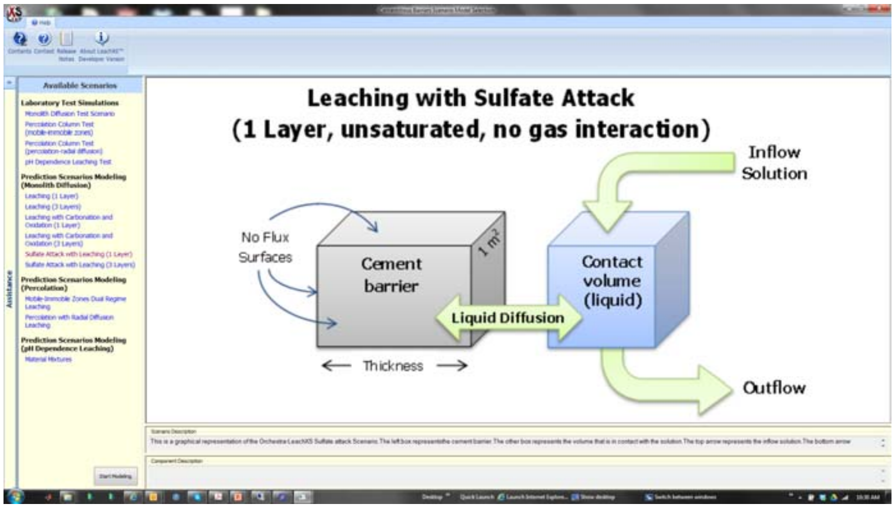
CBP Toolbox—Develop Scenario



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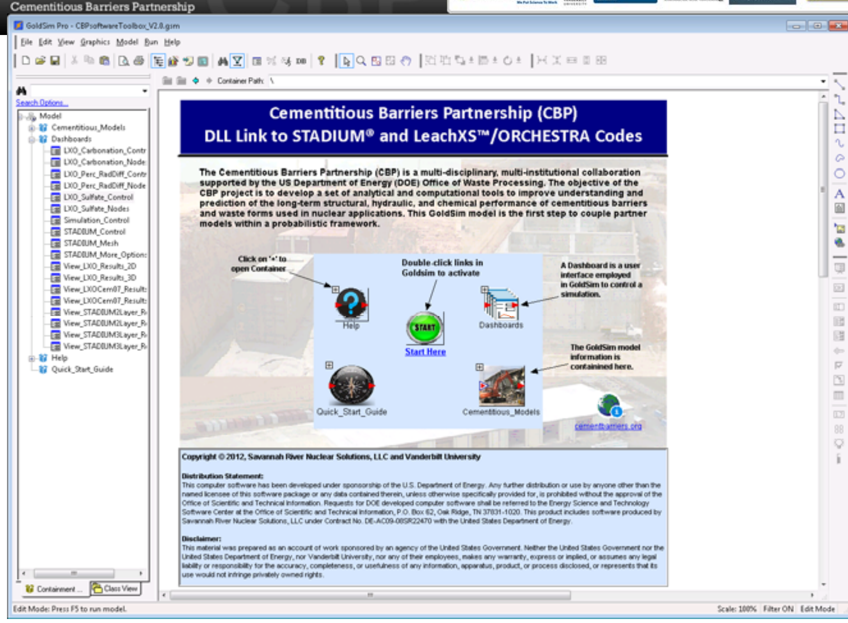

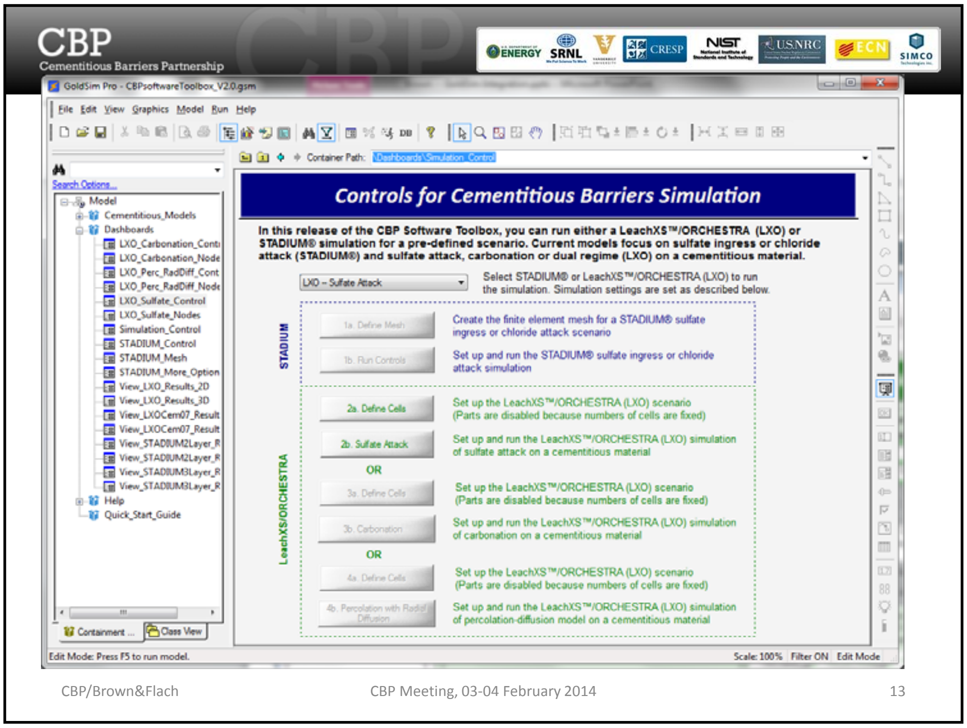
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GoldSim Pro - CBPsoftwareToolbox_V2.0.gsm
Controls for Cementitious Barriers Simulation
In this release of the CBP Software Toolbox, you can run either a LeachXS™/ORCHESTRA (LXO) or STADIUM® simulation for a pre-defined scenario. Current models focus on sulfate ingress or chloride attack (STADIUM®) and sulfate attack, carbonation or dual regime (LXO) on a cementitious material.
Select STADIUM® or LeachXS™/ORCHESTRA (LXO) to run the simulation. Simulation settings are set as described below.
STADIUM
Create the finite element mesh for a STADIUM® sulfate ingress or chloride attack scenario
Set up and run the STADIUM® sulfate ingress or chloride attack simulation
LeachXS/ORCHESTRA
Set up the LeachXS™/ORCHESTRA (LXO) scenario (Parts are disabled because numbers of cells are fixed)
Set up and run the LeachXS™/ORCHESTRA (LXO) simulation of sulfate attack on a cementitious material
OR
Set up and run the LeachXS™/ORCHESTRA (LXO) simulation of carbonation on a cementitious material
Set up and run the LeachXS™/ORCHESTRA (LXO) simulation of percolation-diffusion model on a cementitious material
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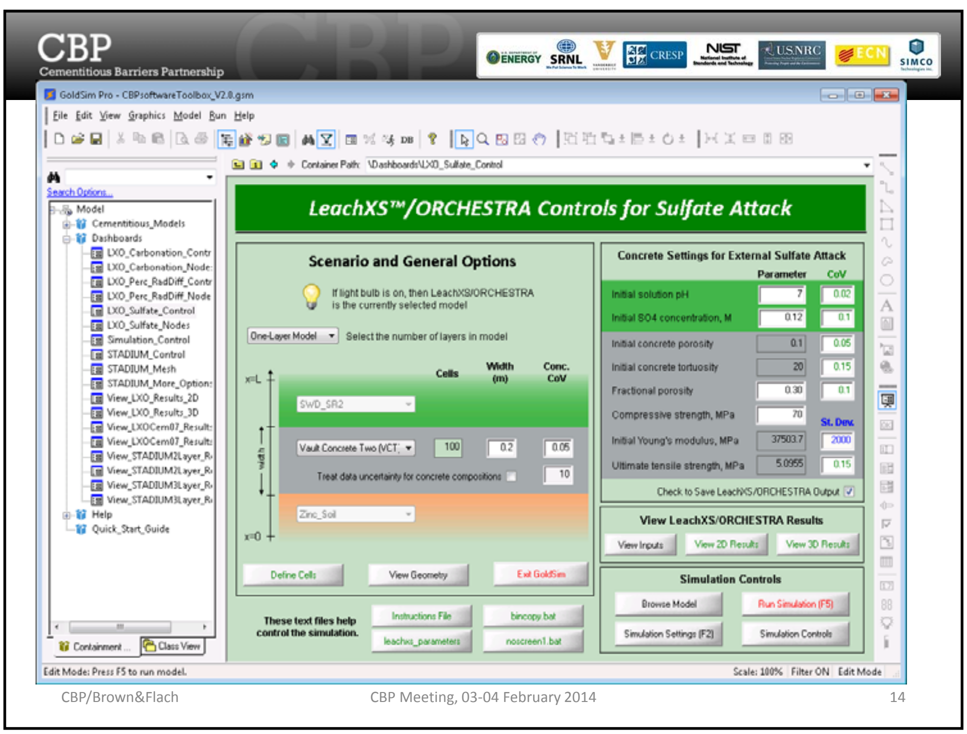
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GoldSim Pro - CBPsoftwareToolbox_V2.8.gsm
LeachXS™/ORCHESTRA Controls for Sulfate Attack
Scenario and General Options
If light bulb is on, then LeachXS/ORCHESTRA is the currently selected model
Select the number of layers in model
Concrete Settings for External Sulfate Attack
Initial solution pH
Initial SO4 concentration, M
Initial concrete porosity
Initial concrete tortuosity
Fractional porosity
Compressive strength, MPa
Initial Young's modulus, MPa
Ultimate tensile strength, MPa
Check to Save LeachXS/ORCHESTRA Output
View LeachXS/ORCHESTRA Results
Simulation Controls
These text files help control the simulation.
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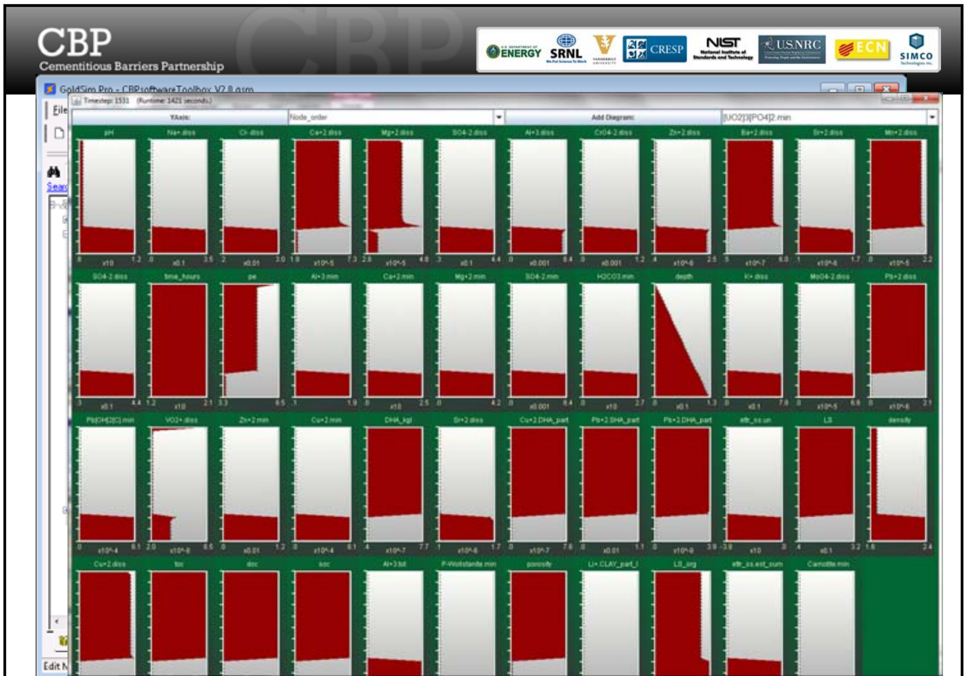

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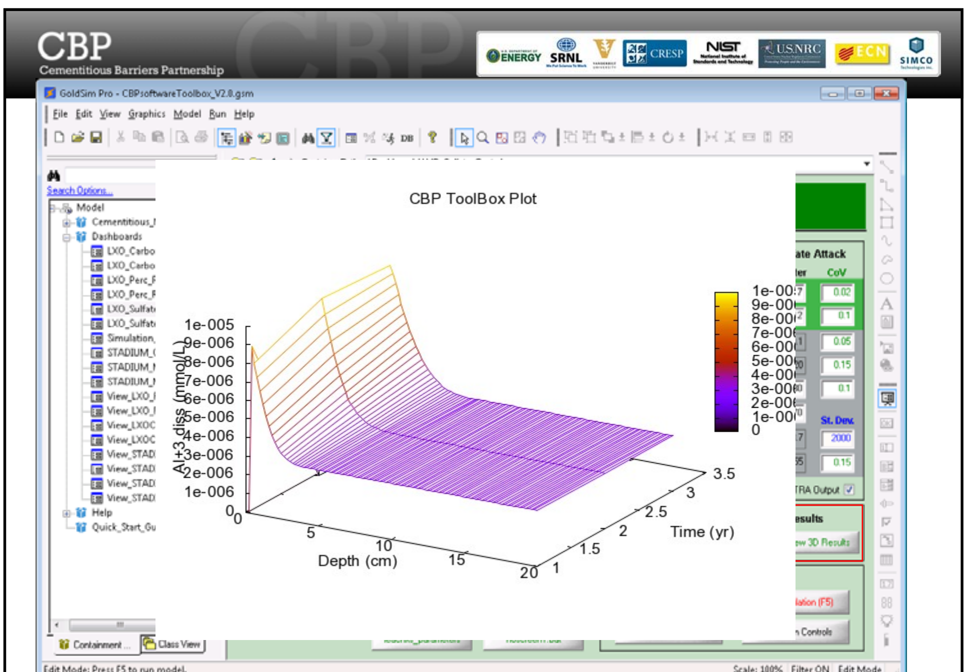

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CBP Software Toolbox Data and Uses

- Characterization of CBP Materials
  - SRNS-STI-2009-00477, Rev. 0 (SIMCO Technologies) and CBP-TR-2010-012-1
- Sulfate Attack and Leaching for SRS Saltstone
  - Sarkar, S, Kosson, DS, Mahadevan, S, Meeussen, JCL, van der Sloot, H, Arnold, JR & Brown, KG 2012, 'Bayesian calibration of thermodynamic parameters for geochemical speciation modeling of cementitious materials', *Cem. Concr. Res.,* vol. 42, pp. 889–902.
- Carbonation and Leaching for a Representative HLW Tank Closure Scenario
  - Brown, K.G., et al. (2013a). "Modeling carbonation of high-level waste tank integrity and closure." *EPJ Web of Conferences*, vol. 56, 05003
- Flow and Leaching through a Cracked HLW Tank Closure Grout
  - Sarkar, et al. (2013). "A dual regime reactive transport model for simulation of high level waste tank closure scenarios." WM2013 Conference, Feb. 24-28, Phoenix, AZ USA.
- Combined Dome Carbonation/Leaching and Subsequent Leaching through a Cracked Grout – Probabilistic Analysis
  - Brown, et al. Presentation at CEM2013, Ghent, Belgium
- Modifying the SDF Performance Assessment (PA) via a Special Analysis

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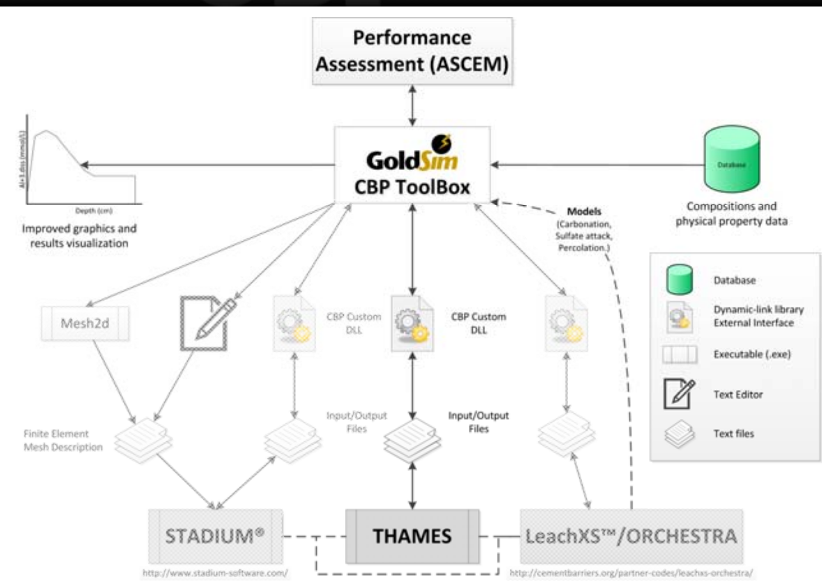
Future Plans for Integration



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CBP Software Toolbox Plans

- CBP Software Toolbox Training
- Work with end-users for implementation and use with specific applications (e.g., ASCEM demonstration, HLW tank closure, Tc-99 retention, Saltstone, ASR)
- Develop new and improved models to represent cementitious materials performance (e.g., STADIUM carbonation, porosity change, cracking, gap flow, multi-layer 1D, and 2D)
- Next major release of CBP Software Toolbox and additional data and test cases needed for verification/validation