Performance Assessment Challenges and Model Abstraction

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CBP
Cementitious Barriers Partnership

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Richland WA

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PA Challenges: Long Time Scales

Disposal of long-lived radionuclides requires effective containment for 1,000 to 10,000 years or more, e.g.,

- Tank closures, saltstone
- Solid waste disposal
- D&D

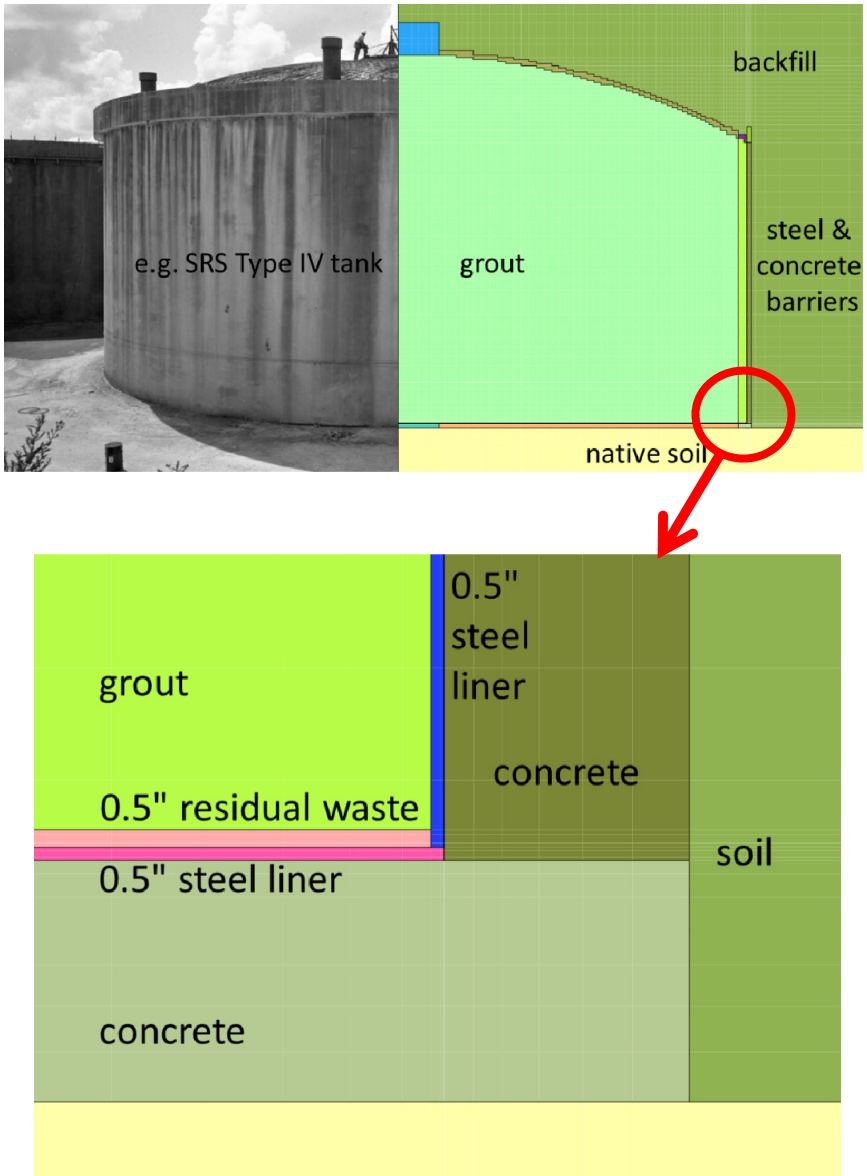
However assumed performance beyond ~500 years requires explicit justification, e.g., NUREG-1573

- "Engineered barriers can . . . be assumed to have physically degraded after 500 years"
- "For timeframes longer than 500 years . . . credit . . . may be taken for the long-term provided the applicant provides suitable information and justification"

PA Challenges: Engineered Materials

Engineered barriers and waste forms introduce significant modeling challenges:

- Reactive chemistry (grout and concrete)
- Evolution of physical and chemical properties over long time periods
- Highly contrasting material properties and fine geometric features (liners and fast flow paths)



PA Challenges: Uncertainties

Significant uncertainties

- Scenarios / conceptual models
- Closure state
- Exposure conditions
- Material properties and evolution

Features
Events
Processes

Uncertainties must be reduced and/or managed

- Experimental measurement
- Field validation
- Sensitivity analysis and uncertainty quantification
- Compliance margin

⇨ **Many modeling cases**

PA Challenges: Ambiguous Objectives

Period of Performance?

- DOE Order 435.1 → 1,000 yrs
- NRC guidance → 10,000 yrs

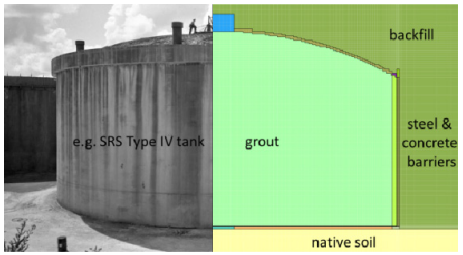
"Reasonable" expectation / assurance?

- Subjective criterion
- Role of behavior beyond period of performance

⇨ **More modeling cases**

PA Challenges: Computing Demands

Savannah River H-Tank Farm example



Vadose zone flow

- 4000 simulations = 5 scenarios · 20 tanks/srcs · 40 flow periods

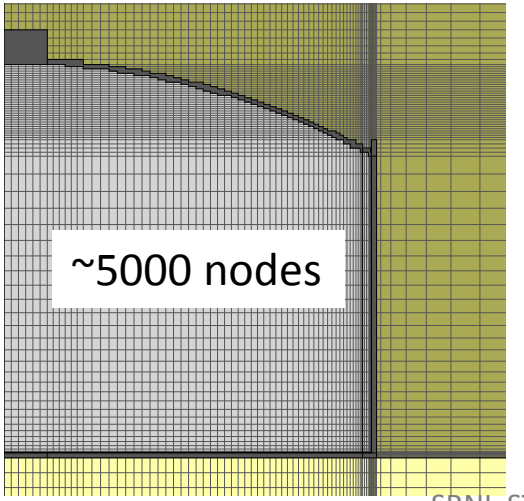
Vadose zone transport

- Base case: 3200 runs = 40 tanks/srcs · 80 species
- Alternative cases: 1000 runs = 4 cases · 25 srcs · 10 species
- Sensitivity cases: 1000 runs = 10 scenarios · 10 srcs · 10 species
- Total: 5200 simulations

Aquifer transport

- 5200 simulations

Total = 14,400 simulations



PA Challenges: Schedule Constraints

Performance Assessment

- Months to one year

Revisions

- Weeks to months

Comment response

- Days to weeks

⇨ **Modeling efficiency**

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PA Challenges: Multiple Models

Higher fidelity models for separate effects/phenomena and/or very-near field

- Cementitious material degradation
- Corrosion
- Reactive chemistry

System models for deterministic and limited sensitivity analysis

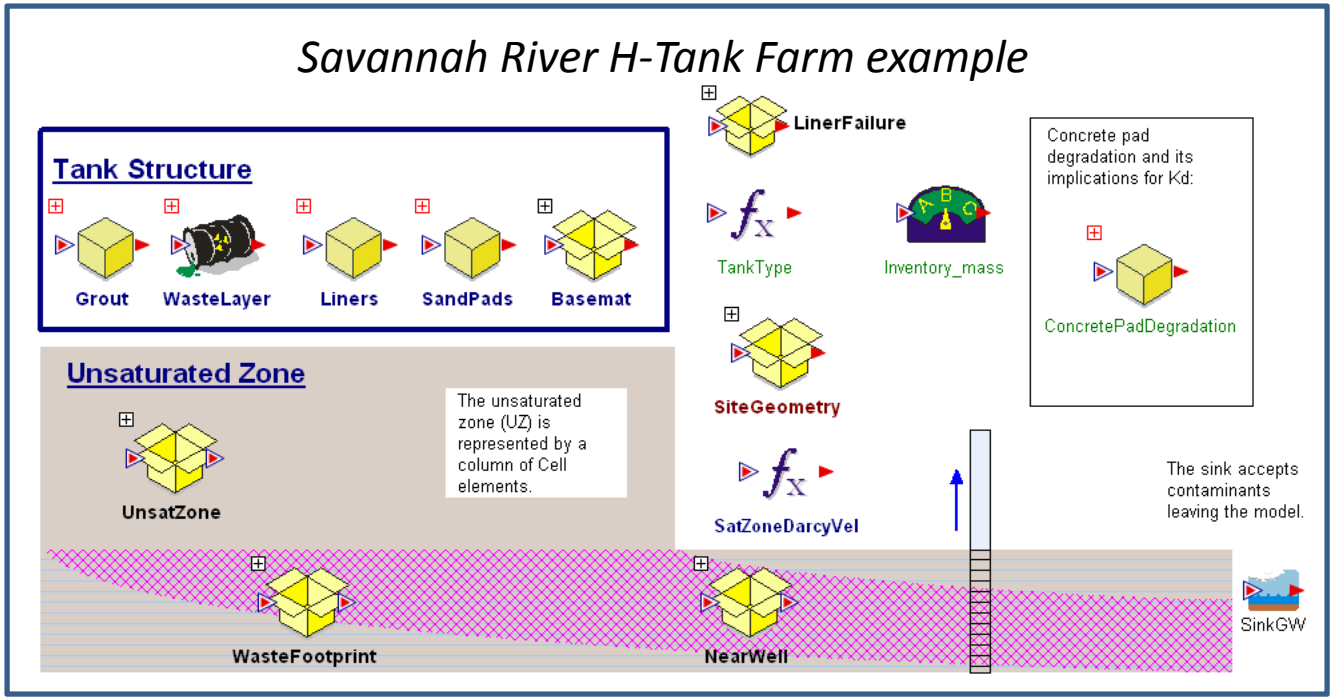
- Vadose zone / near-field
- Aquifer / far-field

Abstracted system model for sensitivity analysis and uncertainty quantification

PA Challenges: Model Abstraction

Model abstraction required for efficiency

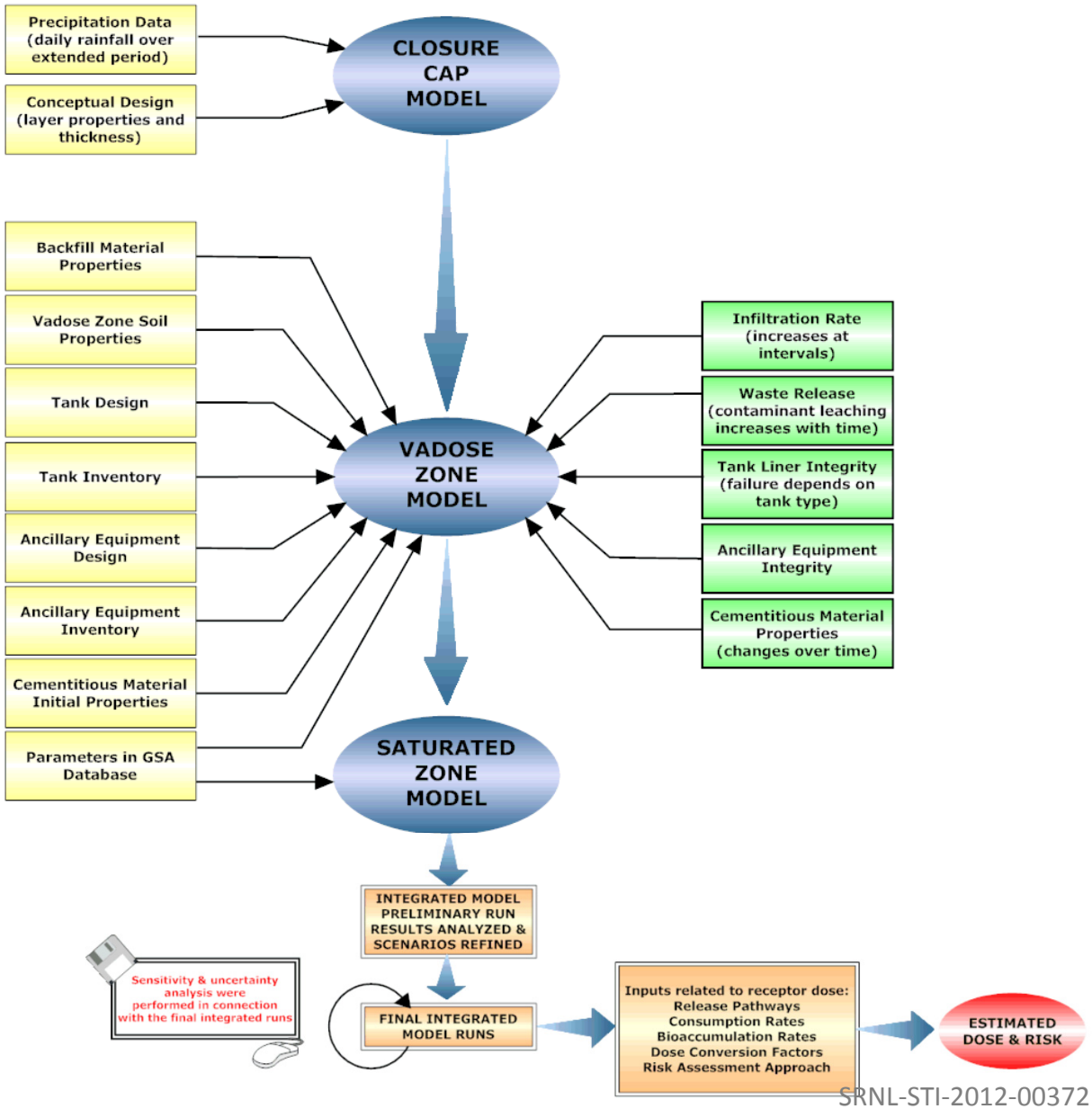
- Dimensionality: 3D → 2D → 1D
- Properties → fcn(time)
- Etc.



PA Challenges: Model Integration

Model integration

- Phenomena
- Regions
- Varying fidelity / abstraction
- Benchmarking



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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 (~FY11)
- Carbonation (~FY12)
- Fractured materials (~FY13)

Experimental data

- Property measurements
- Validation data

Probabilistic framework

- Integration with GoldSim (www.goldsim.com)

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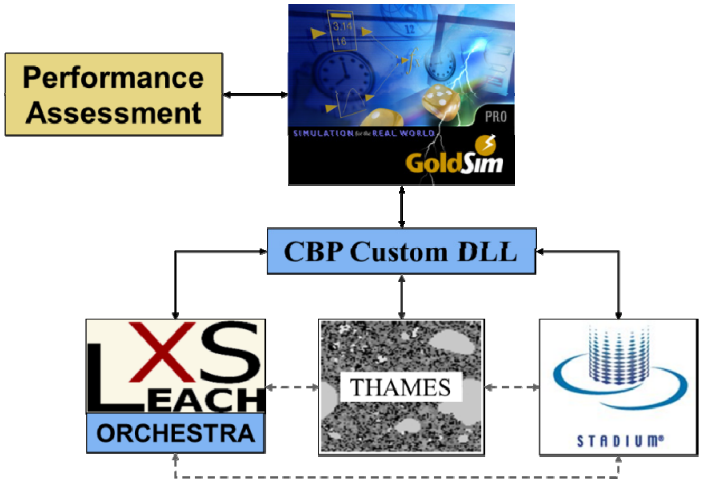
CBP Engagement with PA Process

Conceptual engagement through

- Source-term or boundary condition in near-field
  - for example, radionuclide release from waste form or through barrier
- Material property variations in space and time
  - for example, permeability
- Development of abstracted models



Software engagement through

- GoldSim interface
- Data files (for example, species flux as a function of time)

Performance Assessment Applications of CBP Toolbox Version 1.0 and Prototype Version 2.0

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2012 Hanford Workshop Feedback

Participant feedback in reference to CBP Software Toolbox version 1.0

"As tools mature, it would be beneficial to go through a real scenario on how it was used in DOE complex"

Anonymous

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General Work Scope and Progress

Phenomena	FY2010	FY2011	FY2012	FY2013	FY14 to-date
External Sulfate Attack & Primary Constituent Leaching	Priority need	LXO and Stadium development	CBP Toolbox Version 1.0; workshops	**Contractor deployment / funding**	CBP Toolbox **Version 2.0; DOE-SR/DOE-ORP user**
Carbonation	Priority need	Initial LXO development	CBP Toolbox Version 1.0; workshops	**Contractor citation**; LXO module v2	CBP Toolbox **Version 2.0;** Stadium module
Oxidation		Priority need	LXO development	LXO development; experiments	CBP Toolbox **Version 2.0;** Tc focus
Transport in Fractured Media			Priority need	Dual-regime LXO transport	CBP Toolbox **Version 2.0**
Unsaturated Hydraulic Properties of Fractured Media			Priority need	Exp. method; **Contractor funding**	Sample characterization
Damage Prediction			Priority need	Sulfate Attack	STADIUM development
Microstructure → Material Properties				Priority need	THAMES funding and scope

DOE Complex Applications

Complete (SRR):

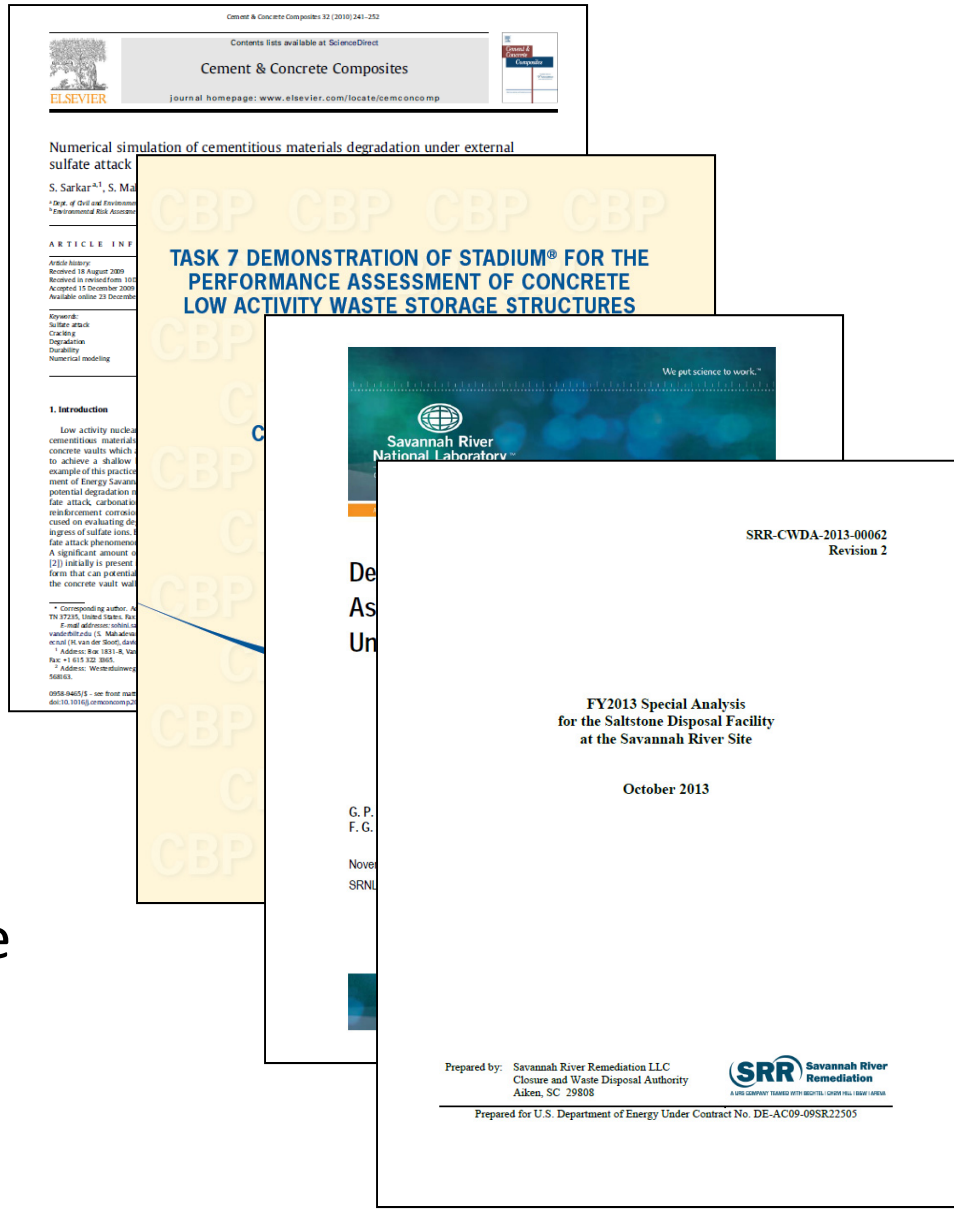
- Sulfate attack on Saltstone concrete for closure scenario

Active (DOE-SR):

- Sulfate attack on Saltstone concrete for operational scenario

Potential:

- Carbonation-influenced steel corrosion damage to concrete
- Primary constituent leaching damage to Saltstone



FY13/14 Saltstone Special Analysis

CBP: Sulfate Attack on Saltstone Concrete (CBP)

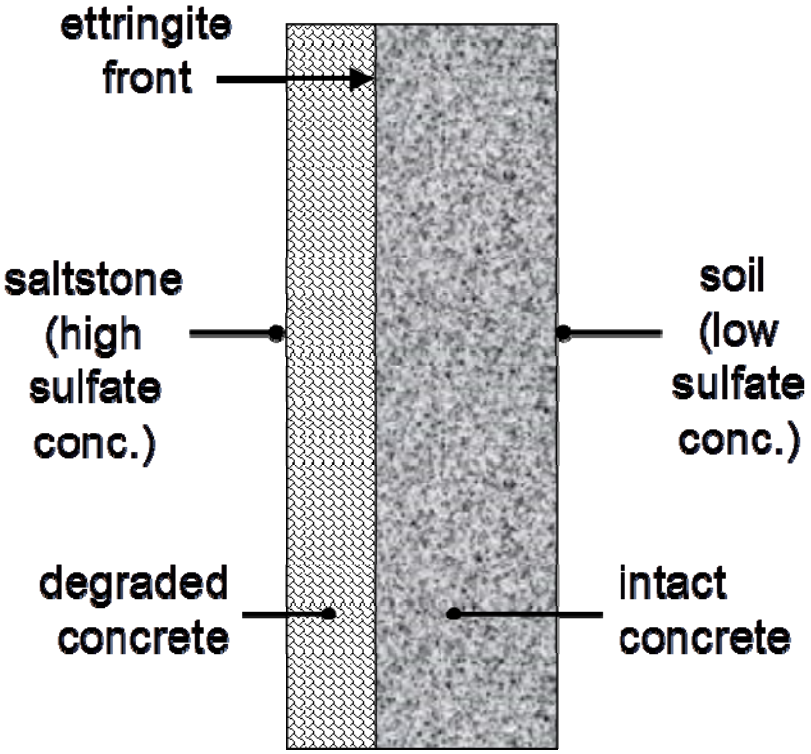
- LeachXS/Orchestra and Stadium predictions of degradation rate
- Defined times for 100% degradation (full penetration)
- Example results for Roof, Floor and Wall components:

	SDU6				SDU2				SDU4			
	Thickness:		NV	BE	Thickness:		NV	BE	Thickness:		NV	BE
Component	(in)	(cm)	(yr)	(yr)	(in)	(cm)	(yr)	(yr)	(in)	(cm)	(yr)	(yr)
Roof delay			0	0			0	0			0	0
Roof delay+degradation	12	30.48	1413	2717	8	20	961	1820	4	10	1106	7237
FloorUMM delay			0	0			0	0			0	0
FloorUMM delay+degradation	12	30.48	1413	2717	12	30	1413	2717	24	61	1404	3868
Wall 5 delay			0	0			0	0				
Wall delay+degradation	8.75	22.23	817	1937	8	20	922	1797				
Wall 4 delay			0	0								
Wall 2 delay+degradation	10.47	26.59	981	2329								
Wall 3 delay			0	0								
Wall 3 delay+degradation	13.5	34.29	1265	3021								
Wall 2 delay			0	0								
Wall 4 delay+degradation	16.55	42.04	1550	3720								
Wall 1 delay			0	0								
Wall 5 delay+degradation	19.5	49.53	1827	4397								

FY13/14 Saltstone Special Analysis

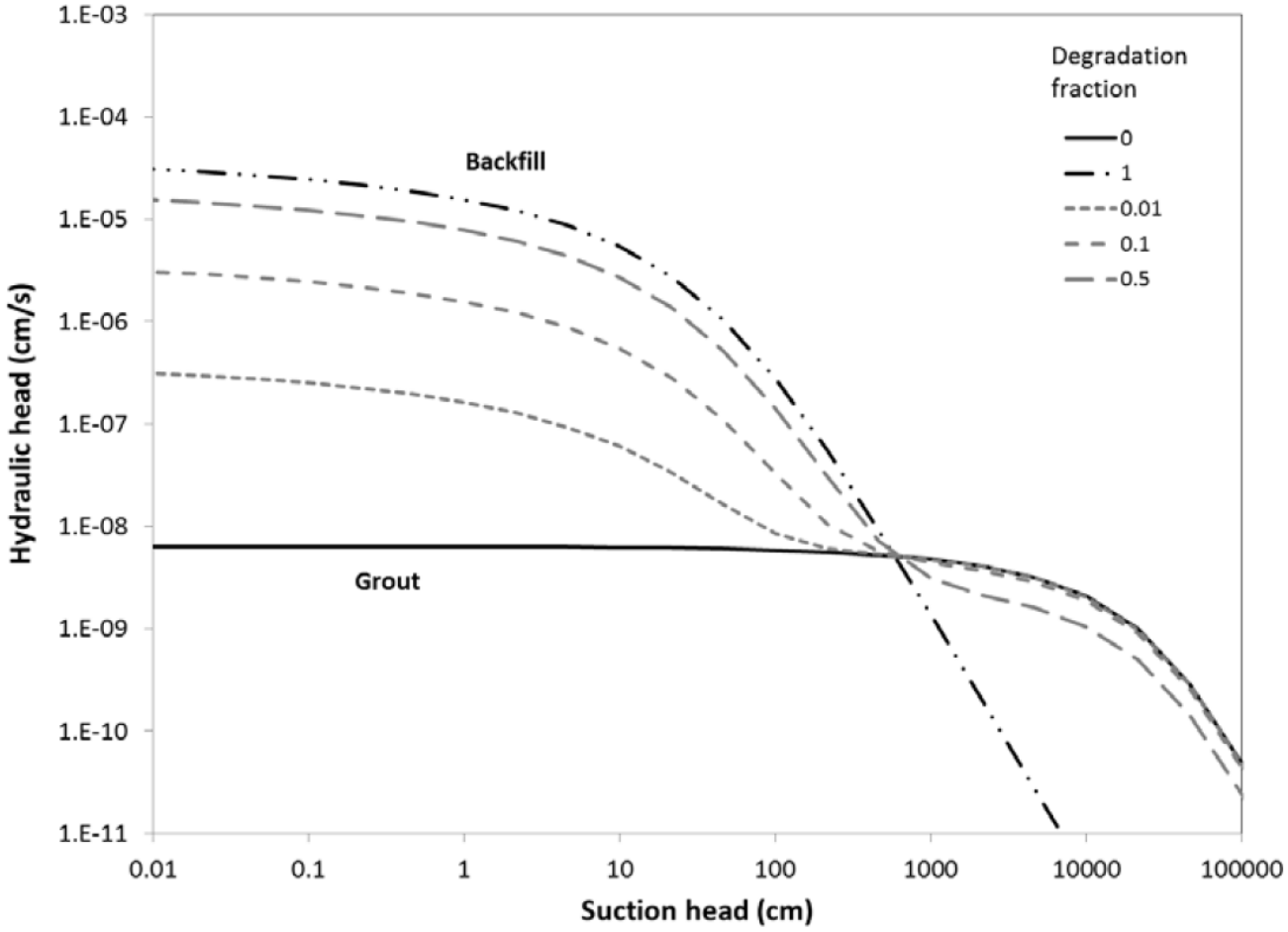
Contractor: Effective Hydraulic Properties of Concrete

- 0% and 100% degradation times defined from CBP analysis
- 100% degradation defined as degradation to a soil-like condition
- Effective hydraulic properties defined by arithmetic averaging based on degraded and intact thicknesses
  - conservative-tending
  - harmonic average alternative



FY13/14 Saltstone Special Analysis

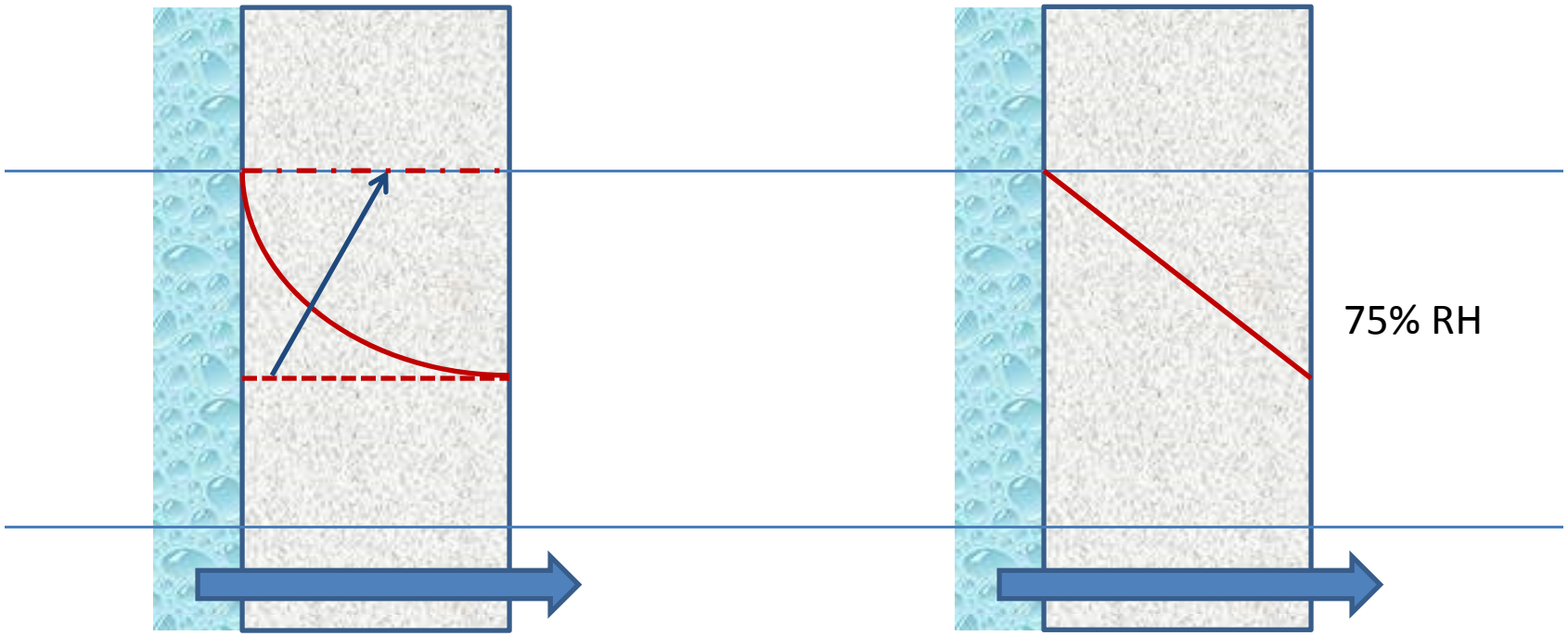
Arithmetic Averaging = Equivalent Continuum Model



Active: Operational Scenarios

Influence of capillary flow driven by

- Initially unsaturated concrete exposed to bleedwater and/or fresh grout
- Concrete exterior exposed to atmosphere



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Summary

- **CBP data and software are designed to address PA challenges arising from**
  - **Long time frames**
  - **Cementitious material degradation**
  - **Uncertainty**
  - **Computing and schedule limitations**
- **CBP software tools can engage the PA process in multiple ways**
  - **Provide higher fidelity models for particular phenomena**
  - **Support model abstraction**
- **CBP tools are 'GoldSim-ready'**