SAVANNAH RIVER NATIONAL LABORATORY
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# Integration of System Components and Phenomena through Multiscale Modeling and Abstraction: Savannah River Examples

Greg Flach

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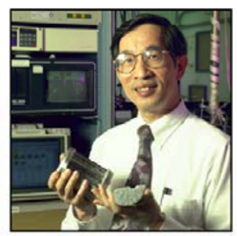
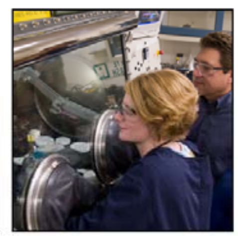
Salt Lake City



**Performance Assessment Community of Practice Technical Exchange Meeting**

Modeling the Performance of Engineered Systems for Closure and Near-Surface Disposal

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# Integration Challenges

- Multiple scales
  - groundwater plume (~100 m)
  - vadoze zone (~10 m)
  - components of engineered system (~0.1 to 1 m)
  - smaller features such as fractures, aggregates, pores (<0.1 m)
- Multiple phenomena (complex / demanding)
  - physical
  - chemical

Difficult to incorporate all scales & phenomena into single model

# Integration Approaches

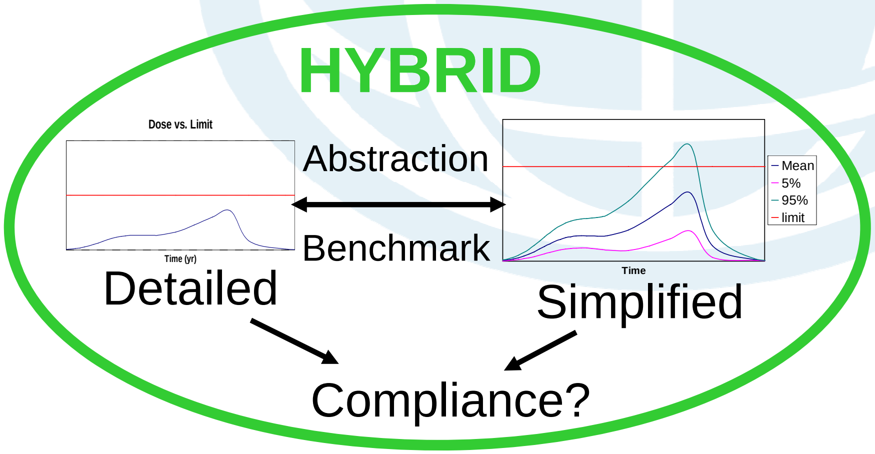
- Couple multiple models
  - various scales and phenomena
  - coupling can be loose or tight
- Abstract or simplify full physics models, e.g.
  - apparent Kd
  - effective hydraulic properties
  - response surface / table
  - analytic approximation
  - lower dimensionality

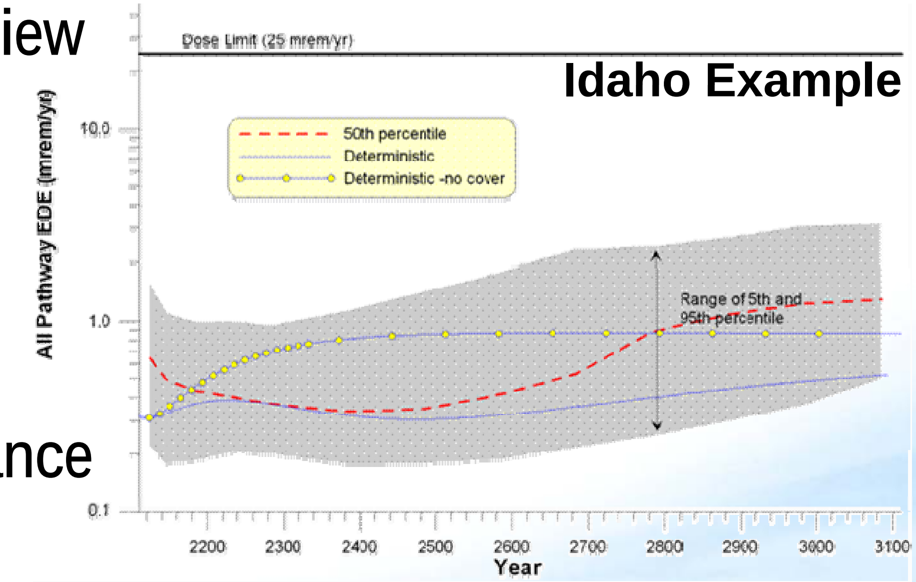
# Typical PA Modeling Practice at Savannah River

- Vadose Zone (2D near field) and Aquifer (3D far field) models for flow and transport
- Single-domain porous medium formulation
  (e.g. fractures / cracks treated as sand or gravel seam)
- Auxiliary analysis of geochemical environment
  (e.g. GeoChemist's Workbench)
- Kd w/o or w/ solubility limits
  - value based on pH and Eh regimes
  - timing based on pore volumes flushed
- More abstractions for probabilistic analysis

# PA Practice - Sensitivity and Uncertainty Analysis

- Deterministic sensitivity calculations for specific cases
- Deterministic model abstracted for probabilistic analysis
- Probabilistic analysis used to provide more comprehensive view of sensitivity/uncertainty
- Hybrid approach combining detailed deterministic and simplified probabilistic models provides useful check and balance and multiple lines of reasoning

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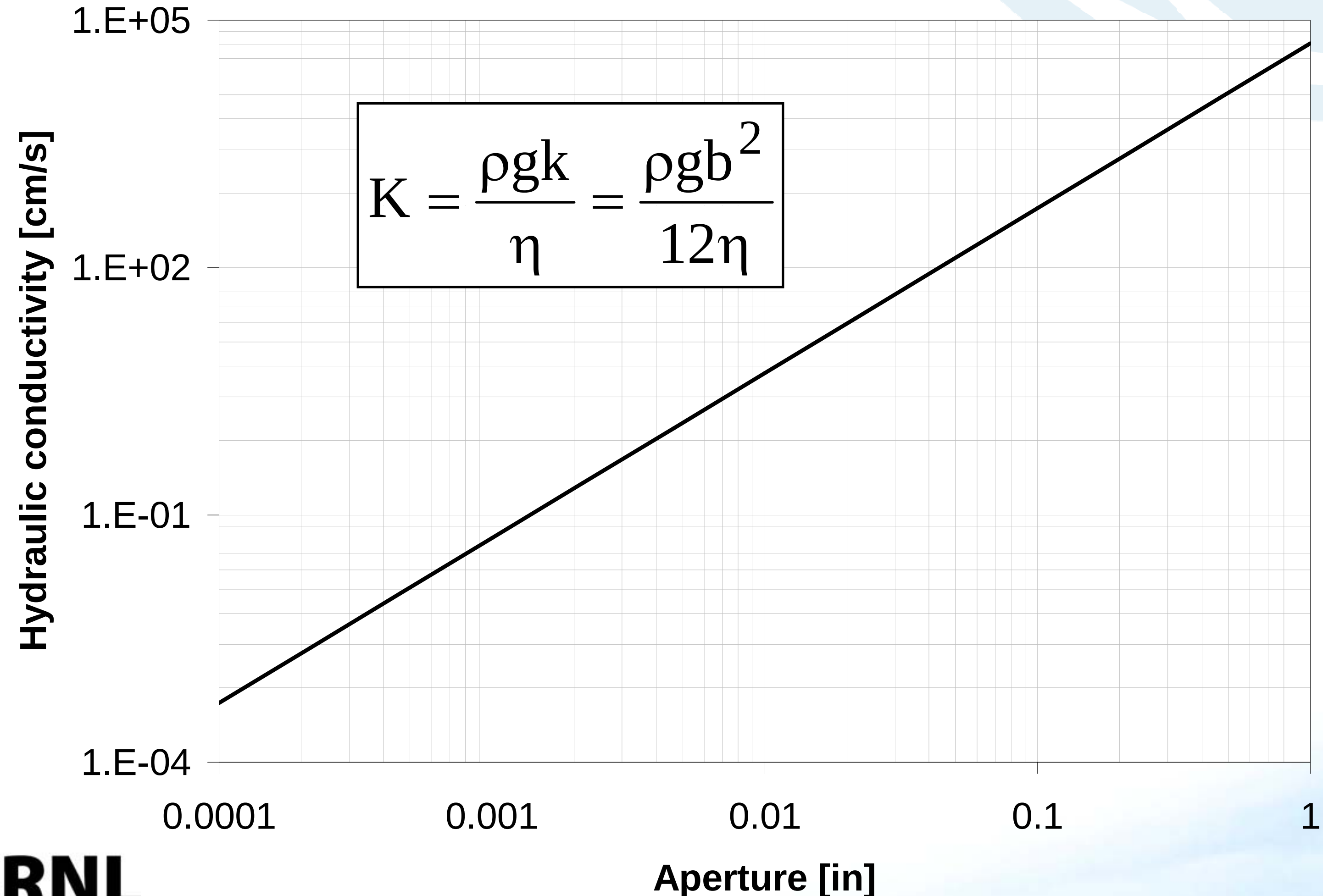
# Some Better Examples of Abstraction and Coupling

- Effective properties of cracked concrete under unsaturated conditions - 2009 Saltstone PA (draft)
- Abstraction of ~full physics external sulfate attack model - 2009 Saltstone PA (draft)
- Small scale diffusion from concrete rubble coupled to larger scale vadose zone transport - 2005 E-area Special Analysis (SA)

# Effective Hydraulic Properties of Cracked Concrete

**Saturated fracture:**

Fractures typically dominate saturated transport




$$K = \frac{\rho g k}{\eta} = \frac{\rho g b^2}{12\eta}$$

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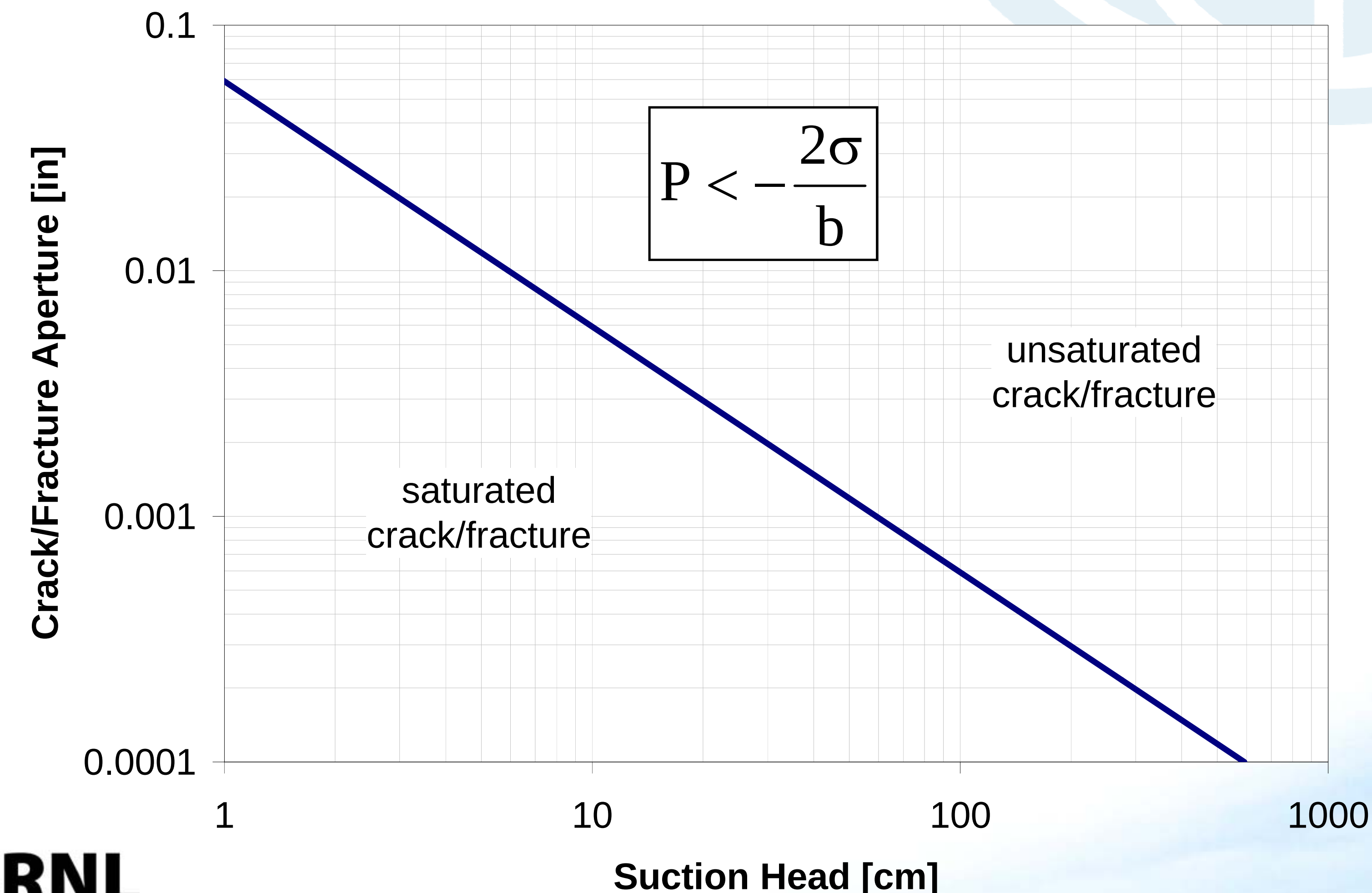
# Effective Hydraulic Properties of Cracked Concrete

**Unsaturated fracture:** Fractures typically "dewater" at low suctions

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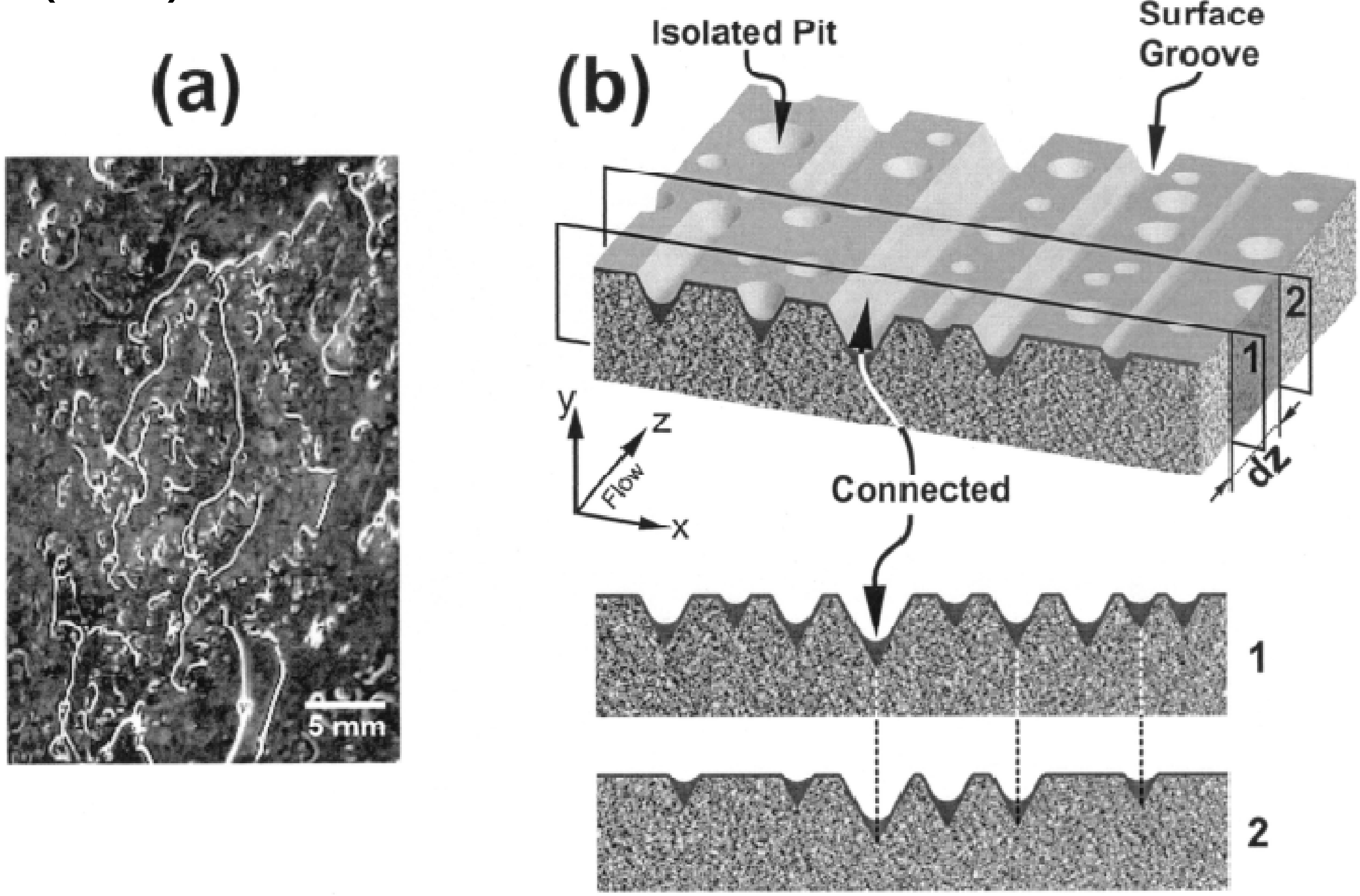
# Effective Hydraulic Properties of Cracked Concrete

Or and Tuller (2000):

a) Wet fracture surface of Apache Leap Tuff (Arizona)

b) Idealized geometry




WATER RESOURCES RESEARCH, VOL. 36, NO. 5, PAGES 1165–1177,

# Effective Hydraulic Properties of Cracked Concrete

Or and Tuller (2000) continued:

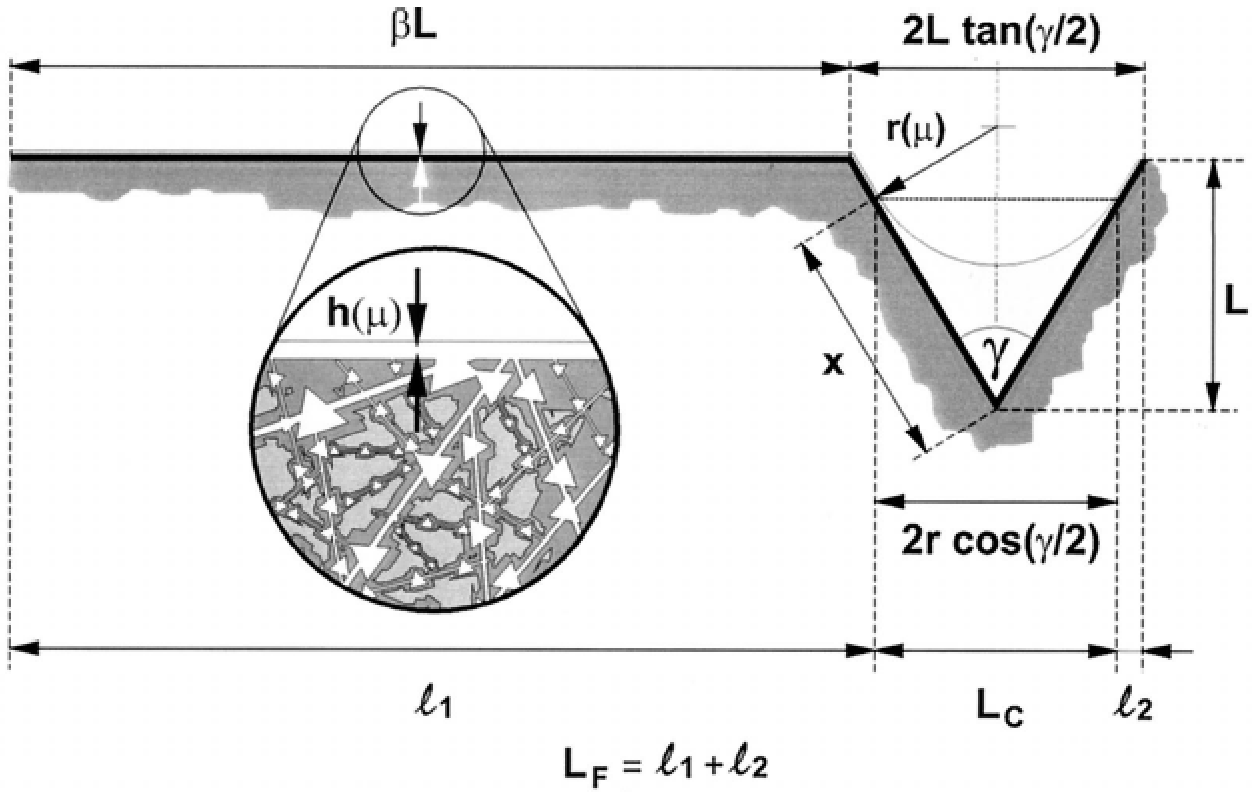


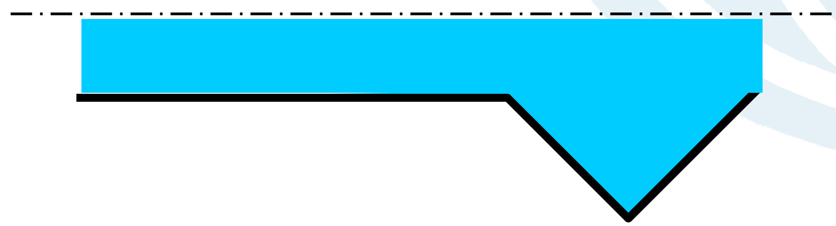

**Figure 1.** Definition sketch for a unit element representing unsaturated fracture surface with a single pit of depth $L$ and angle $\gamma$. Liquid-vapor interfaces are functions of the matric potential $\mu$, which determines the radius of curvature in the pit $r(\mu)$ and film thickness $h(\mu)$. The inset represents the partially saturated porous rock matrix forming the fracture; water in the rock matrix pore space is in equilibrium with water on the fracture surface.

# Effective Hydraulic Properties of Cracked Concrete

Three flow regimes:

Saturated flow

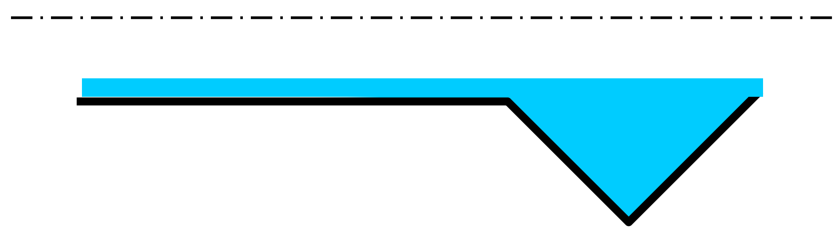
$$P > -\frac{2\sigma}{b}$$



Water filled fracture

Thick film flow

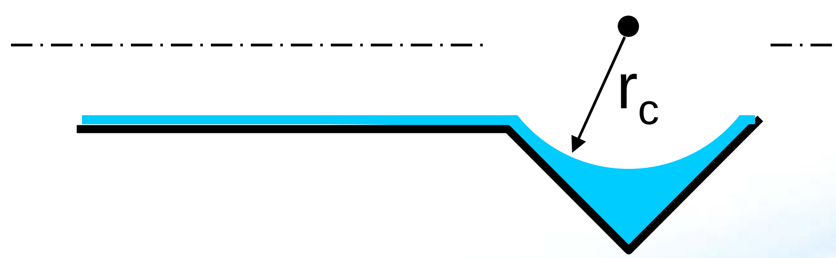
$$-\frac{\sigma}{r_c} < P < -\frac{2\sigma}{b}$$



Water filled groove

Thin film flow

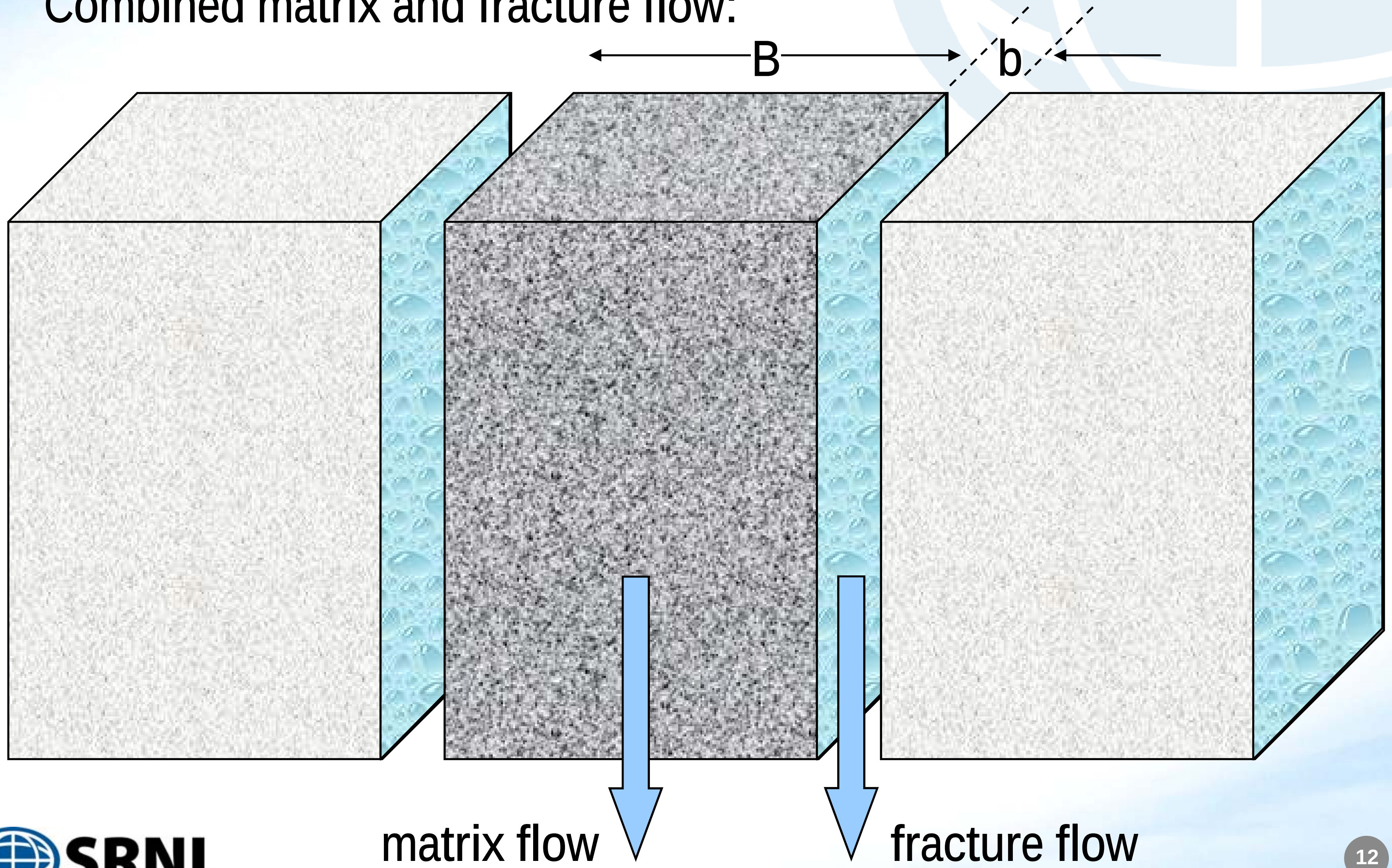
$$P < -\frac{\sigma}{r_c}$$




Water recedes into groove

# Effective Hydraulic Properties of Cracked Concrete

Combined matrix and fracture flow:

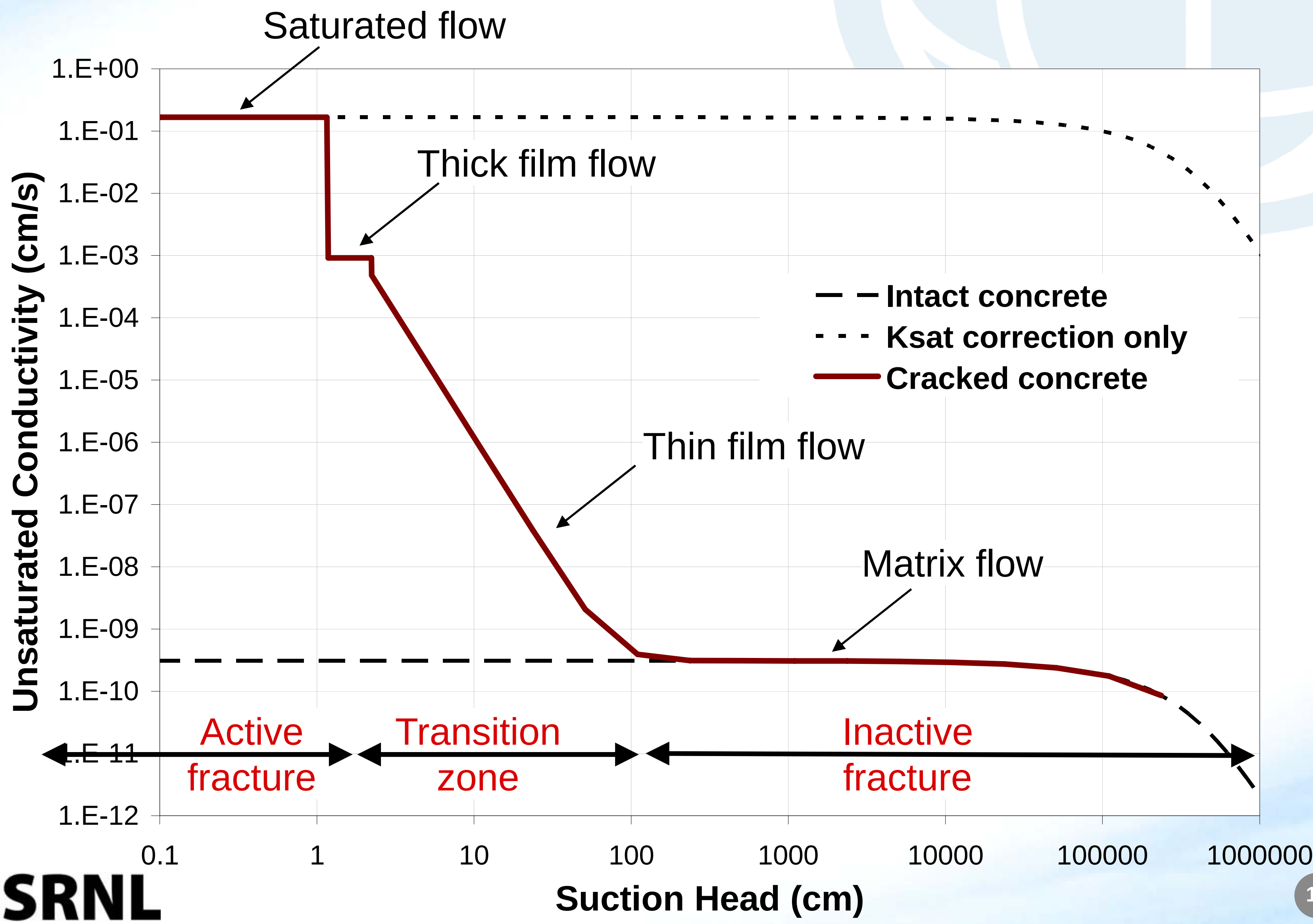


# Effective Hydraulic Properties of Cracked Concrete

Example crack parameters

| Parameter | Symbol (Or and Tuller 2000) | Value | Units |
|---|---|---|---|
| ratio of pit spacing to pit depth | *b* | 1 | unitless |
| pit connectivity factor | *δ* | 1 | unitless |
| pit angle | *γ* | 60 | deg |
| pit depth | *L* | 5.0E-04<br>0.500<br>0.020 | m<br>mm<br>in |
| width of unit element | *W* | 1.08E-03 | m |
| aperture | b | 1.27E-03<br>0.05<br>50<br>1.27<br>1270 | m<br>in<br>mil<br>mm<br>micron |
| spacing between fractures | *B* | 1<br>100 | m<br>cm |
| saturated matrix conductivity | *K* | 3.1E-12<br>3.1E-10 | m/s<br>cm/s |

# Effective Hydraulic Properties of Cracked Concrete

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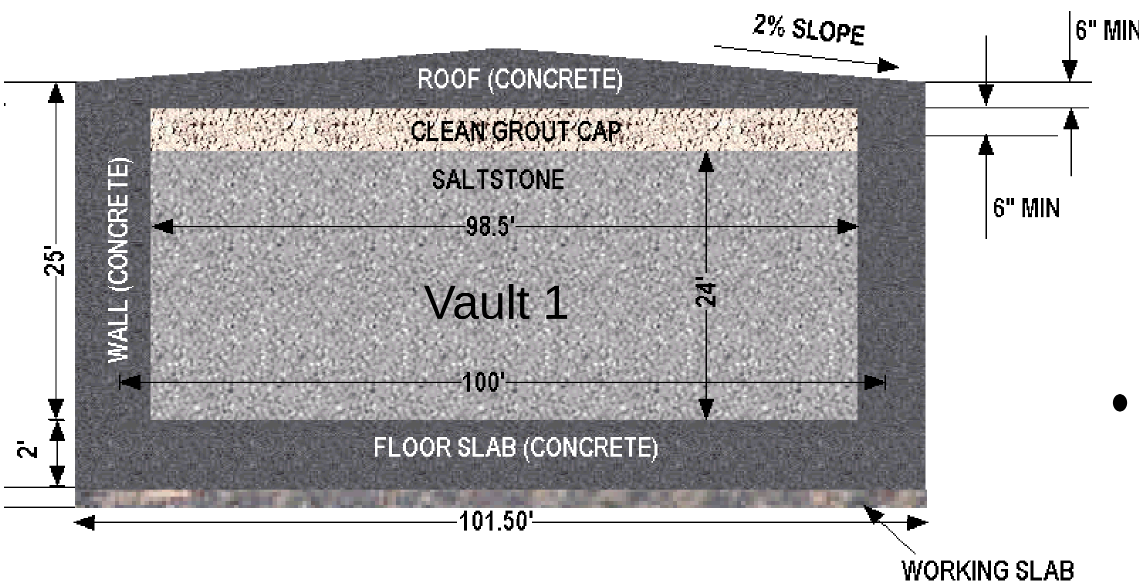
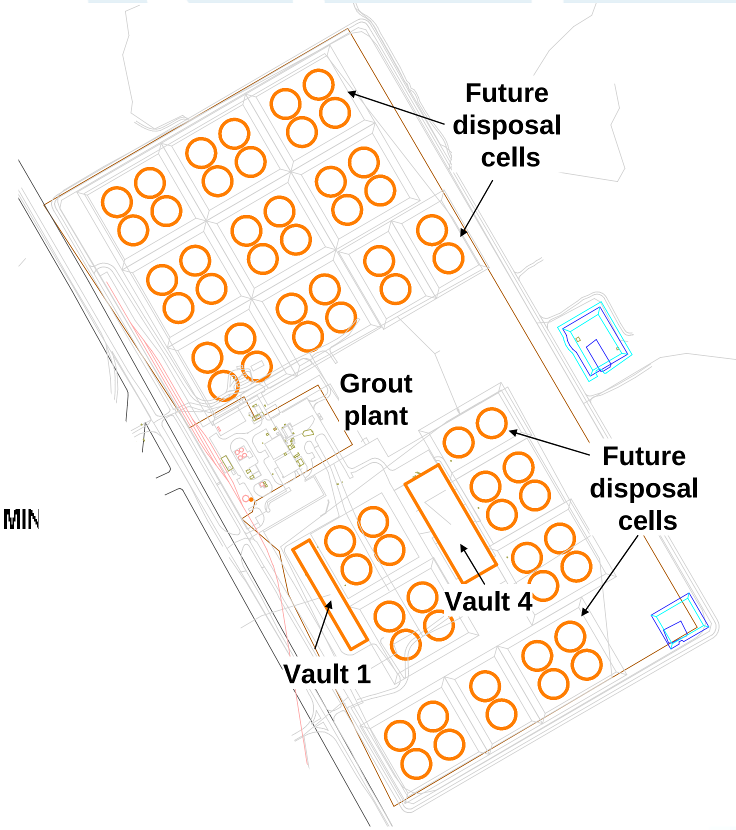
# External Sulfate Attack on Concrete Barrier

Saltstone Facility:

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



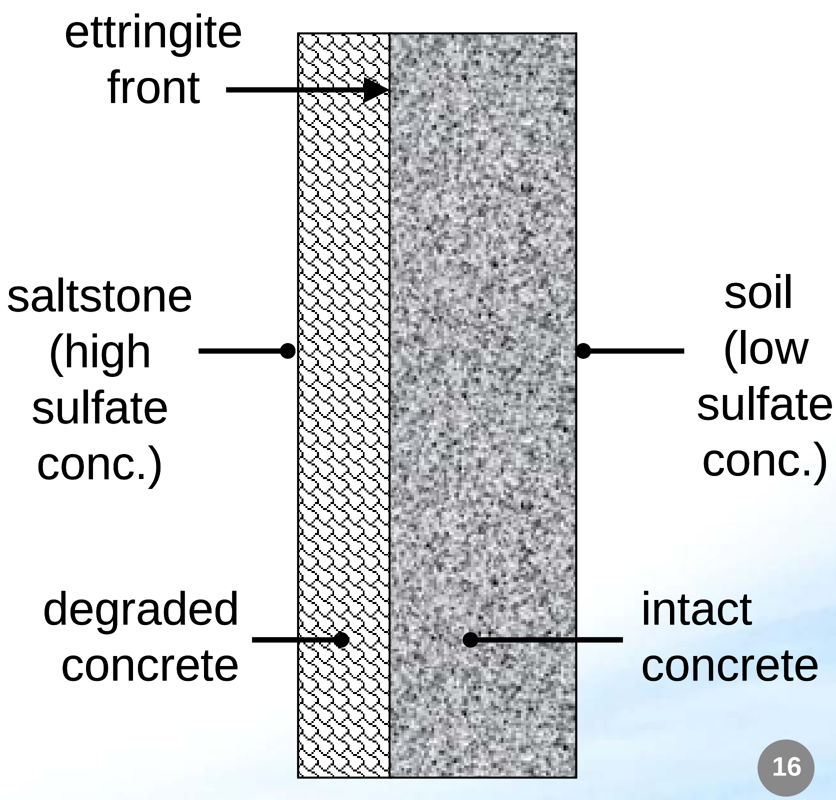




- Sulfate attack identified as primary concrete degradation mechanism

# External Sulfate Attack on Concrete Barrier

Approach:

- STADIUM® code used to predict formation of ettringite (coupled chemistry and transport analysis of major dissolved and solid species)
- Simple damage model (baseline)
  - Ettringite = physical damage (e.g. cracking, spalling)
  - Transport properties not affected by ettringite front
- Effective hydraulic properties by averaging



# External Sulfate Attack on Concrete Barrier

STADIUM® code:

- Multi-ionic transport model based on a split operator approach that separates ionic movement and chemical reactions
- Ionic transport is described by the extended Nernst-Planck equation applied to unsaturated media
- Accounts for the electrical coupling between ionic species, chemical activity, transport due to water content gradient, and temperature effects
- http://www.mslexperts.com/slm/stadium_help/index.html for more information

# External Sulfate Attack on Concrete Barrier

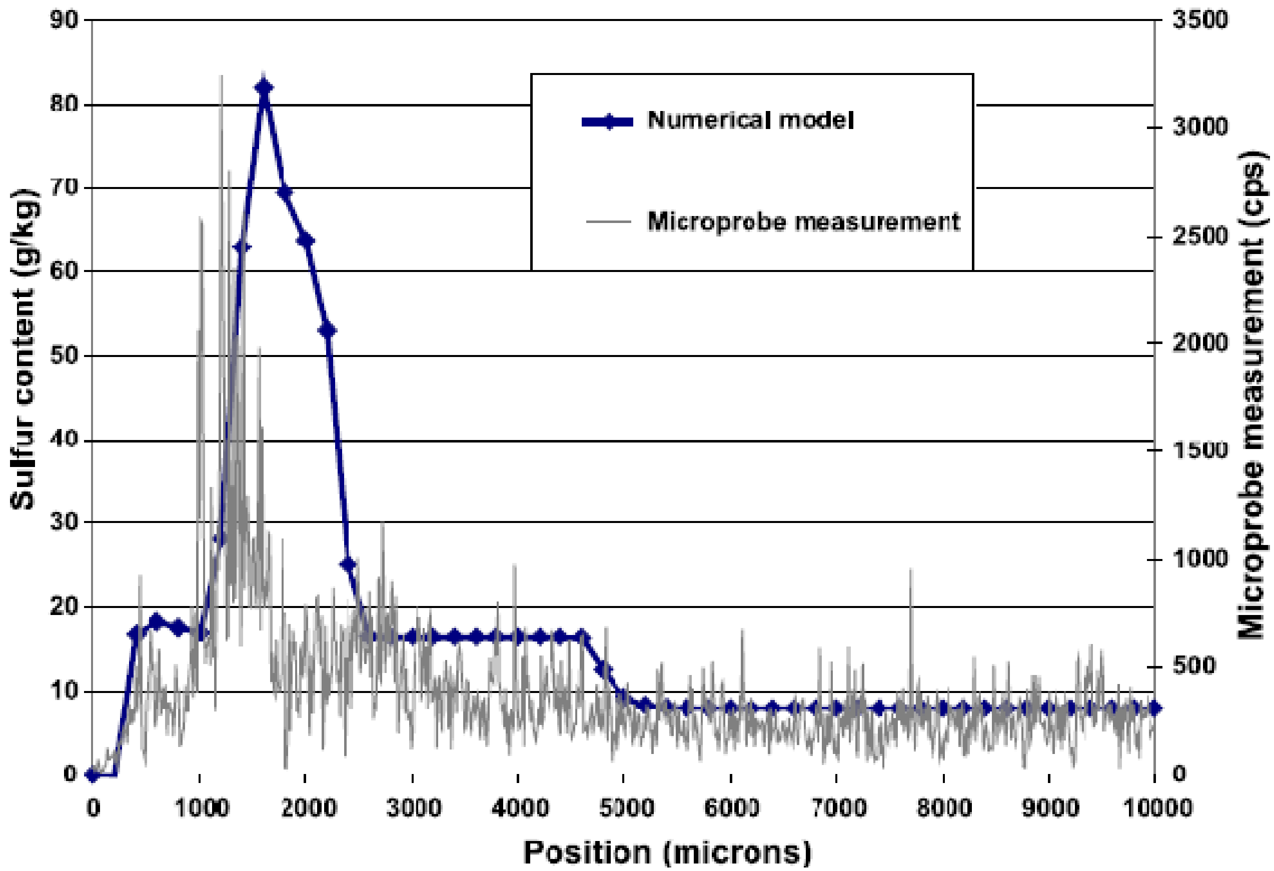
STADIUM® validation:
Maltais, Samson and Marchand (2004)

CSA Type 10
w/c 0.60

3 month exposure

0.05 mol/L
$Na_2SO_4$

saturated
conditions




Cement and Concrete Research 34 (2004) 1579–1589

# External Sulfate Attack on Concrete Barrier

Abstraction:

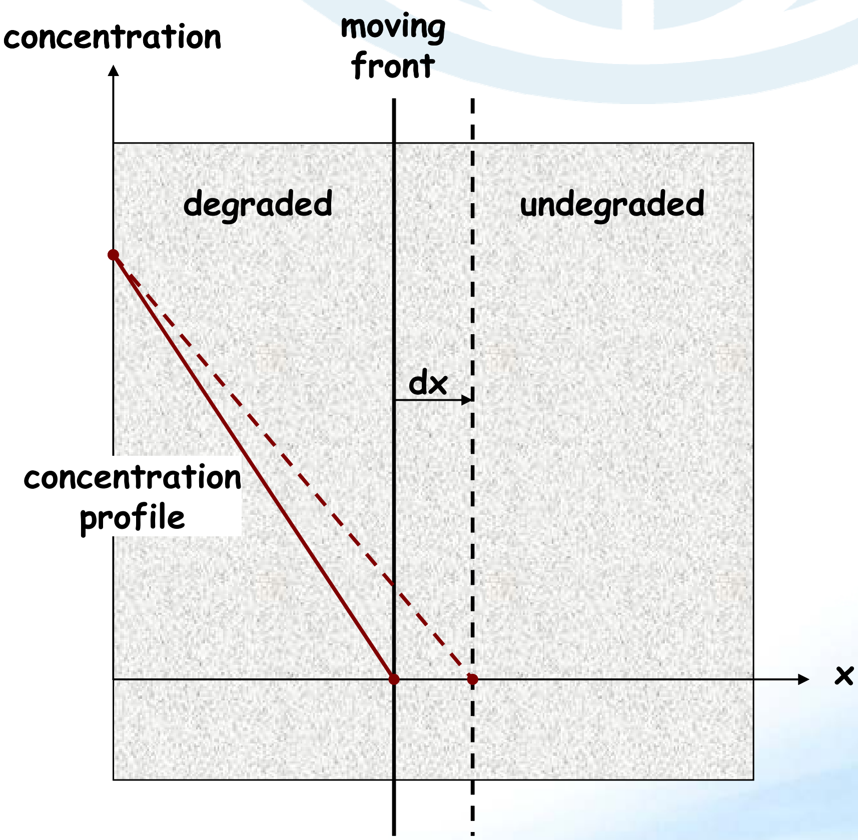
- Ettringite formation controlled by reaction capacity of concrete, R, and diffusion to front

$$R\frac{dx}{dt} = \frac{nD_e c}{x}$$

reactant consumption rate — reactant delivery rate

- Analytic solution for ettringite front

$$x = \left[\frac{2nD_e ct}{R}\right]^{1/2}$$

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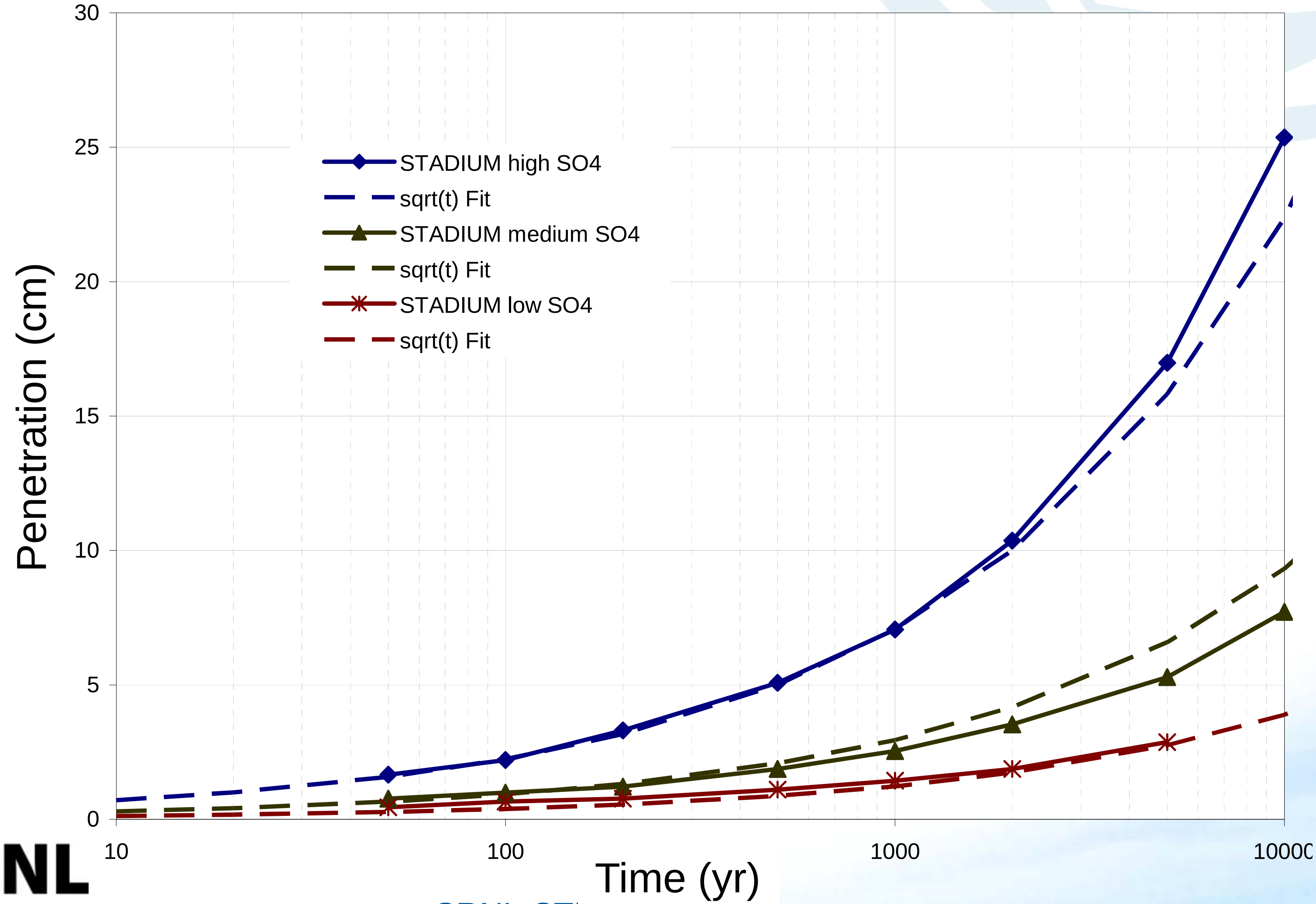
# External Sulfate Attack on Concrete Barrier

Deduce reaction capacity from full-physics STADIUM simulation:

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# External Sulfate Attack on Concrete Barrier

Generalize for varying conditions:

- Lump fixed parameters

$$x = Ac^B \sqrt{\frac{D_e}{D_{ref}}} \sqrt{t}$$

- Assume time-dependent parameters in penetration rate

$$\frac{dx}{dt} = Ac(t)^B \sqrt{\frac{D_e(t)}{D_{ref}}} \frac{1}{2\sqrt{t}}$$

- Integrate (numerically in practice)

$$x = \int_0^T Ac(t)^B \sqrt{\frac{D_e(t)}{D_{ref}}} \frac{1}{2\sqrt{t}} dt$$

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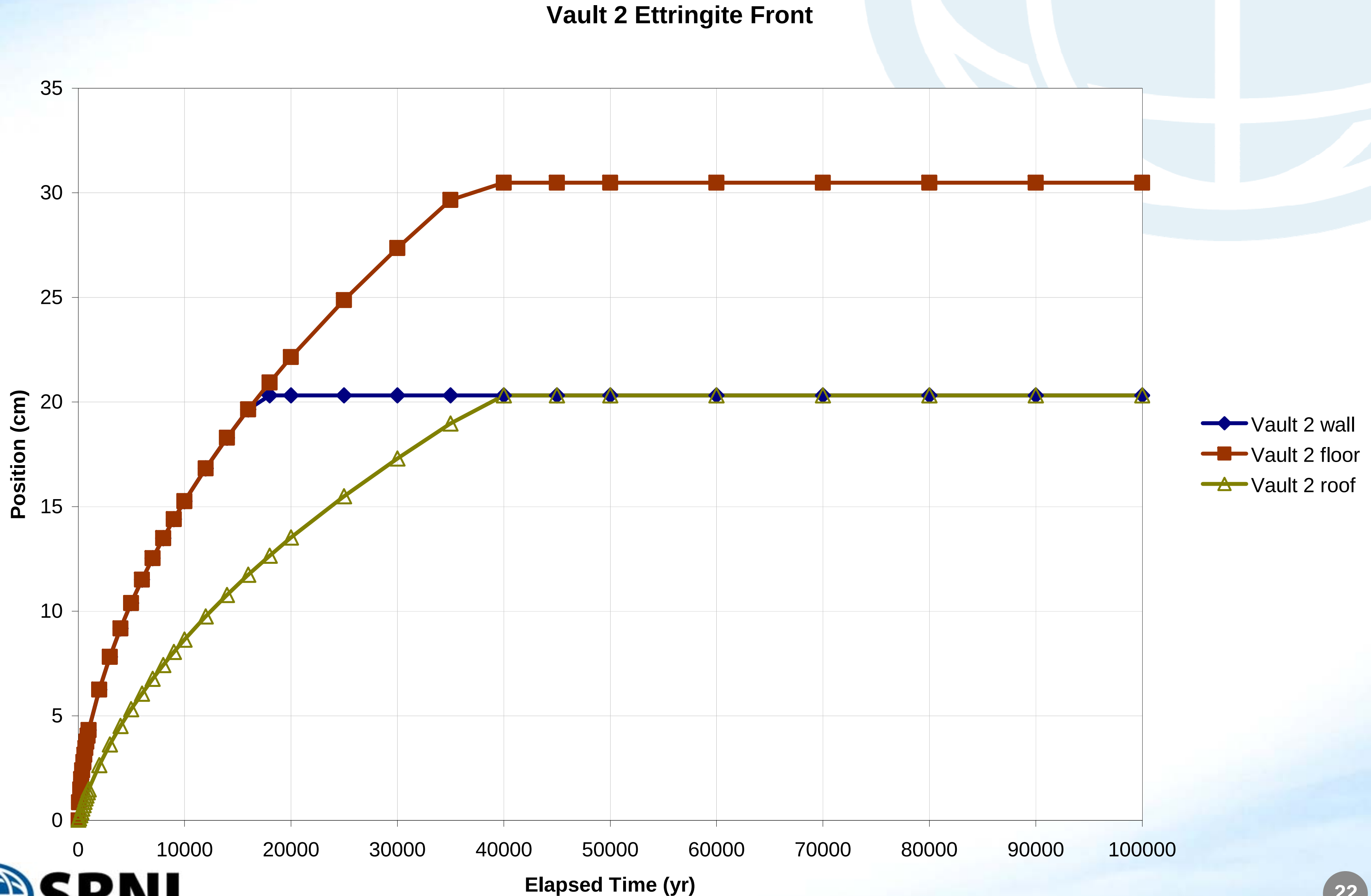
# External Sulfate Attack on Concrete Barrier

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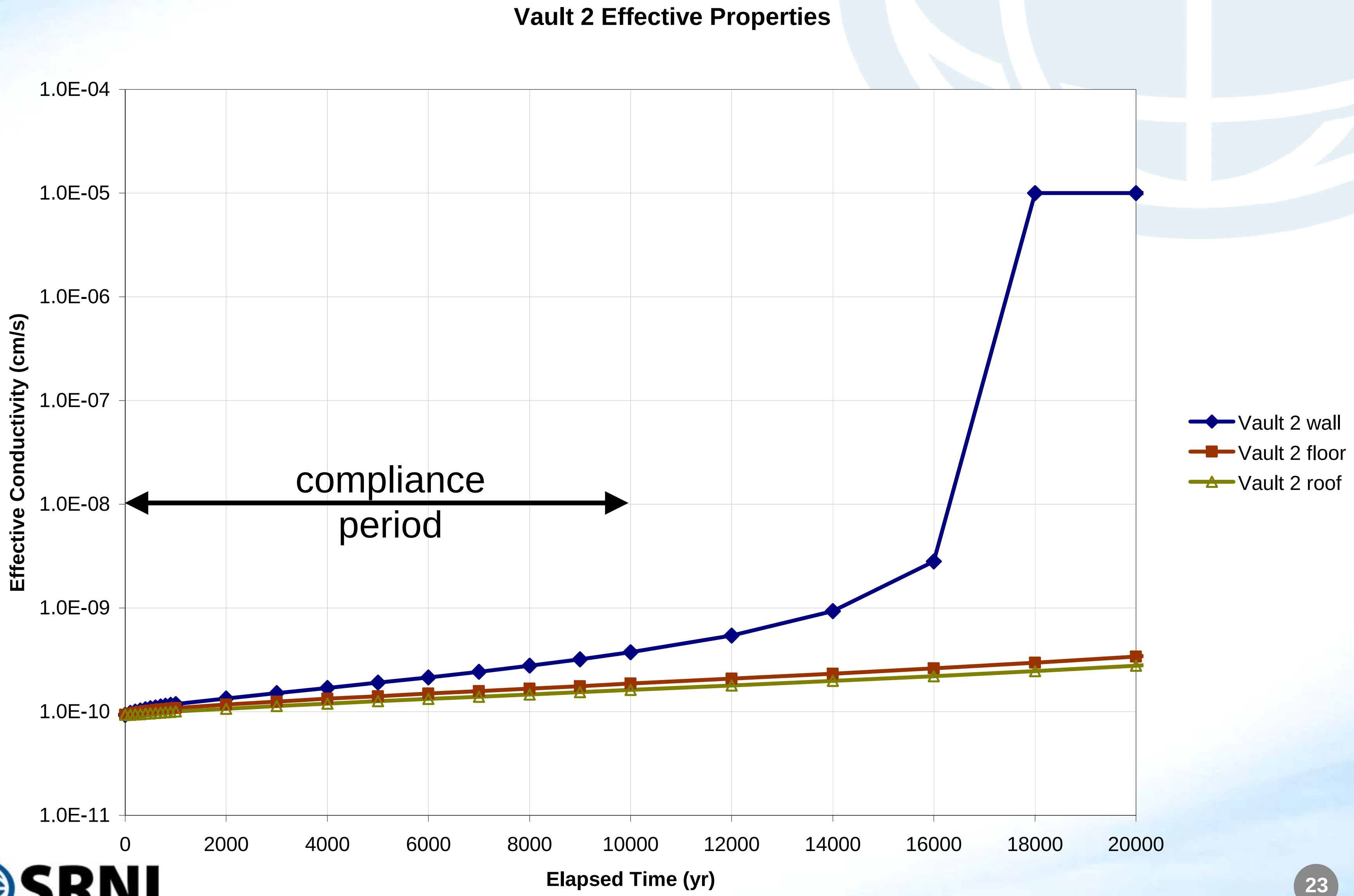
# External Sulfate Attack on Concrete Barrier



# Multiscale Solute Transport from Concrete Rubble

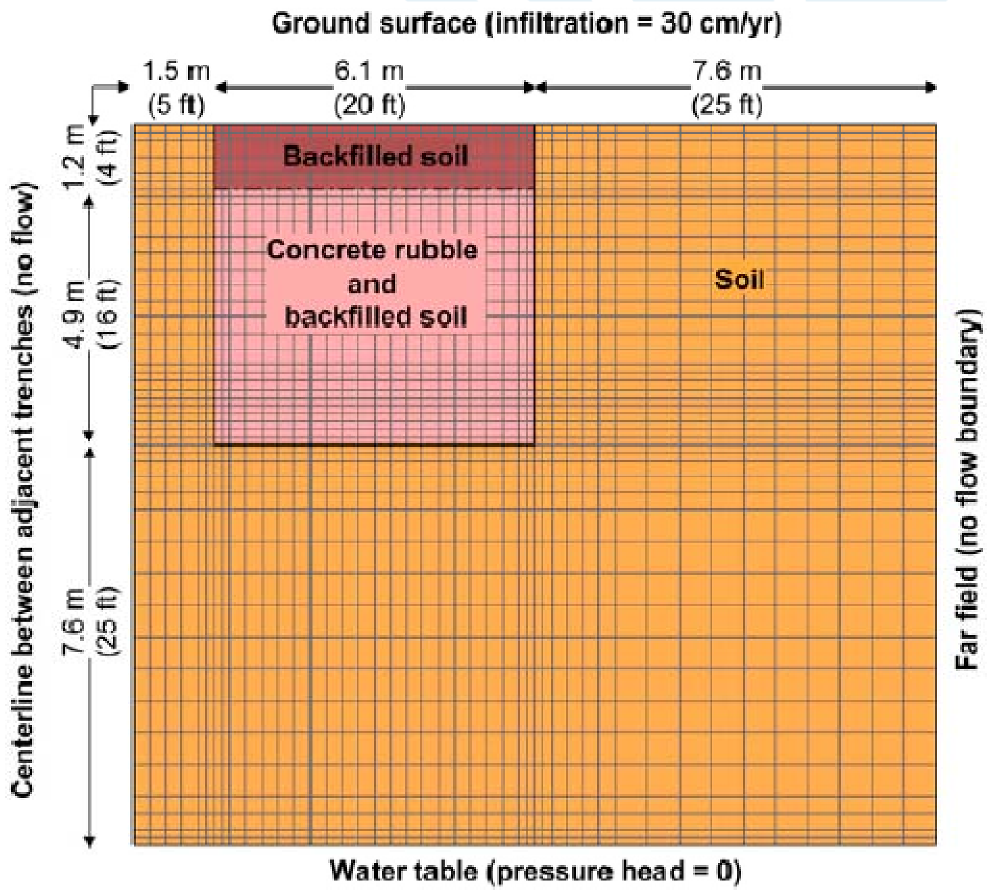
Building 232-F rubble:

- Former tritium extraction facility
- D&D produced concrete rubble contaminated with HTO moisture
- Onsite disposal in E-area Slit Trenches
- Accurate analysis needed to show compliance with performance objectives


# Multiscale Solute Transport from Concrete Rubble

Disposal trench:

- Heterogeneous mixture of coarse aggregate sizes, shapes, and internal tritium distributions
- Diffusional release from concrete to backfilled soil (~ 0.1 m length scale)
- Advective transport from soil to water table (~ 10 m length scale)

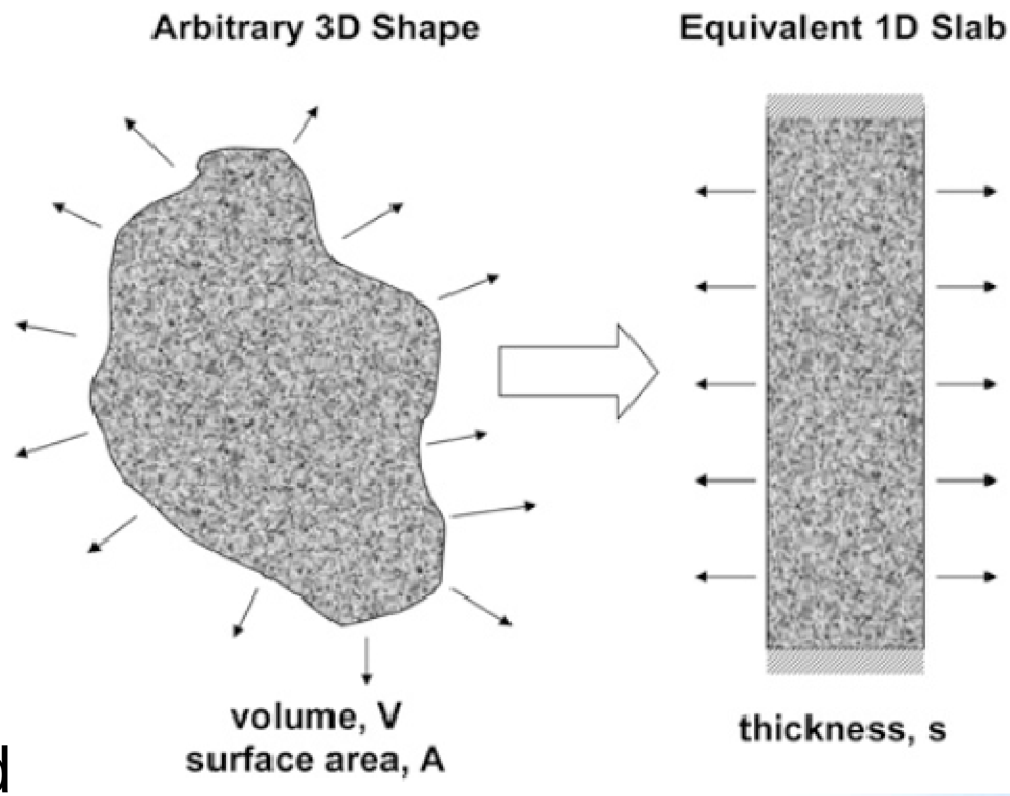


# Multiscale Solute Transport from Concrete Rubble

"Unsteady" dual-porosity formulation:

- 1D slab surrogate for 3D coarse aggregate
- 1D diffusion in immobile domain (concrete slab)
- 2D advection / dispersion in mobile domain (soil)
- Iterative coupling through soil concentration C(t) and waste flux F(t)

(geometric abstraction)




Vadose Zone J. 6:336–343
doi:10.2136/vzj2006.0051

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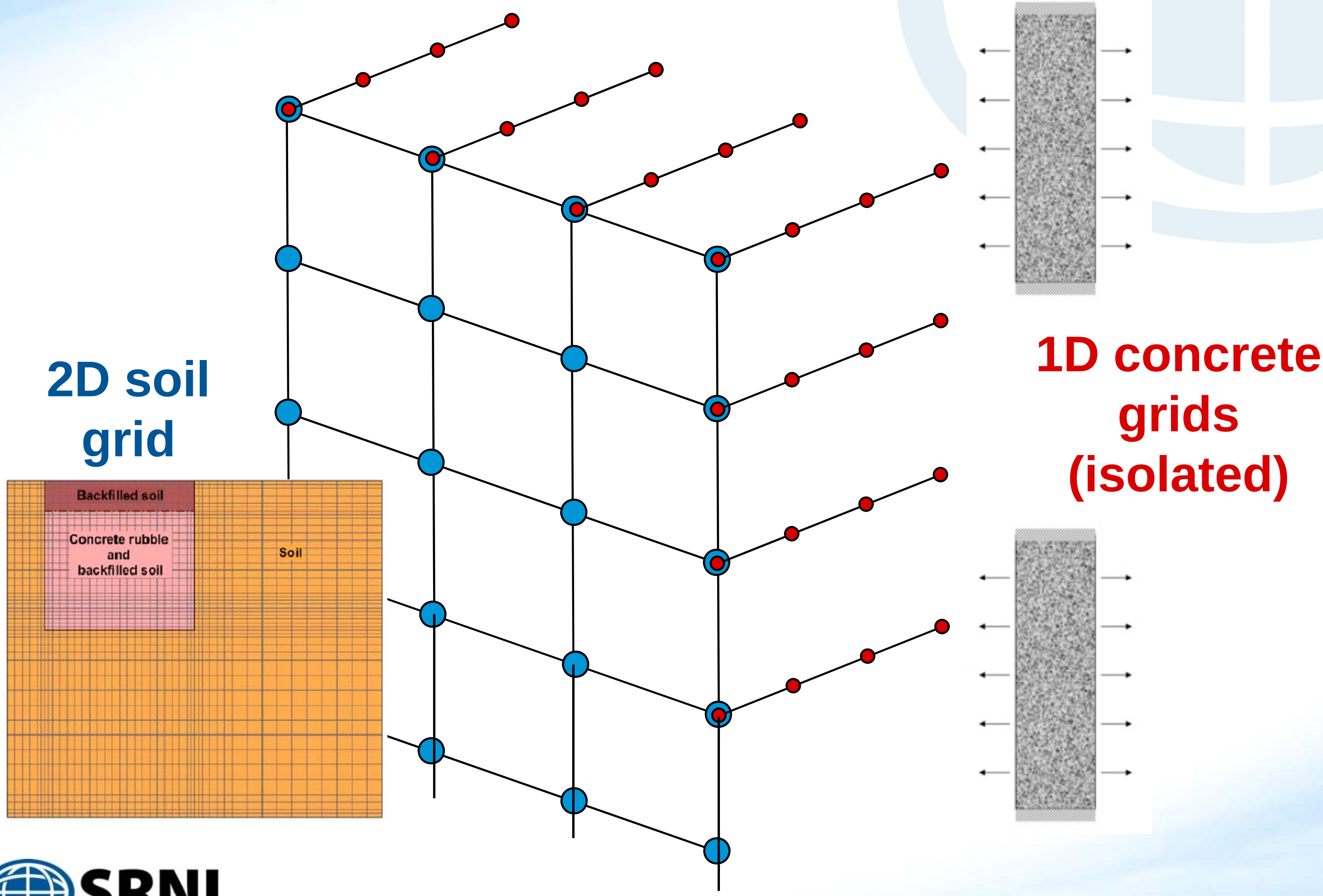

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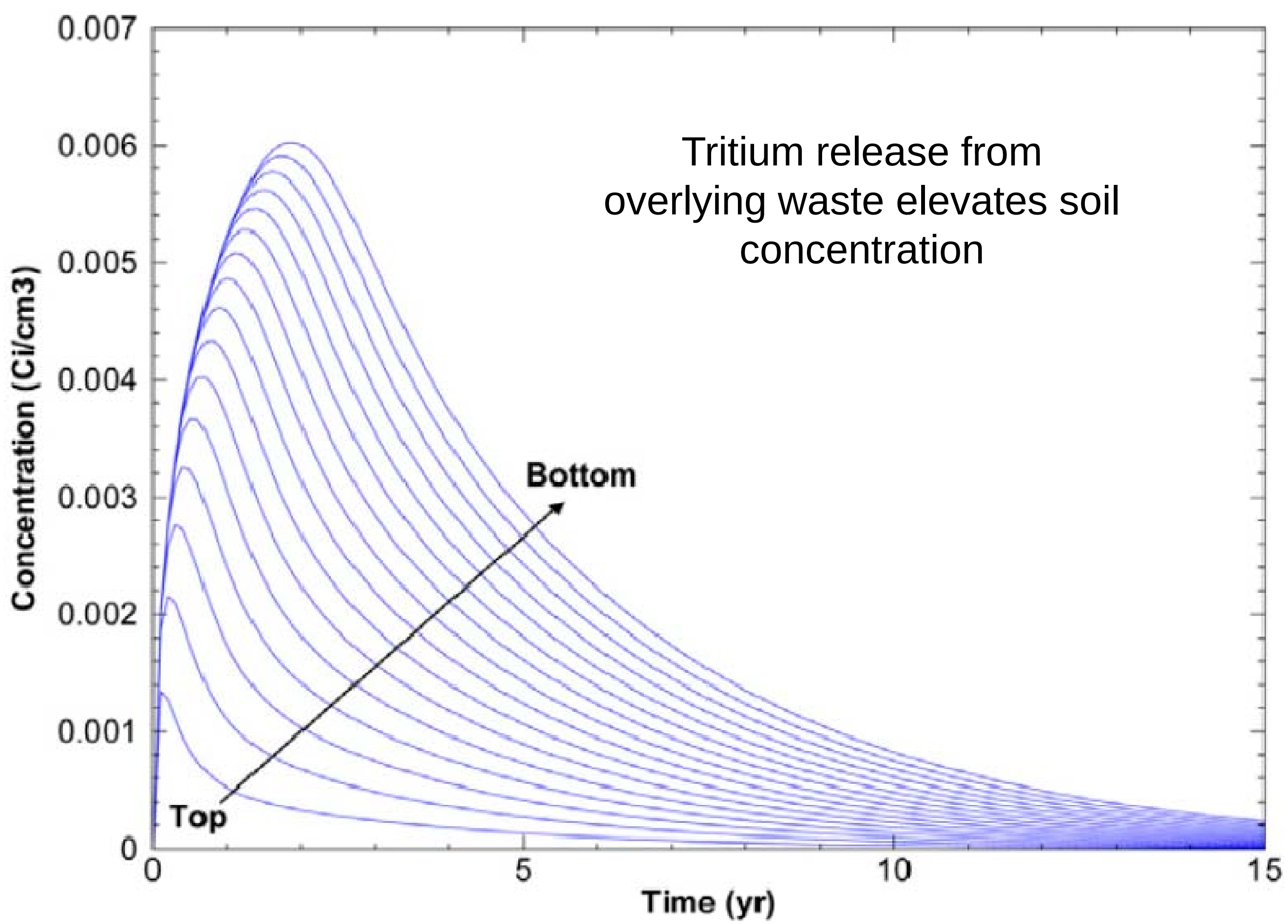

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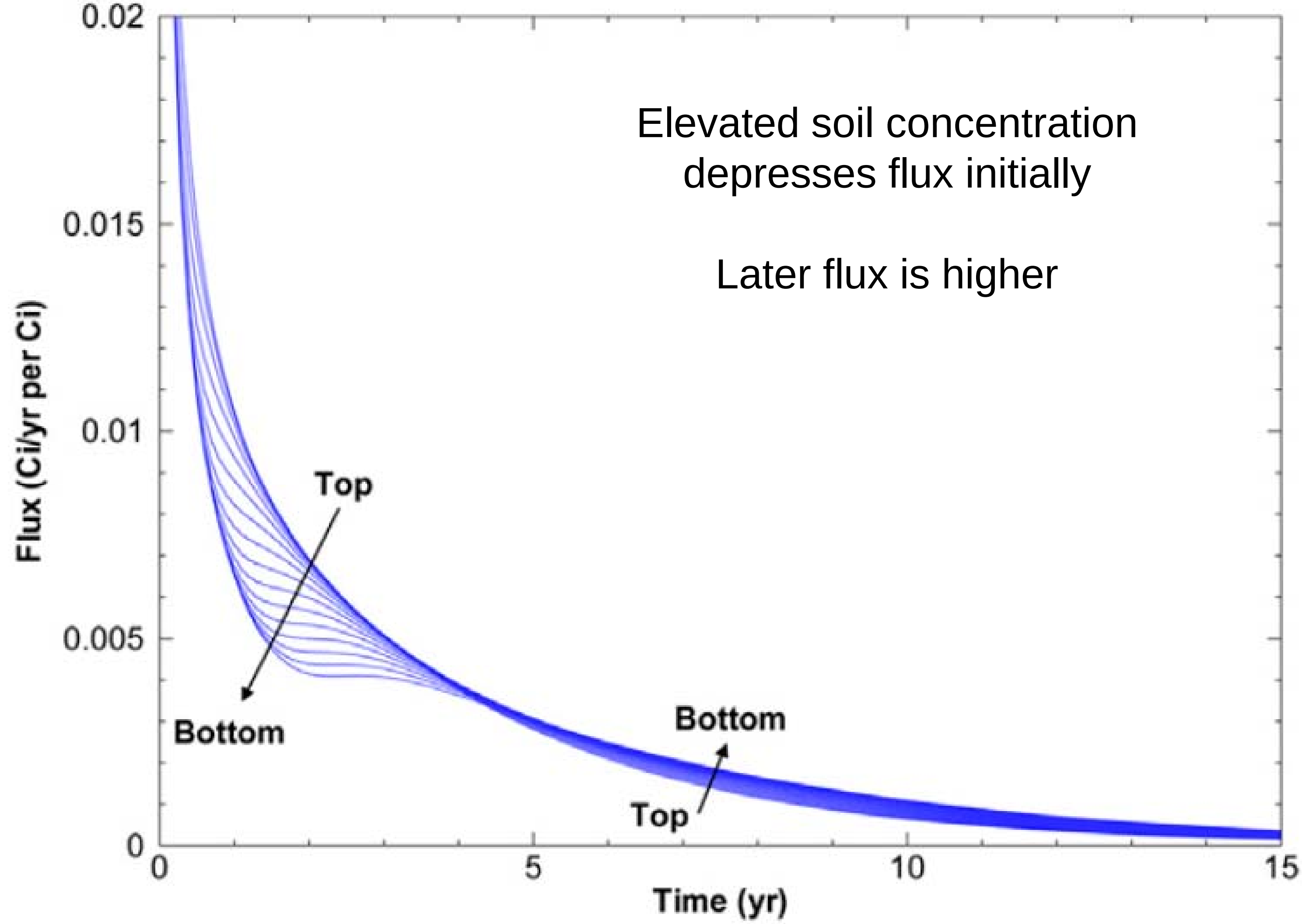


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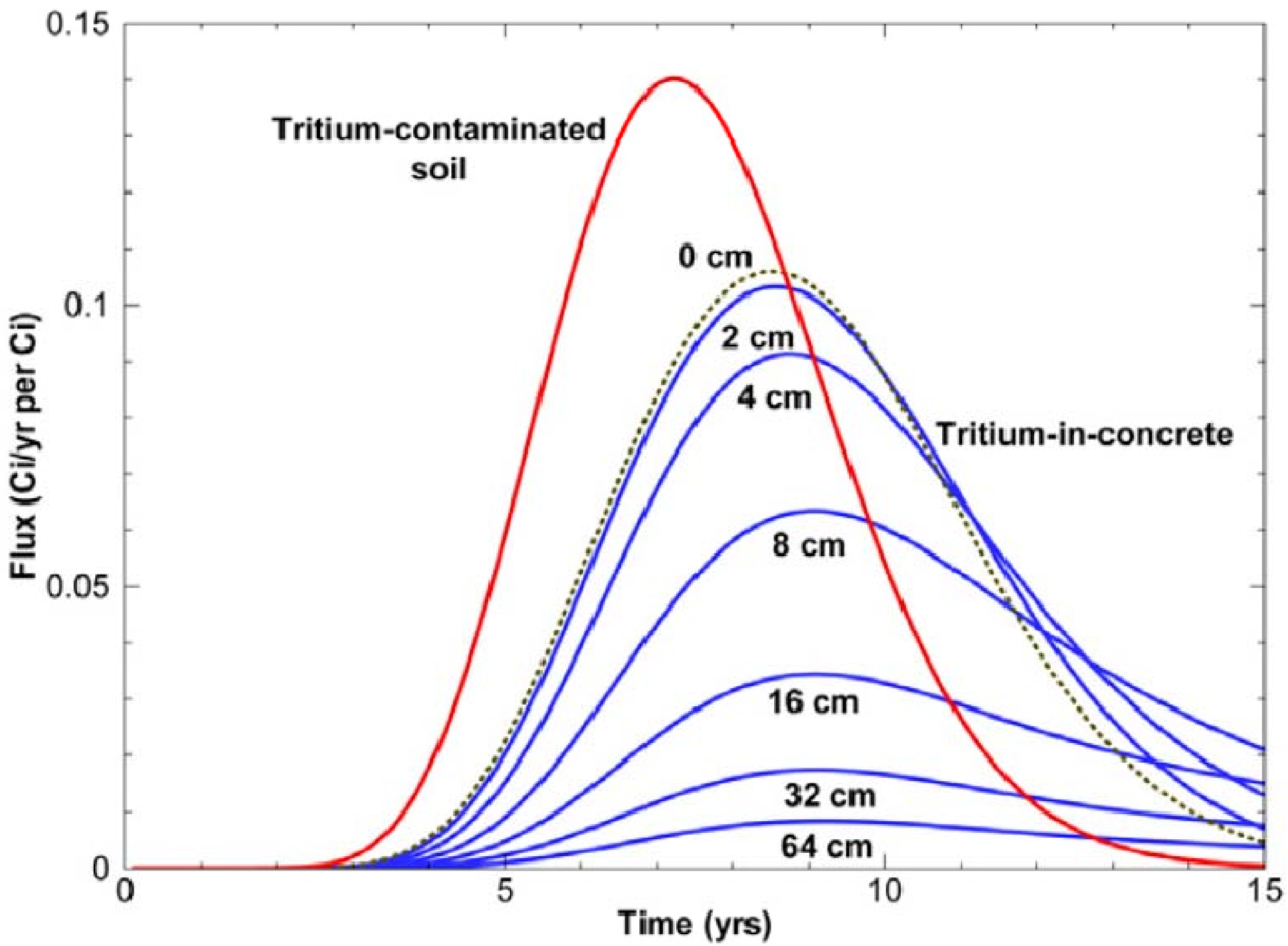
# Multiscale Solute Transport from Concrete Rubble

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# Opportunities for Improvement

- Coupled equilibrium chemistry and solute transport
- Dual-domain transport formulation
- What else?