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Operated by Savannah River Nuclear Solutions, LLC

We Put Science To Work

Modeling of Engineered Systems in the Vadose Zone

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Performance Assessment Community of Practice Technical Exchange

Richland WA

SRNL-MS-2010-00070

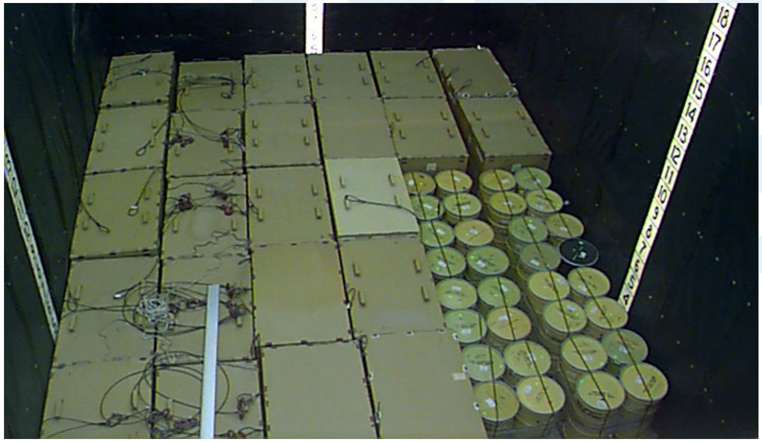
Outline

- Engineered Systems at the Savannah River Site
- Key failure / degradation modes
- Modeling philosophy
- Modeling practice
- Opportunities for ASCEM and CBP

Engineered systems

- **Solid waste disposal, E-area**
  - Intermediate-level and low-activity waste vaults
  - Components-in-grout trench disposal
- **Tank closures, F- and H-area**
- **Saltstone disposal facility, Z-area**
- **Decontamination and Decommissioning (D&D)**
  - reactor buildings
  - canyons
  - other building slabs and below-grade infrastructure

Intermediate Level Vault (ILV)



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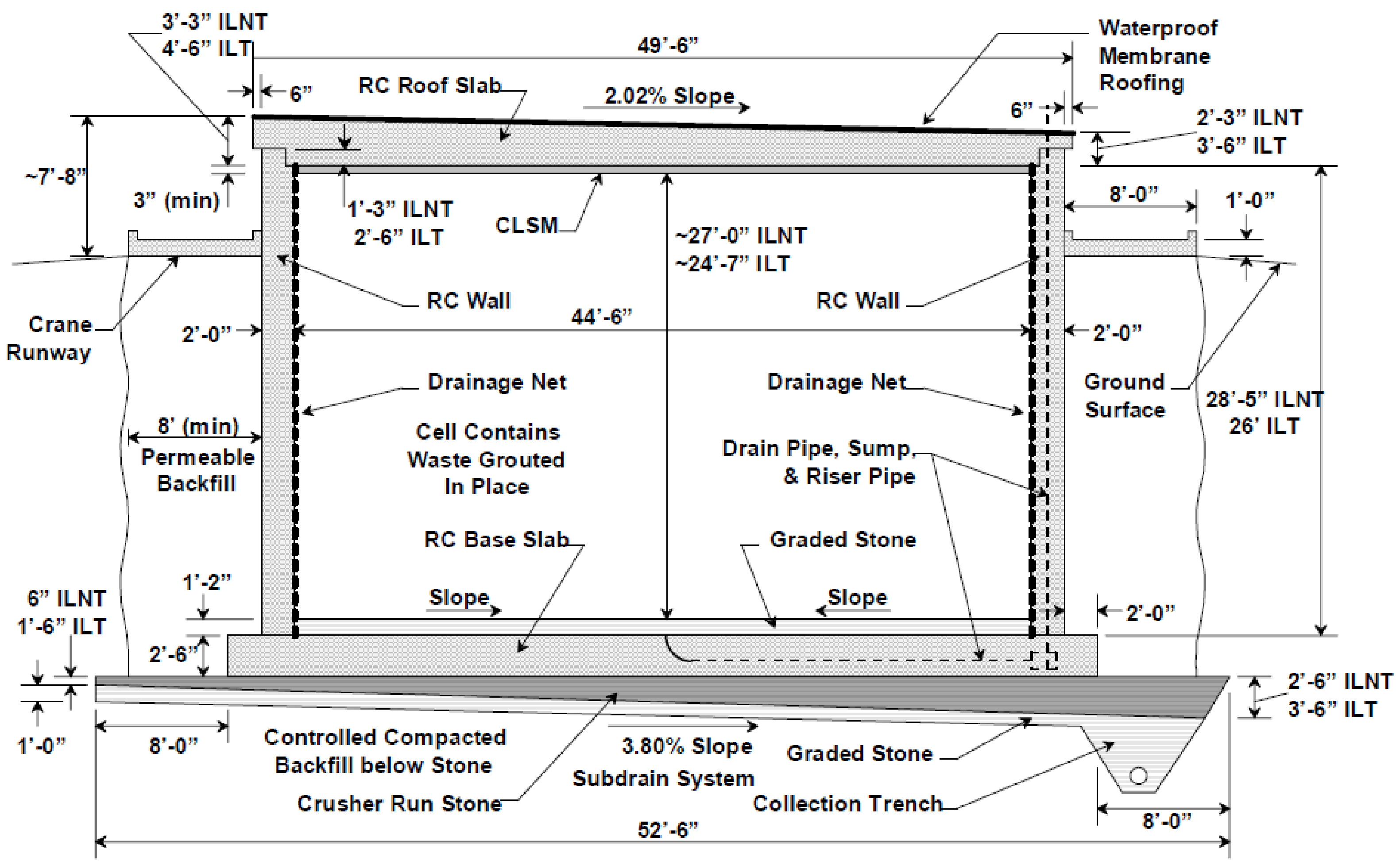

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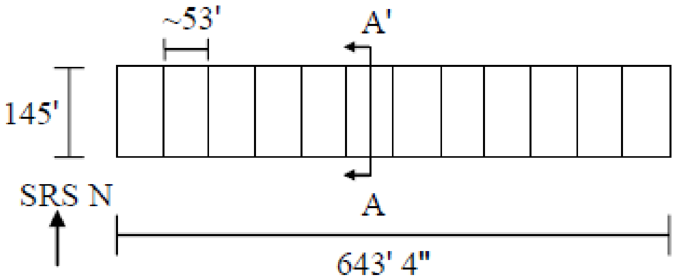
Low Activity Waste (LAW) Vault



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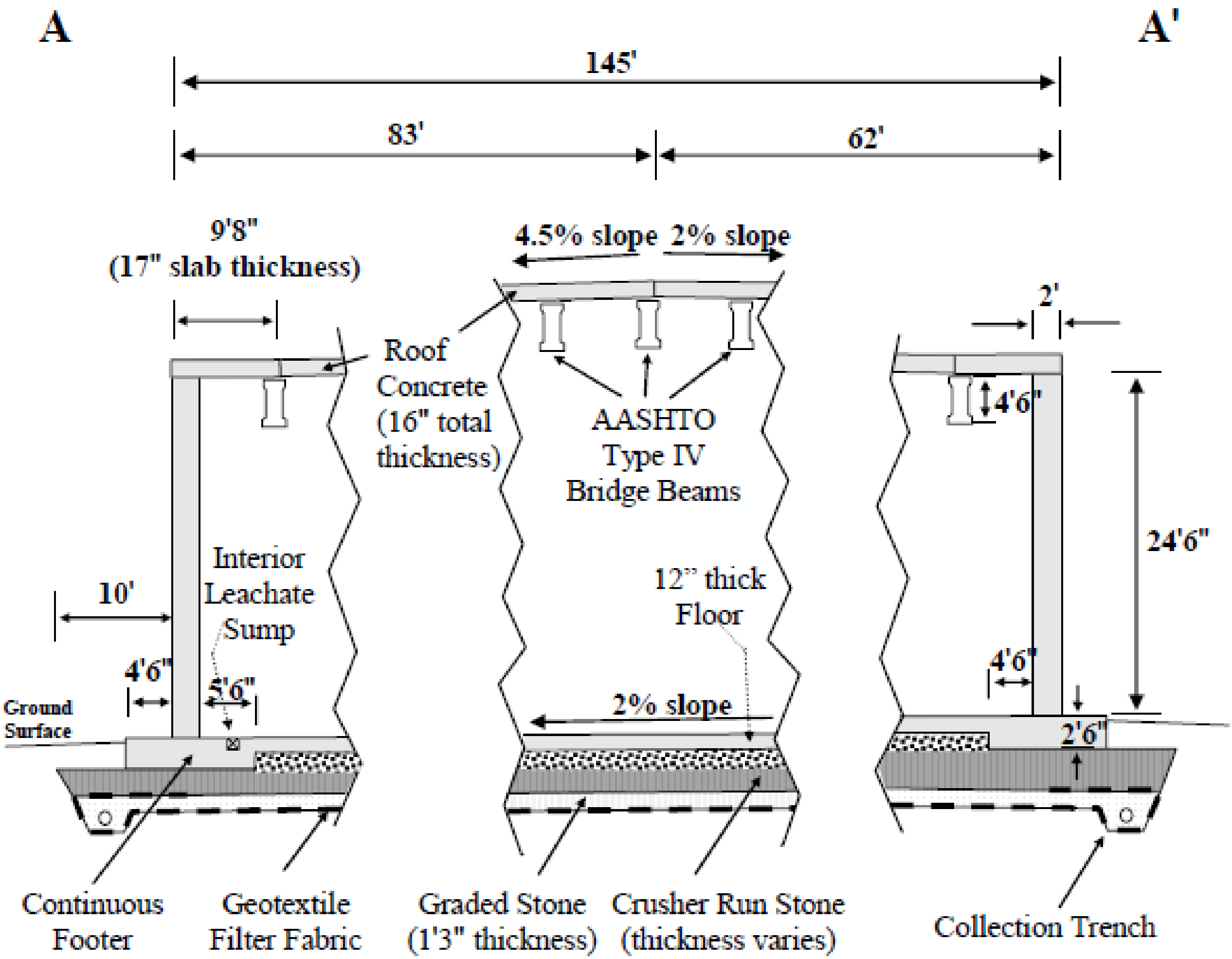

Components-In-Grout (CIG) trench disposal

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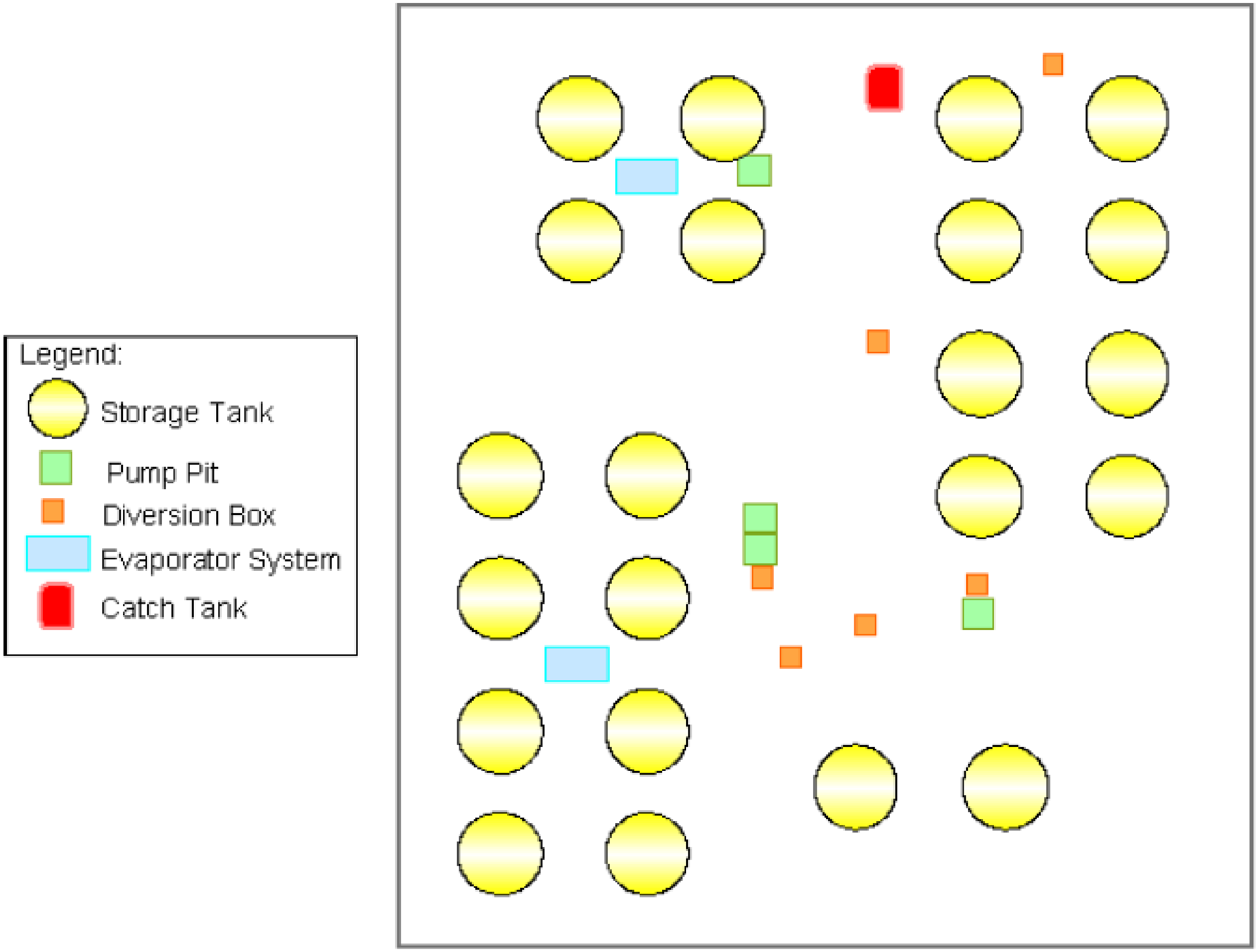
Components-In-Grout (CIG) trench disposal

Tank closures

Figure 3.2-1: General Layout of F-Tank Farm Including Ancillary Equipment



[NOT TO SCALE]

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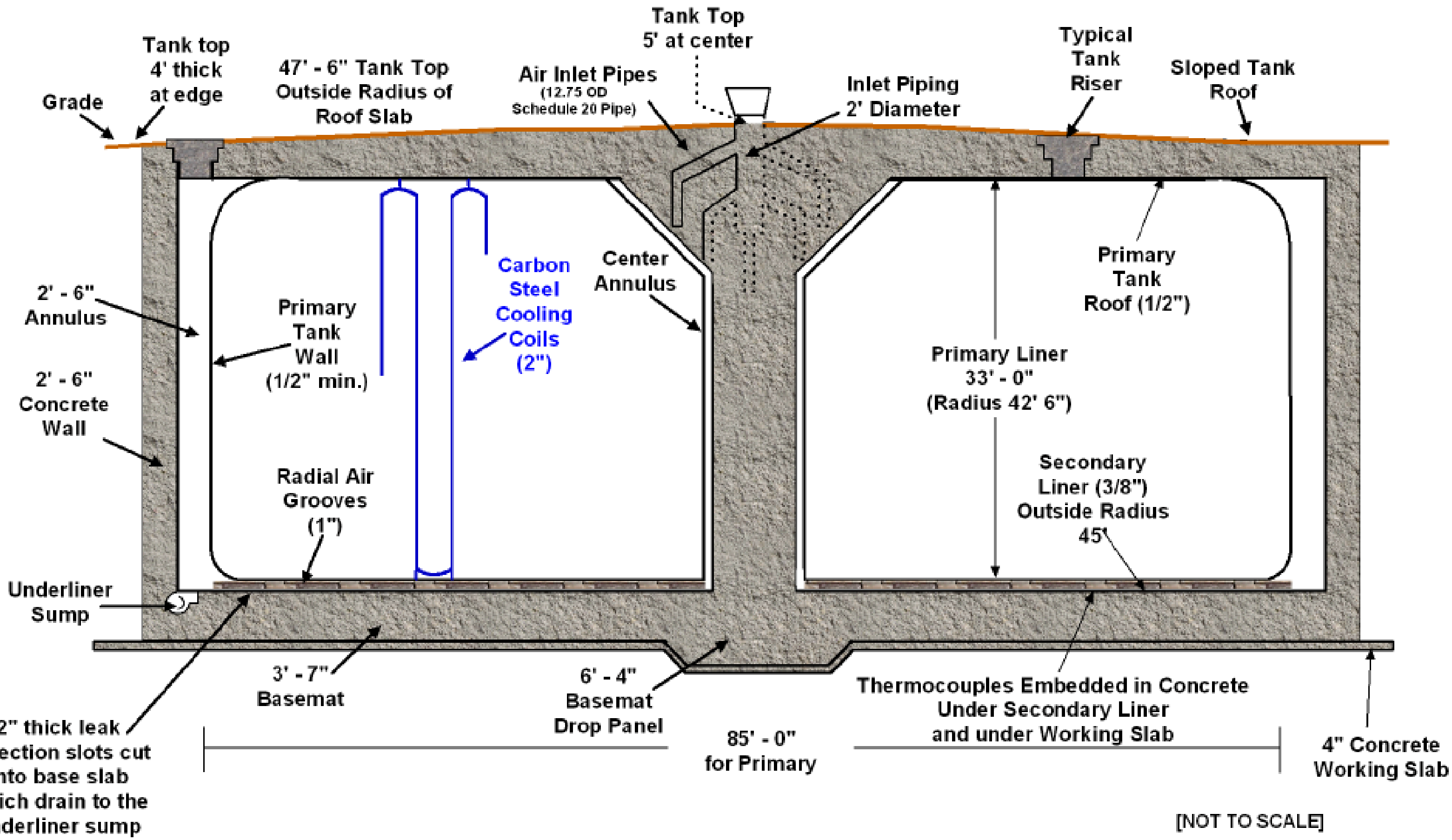
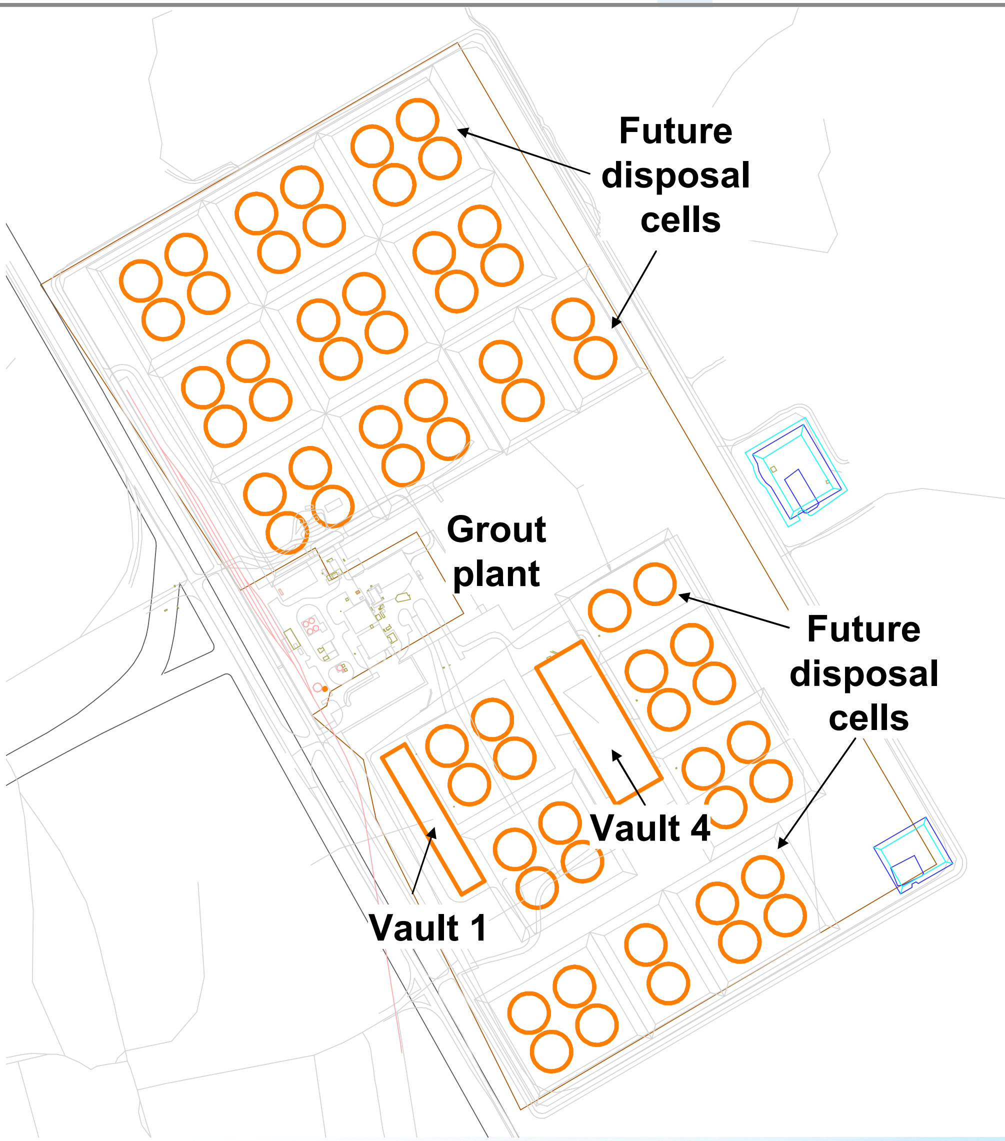
Tank closures

Figure 3.2-14: Sketch of Typical Type IIIA Tank (Cross-sectional View)



Saltstone Disposal Facility



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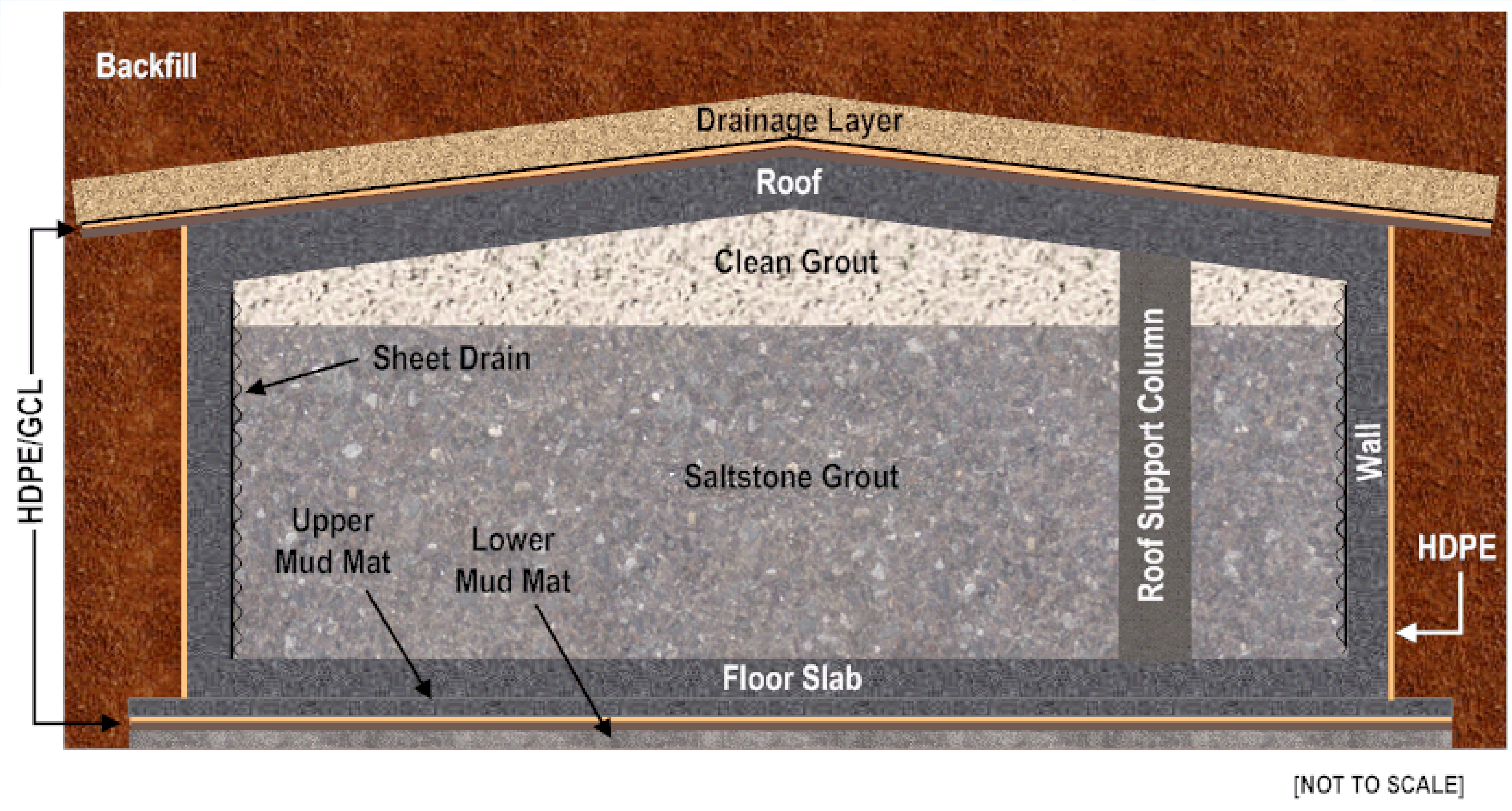
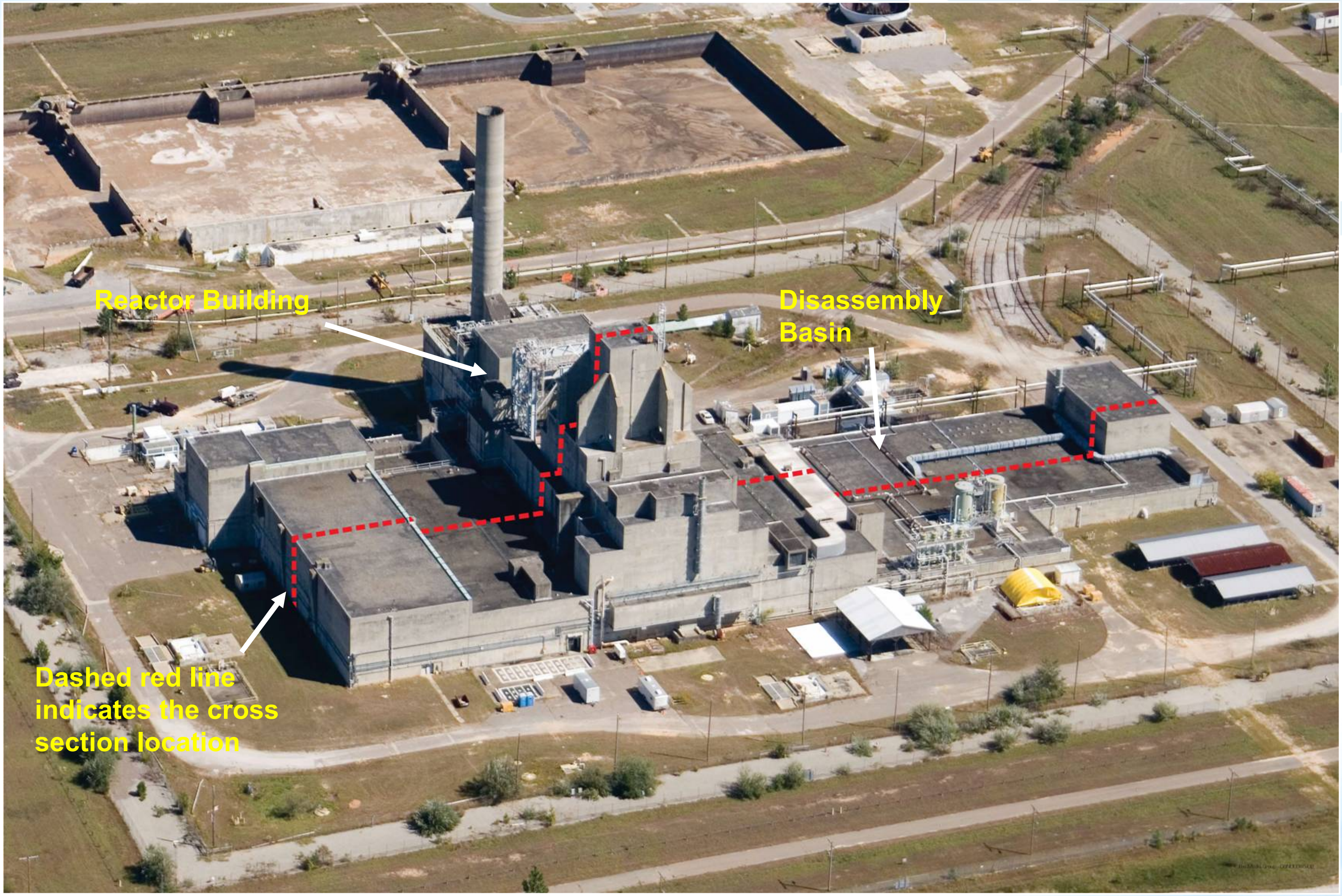


Decontamination and Decommissioning (D&D)



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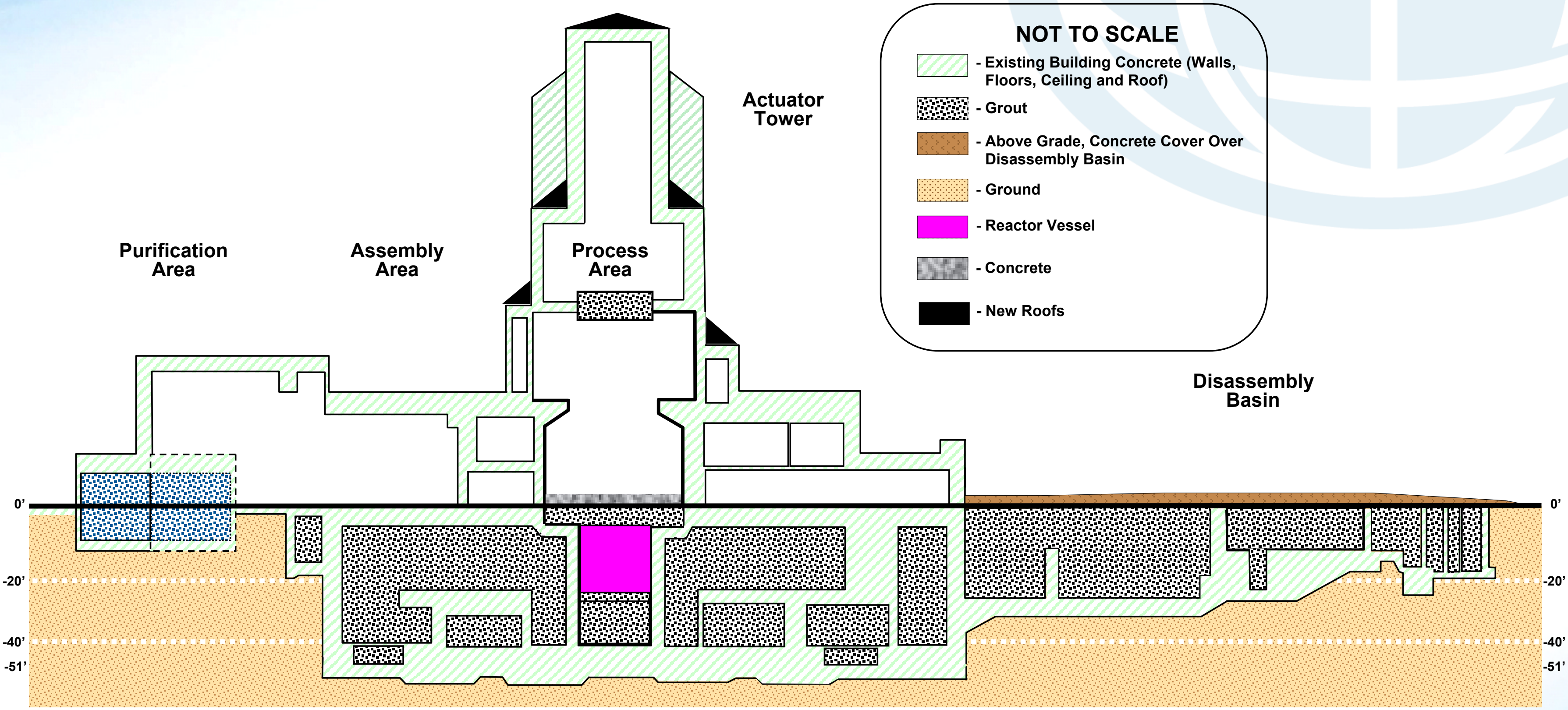

Alternative 2A:

- reactor vessel remains (capped with concrete)
- below-grade portions of building grouted
- above-grade portion of disassembly basin removed

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Key failure / degradation modes

- **Saltstone**
  - sulfate attack and rebar corrosion for concrete
  - oxidation for HDPE liners
  - differential settlement / seismic events for structure
- **Waste tanks**
  - acid leaching/decalcification for saturated concrete
  - carbonation / rebar corrosion for unsaturated concrete
  - general and pitting corrosion for steel tank

Key failure / degradation modes (continued)

- **E-area vaults**
  - structural cracking due to seismic events and cover system overburden
  - rebar corrosion for concrete
- **Components-In-Grout trenches**
  - grout credited for 300 years
- **D&D**
  - varies

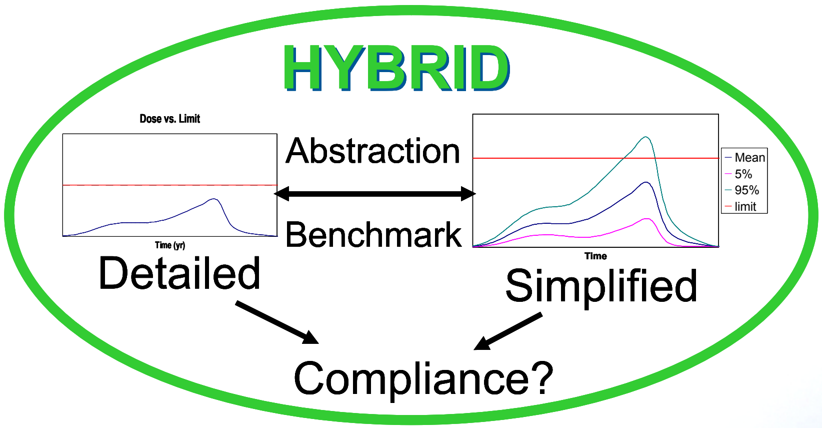
Modeling philosophy

- **Under, but close to, performance objective**
  - simple is often sufficient
  - tailor waste stream to disposal options
    - no containment
    - components-in-grout
    - vaults
  - avoid unnecessary decontamination, cleaning, pre-treatment, and over-engineered closures

→ Graded approach

Modeling philosophy (continued)

- **Reasonable assurance**
  - historically
    - deterministic analysis with conservative assumptions
    - sensitivity analysis
  - increasingly
    - probabilistic analysis
    - using abstracted models
  - typically a <u>hybrid blend</u>
    - deterministic results from higher fidelity model
    - probabilistic results from simpler, abstracted, model



Modeling philosophy (continued)

- **Core team approach**
  - "core team" of stakeholders and subject matter experts
  - consensus on conceptual approach and anticipated outcomes
  - vetting of key results and interpretations
  - formalized for CERCLA / RCRA work

Modeling philosophy (continued)

- **Regulator constraints and considerations**
  - CERCLA/RCRA
    - formal "core team" approach and decisions
    - agreement to use Groundwater Modeling System (GMS) graphical user interface and GMS supported codes by default
  - ready access to familiar software preferred
    - free, commonly used, well documented, open source
  - strong software pedigree preferred
    - QA, large user base and associated track record

Modeling practice

- **Typical practice is described**
- **Vadose zone modeling only**
  - no aquifer
- **Emphasis on**
  - Performance Assessments
  - PORFLOW modeling

Software

- **HELP**
  - cover system
- **PORFLOW**
  - 2D deterministic
- **GoldSim**
  - 1D probabilistic
- **The Geochemist's Workbench**
  - pH and redox transitions, solubilities
- **STADIUM**

Computational demands

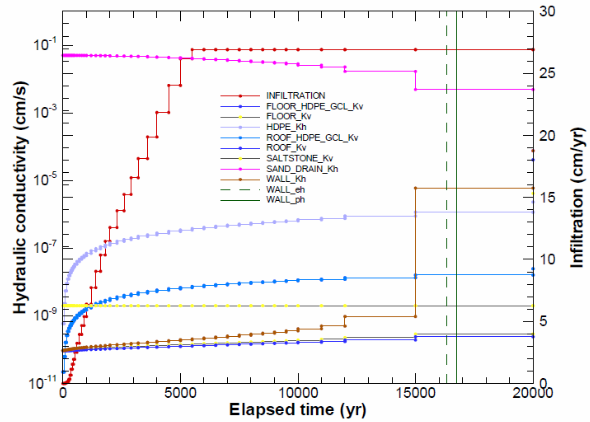
- **Thousands of runs required**
  - geometries
  - cases (best-estimate, sensitivity, . . .)
  - flow periods
  - transport species
  - re-runs (learning, do-overs, updated information, . . .)
- **Need turnaround in one to a few days**
  - 2D vadose zone with (only) several thousand nodes
  - temporal variability defined by a sequence of steady-state flow fields

Computational resources

- **Windows (~50%)**
  - typically multi-core personal desktops
  - interactive
- **Linux (~50%)**
  - typically SRNL clusters
  - 500 cores (subset available)
  - batch
- **Licenses**
  - 13 network for PORFLOW, 1+ node-locked for GoldSim

Workflow

- **Auxiliary supporting calculations**
  - pH/Eh transitions
  - material degradation
- **Pseudo-transient vadose zone flow**
  - sequence of steady-state flow solutions
  - single-phase, single-component
  - single-domain, porous-medium



- **Transient vadose zone transport**
  - abbreviated radionuclide chains
  - linear sorption, sometimes with solubility constraints

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Scripting for PORFLOW simulations

- **Manual approaches are often not practical**
  - too many cases, materials, properties, species, etc.
  - do-overs in response to errors, new inputs, evolving needs
  - difficult to document and reproduce
- **Extensive use of pre- and post-processing scripts**
  - more efficient, and provide a valuable electronic record
  - ad hoc development of several years by multiple analysts
  - often extensive linking (piping) of existing software
    - many languages and utilities
  - often unwieldy

Visualization

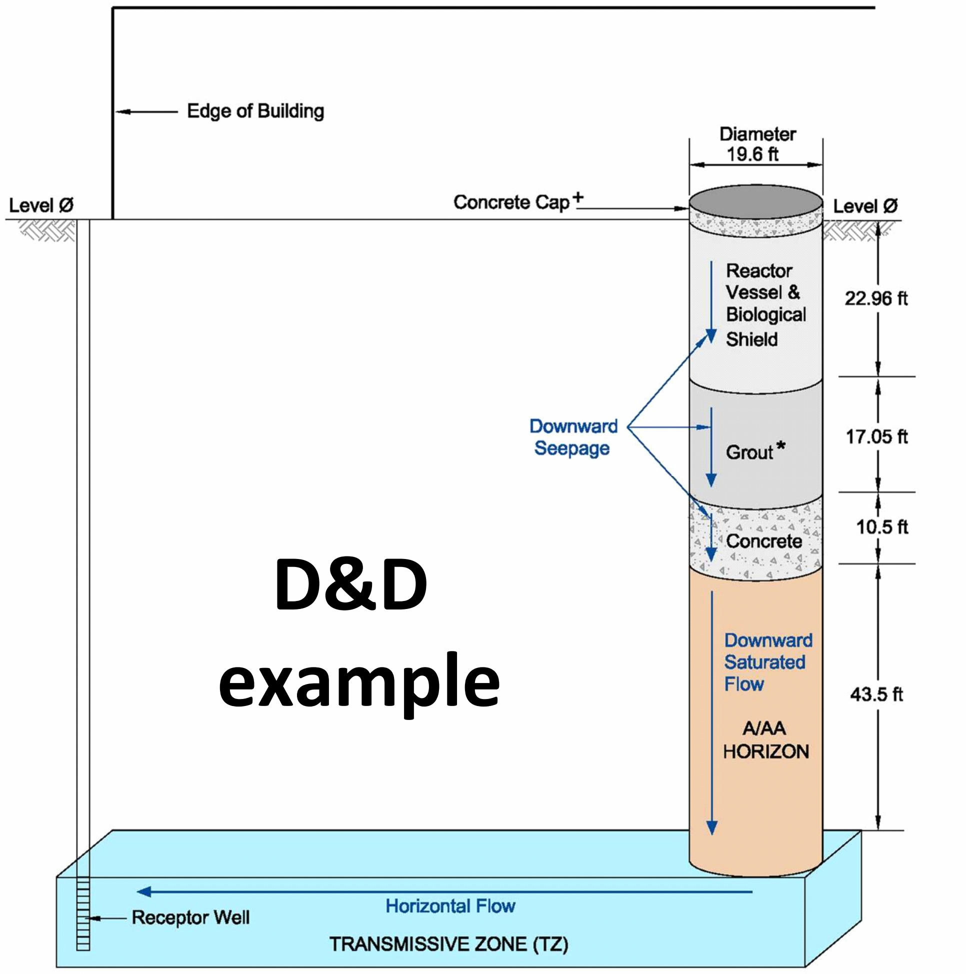
- **PORFLOW**
  - Tecplot
  - Excel
  - Python
- **GoldSim**
  - GoldSim GUI
  - Excel

Data management

- **Primary**
  - Excel
  - Text files
  - GoldSim
- **Infrequent**
  - "Capital D" Databases (e.g. Access)

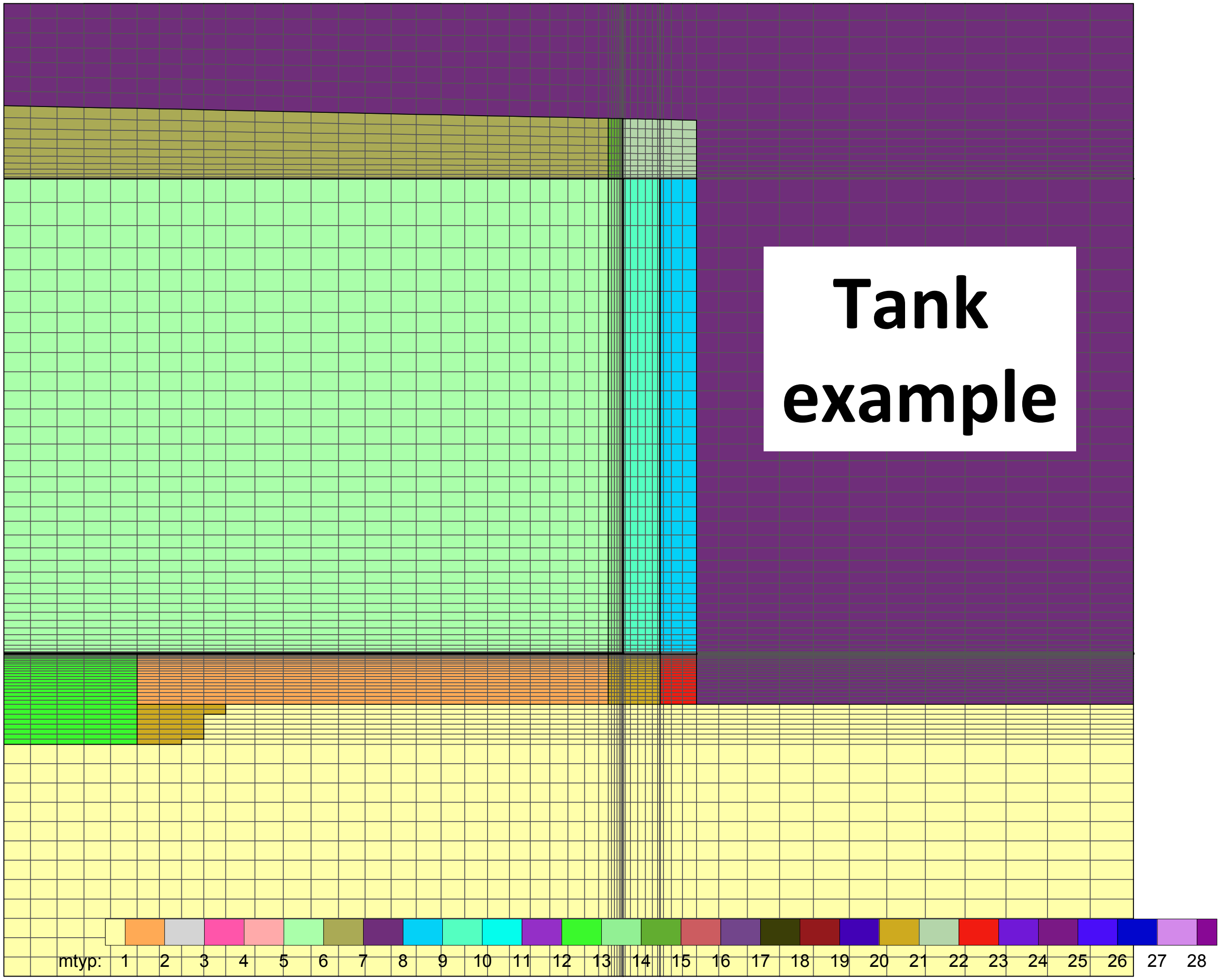
Dimensionality

- **1D**
  - probabilistic and deterministic analyses
- **2D**
  - deterministic
  - axisymmetric or half-width
- **3D**
  - rarely



Grid resolution

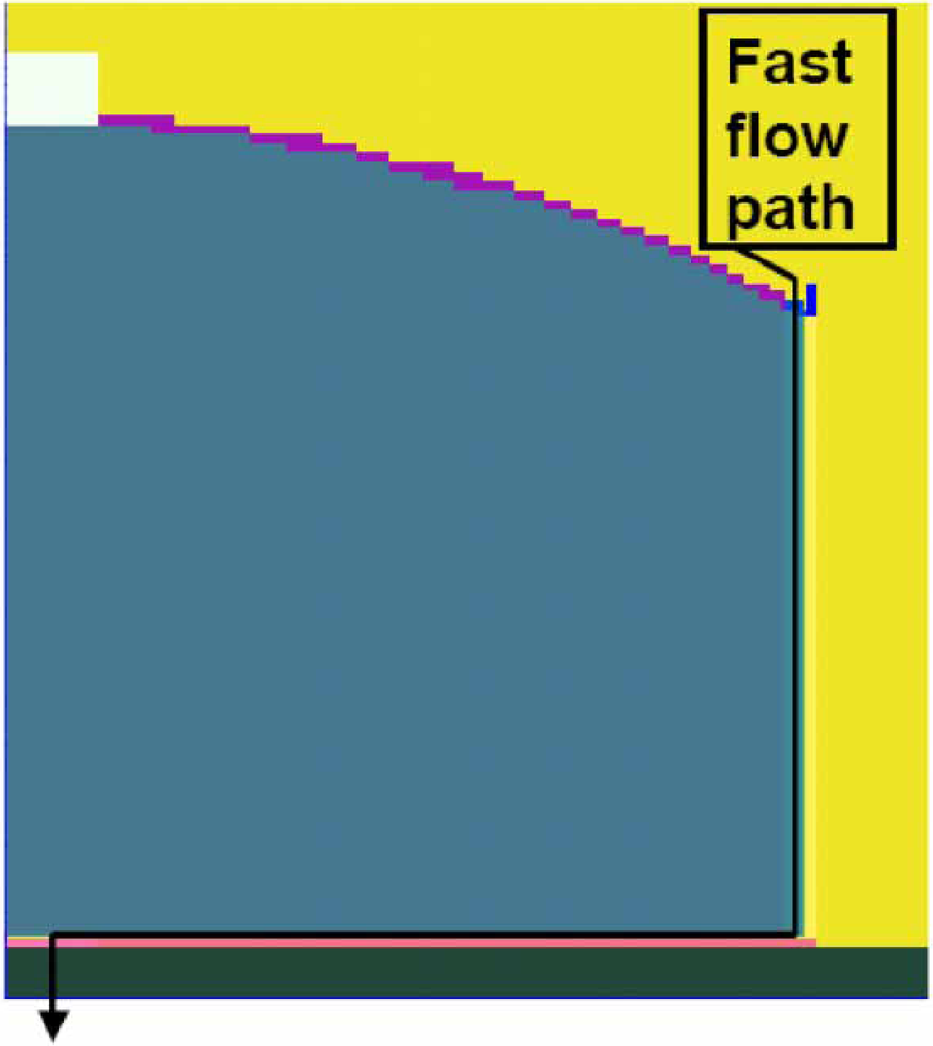
- **5-10k nodes**



Fast flow paths and fractures

- **Explicit fast-flow paths**
  - usually a postulated condition
  - modeled as thicker seam of sand or gravel
  - one to a few in number
- **Smaller scale fractures**
  - cracking is assumed form of concrete physical degradation
  - compute effective properties based on combined matrix and fracture flow
  - matrix and fracture assumed to be in equilibrium

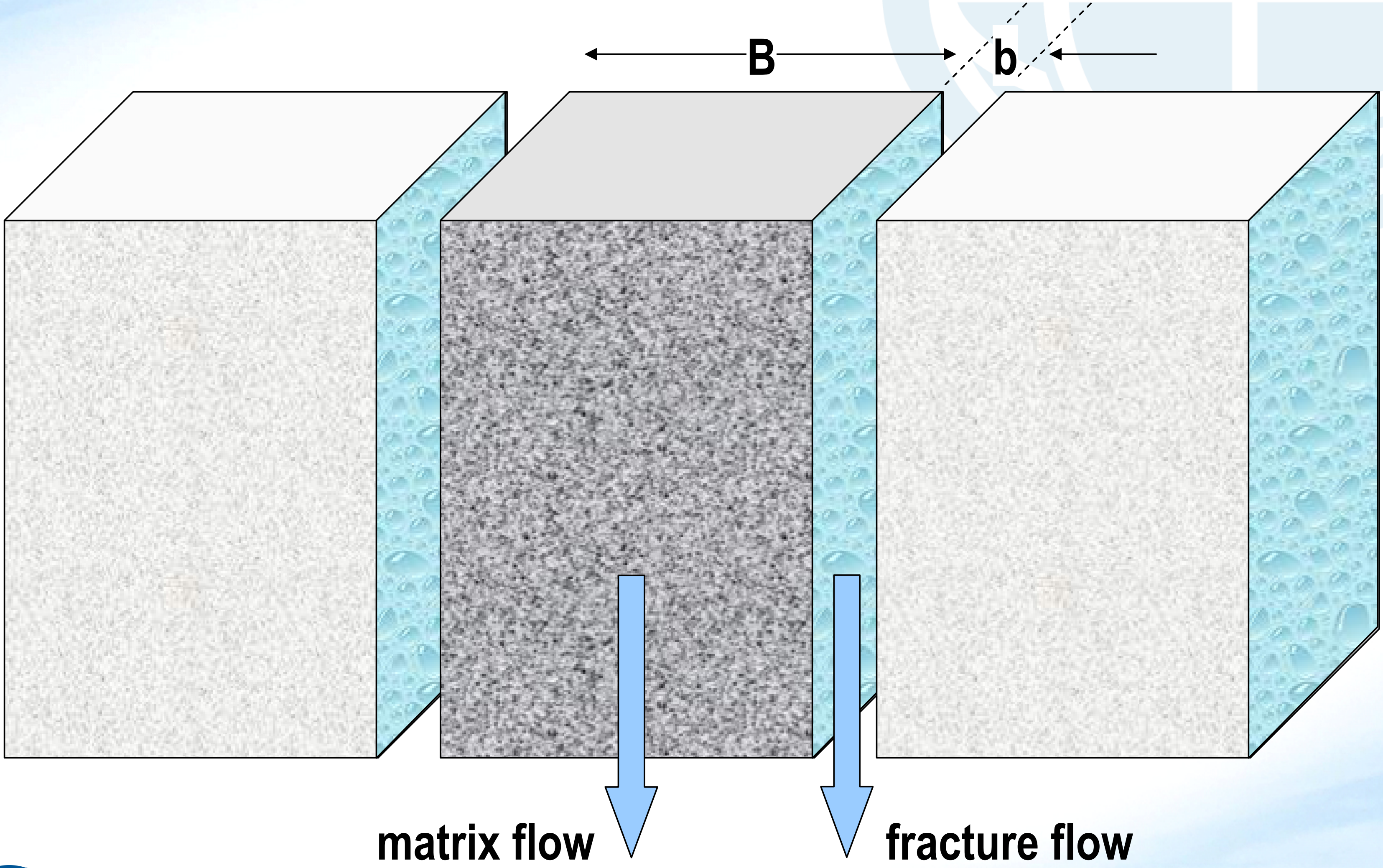
Postulated fast flow path through Type IV tank



Hydraulic property variations (cementitious materials)

- **Frequently,**
  - Instantaneous failure to a soil surrogate, or
  - Gradual increase in saturated conductivity, retaining characteristic curves (water retention, relative perm.)
  - Postulated or assumed degradation / failure
- **Increasingly,**
  - Modified saturated conductivity and characteristic curves to reflect combined matrix and fracture flow
  - Degradation based on an auxiliary, mechanistic, analysis (e.g. STADIUM for sulfate attack)

Combined matrix and fracture flow example



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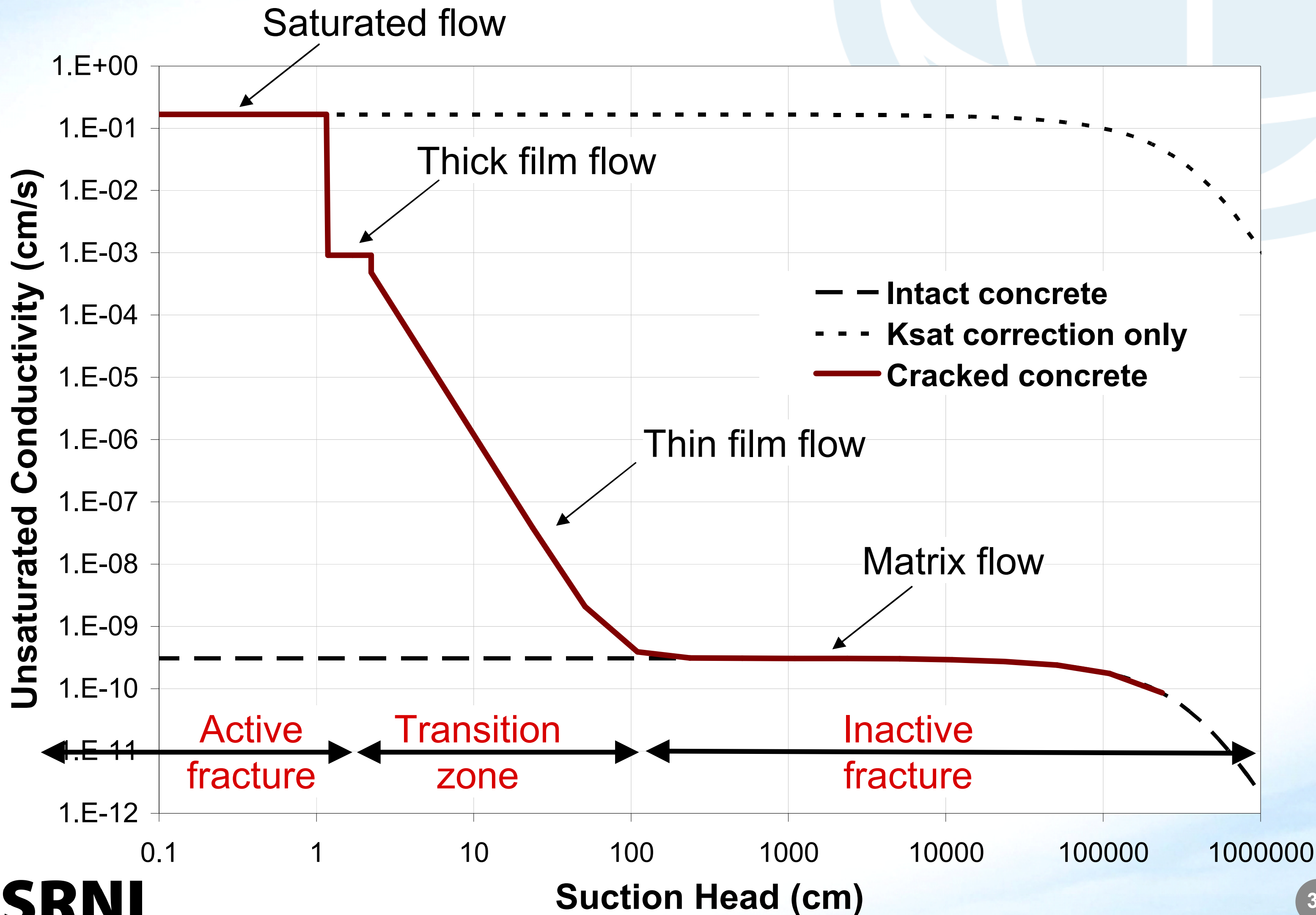
Effective unsaturated K based on Orr and Tuller (2000)



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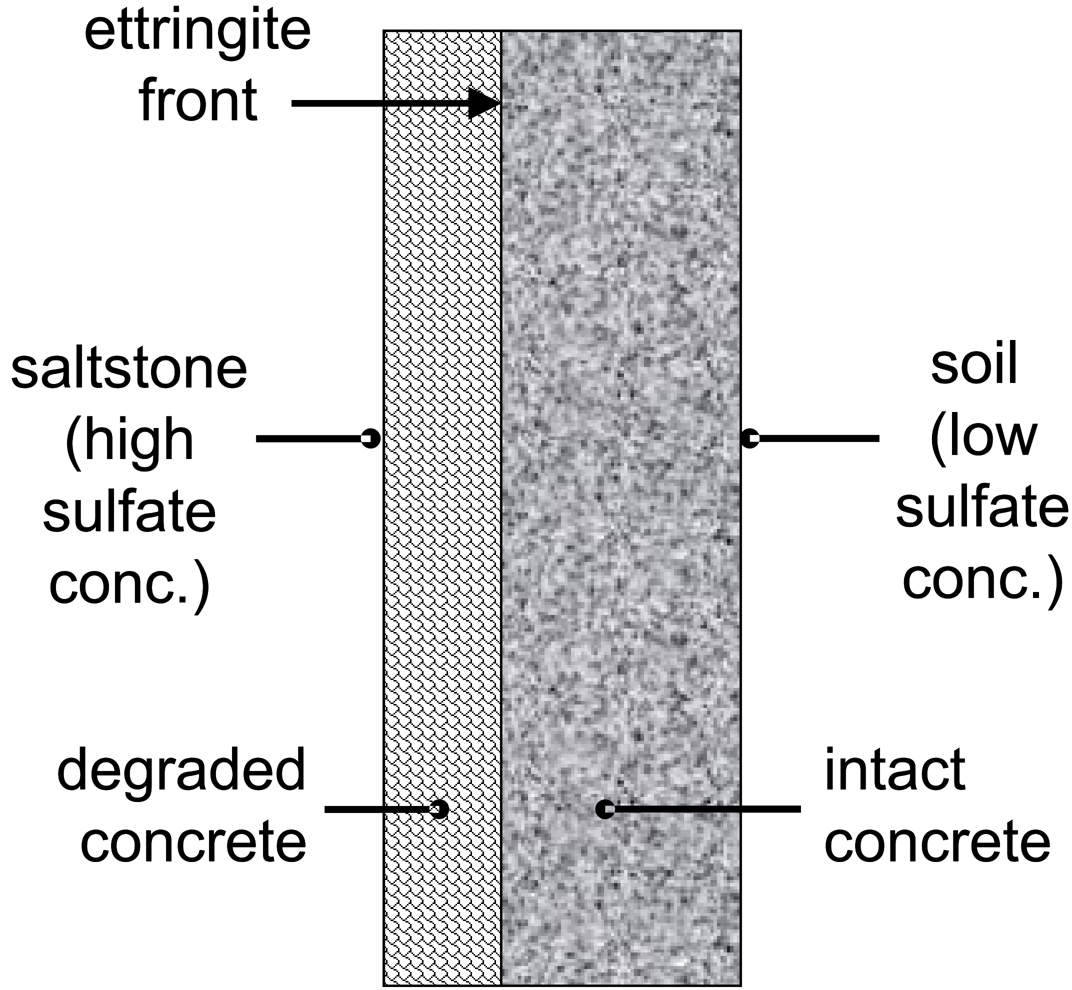
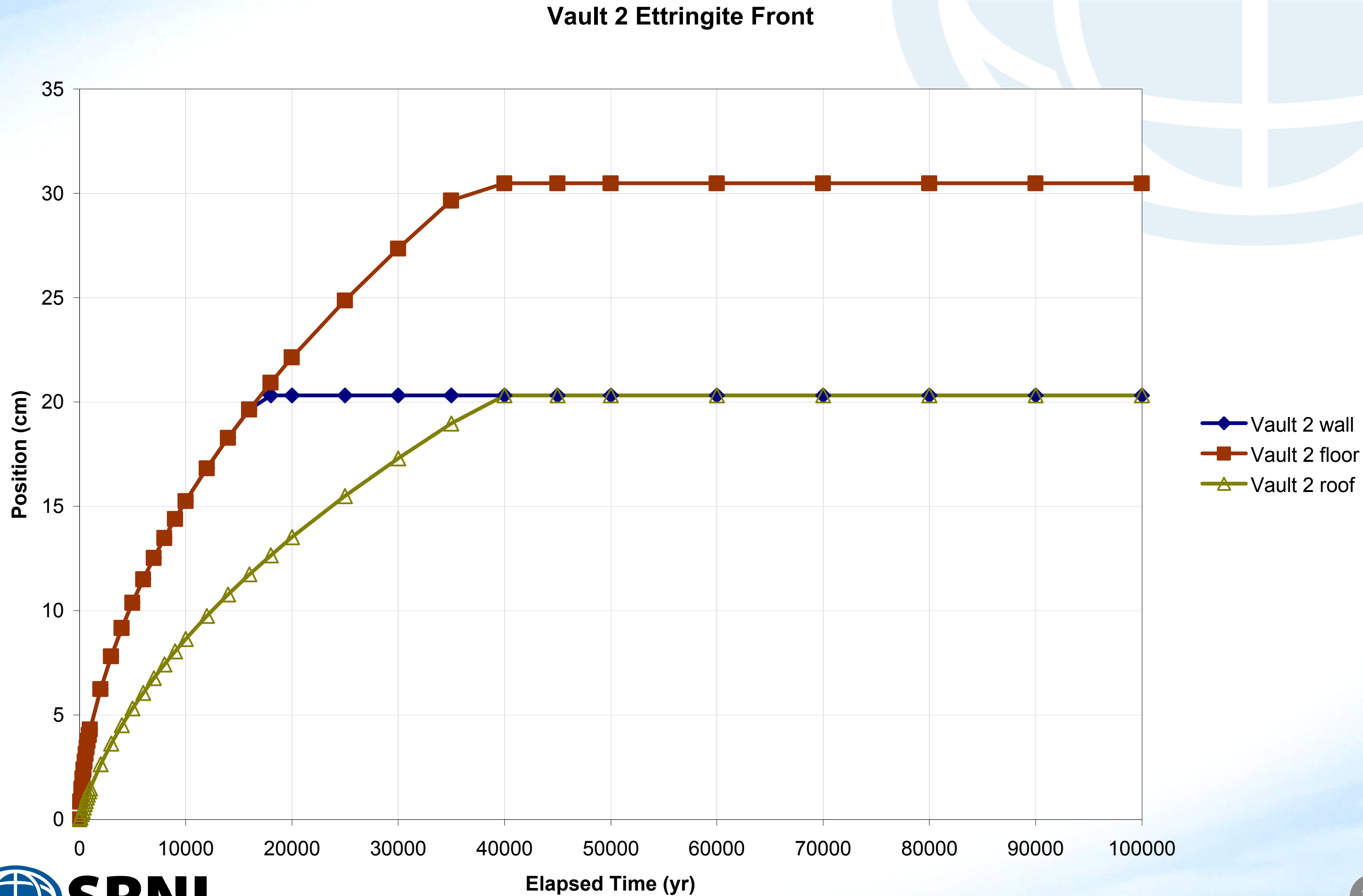
Sulfate attack example



Ettringite formation based on STADIUM simulations



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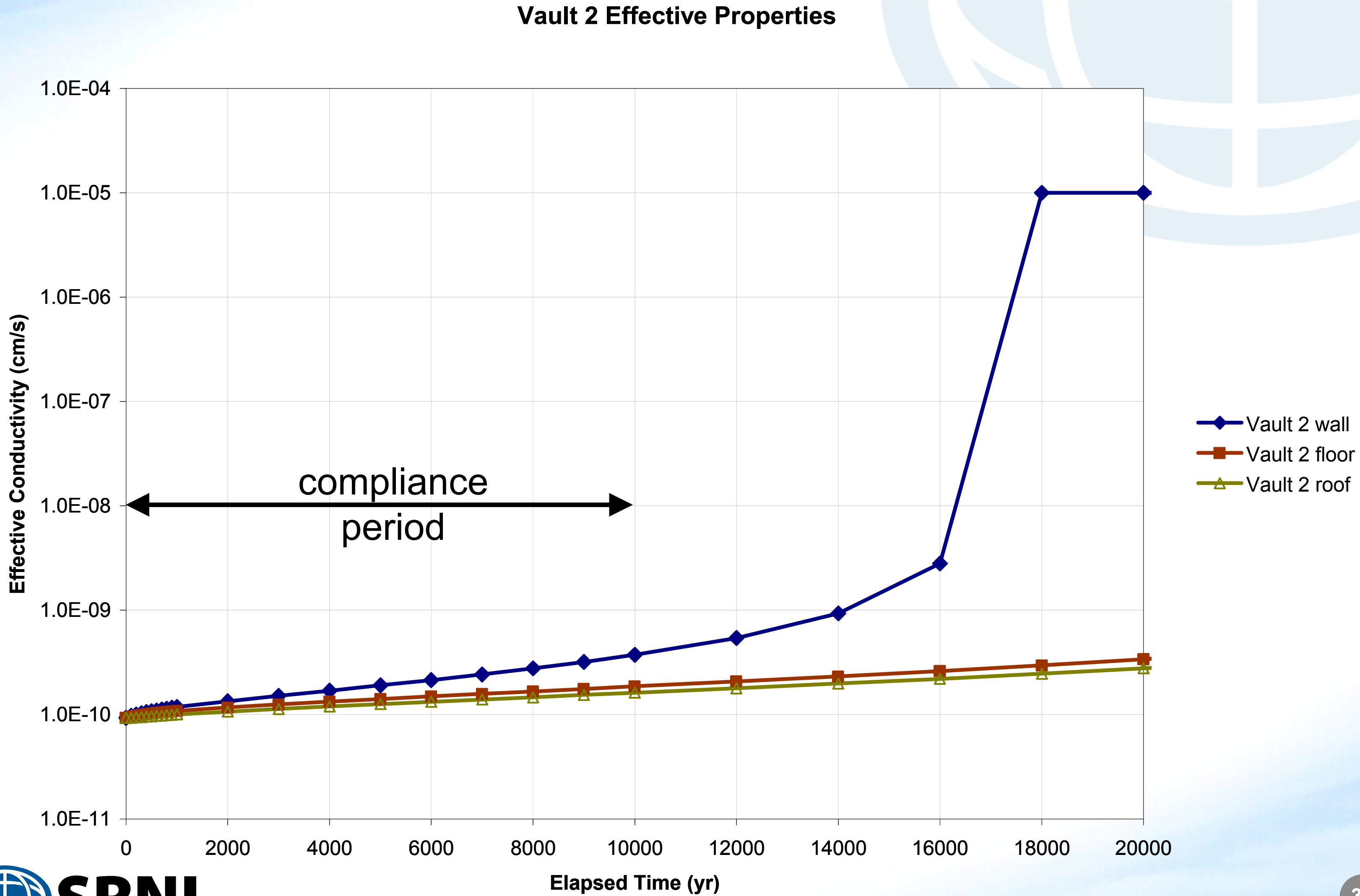
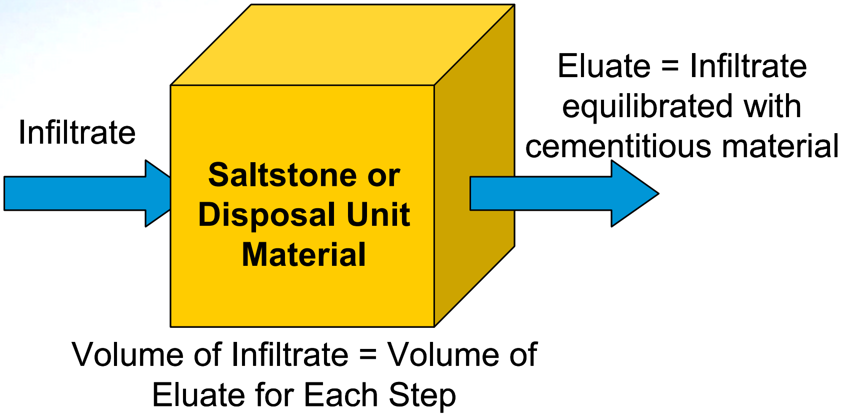
Effective saturated conductivity

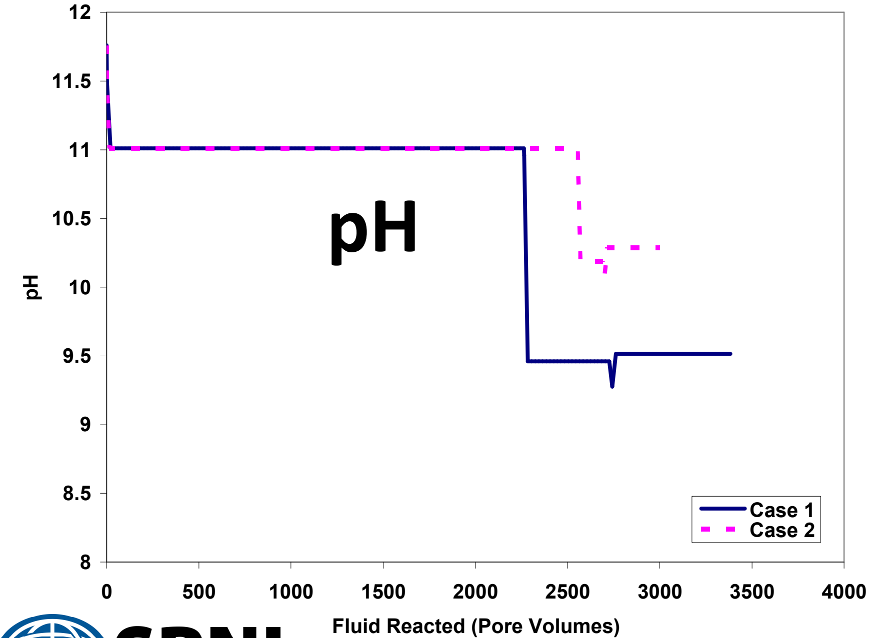


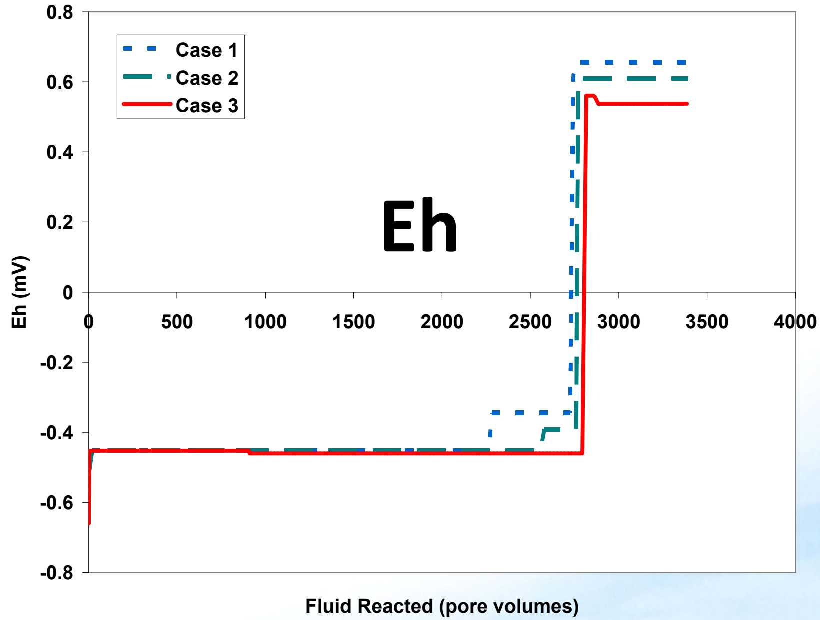
Chemical property variations

- **Chemical equilibrium analysis**
  - The Geochemist's Workbench
  - pH, Eh transitions defined in terms of pore volumes
- **Timing defined by flow simulation**
- **Kd and solubility defined by pH / Eh regime, e.g.**
  - Region II versus III in parlance of Bradbury and Sarott (1995)
  - Oxidizing versus reducing conditions
  - literature and/or SRNL experiments

Saltstone example







SRS modeling interests

- **Multiphase, multicomponent, reactive transport**
  - predict evolution of bulk chemistry
    - pH, Eh (x, t) + empirical Kd (pH, Eh) $\rightarrow$ Kd (x, t)
  - oxidation / carbonation of unsaturated concretes and grouts
    - especially for Tc-99 in Saltstone slag concretes and grouts
  - gas-liquid partitioning and transport in air pathway analysis
- **Probabilistic "full-physics" analyses**
  - take advantage of evolving hardware

SRS modeling interests (continued)

- **Fractured-media approaches for cracked materials**
  - dual-porosity? explicit fracture networks?
- **Open-source flow and transport code**
  - PORFLOW replacement?
  - eliminate licensing limitations and "black-box" mysteries
  - expanded accessibility and user base
- **Mechanistic material degradation predictions**
  - damage mechanics and associated properties
  - corrosion