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We Put Science To Work

Implementation of Model Abstraction for LLW Disposal

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Workshop on Performance Assessments of Near-Surface Disposal Facilities

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Overview

- Abstraction types
- LLW PA challenges
- Abstraction in DOE LLW practice
- Abstraction examples
- Drivers for abstraction
- Abstraction challenges
- Lessons learned and best practices
- Key points

Abstraction Types

Physical reality → conceptual and/or mathematical model

- Conceptual model derived from FEPs
- Richards + van Genuchten + Mualem representation of vadose zone flow

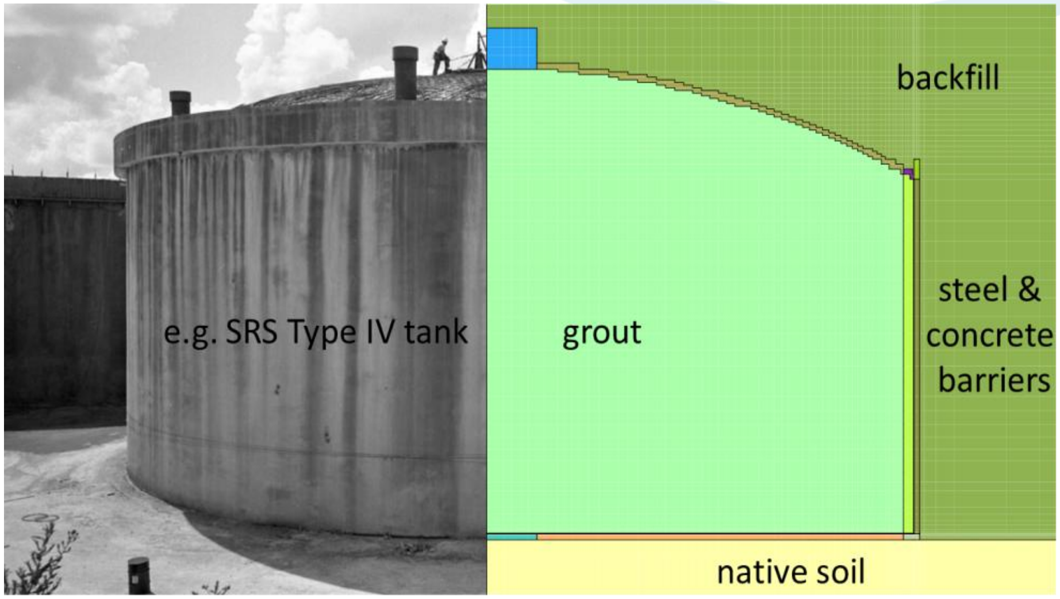
"Full" physics mathematical model → "abstracted" model

- 3D flow field → 1D streamtube
- Neglect secondary chemical species

LLW Performance Assessment Challenges

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

- Tank closures
- Salt waste disposal
- Solid waste disposal
- Facility D&D



Engineered barriers and waste forms are not stable over these geologic time scales

Abstraction Hierarchy in Typical Practice

Higher fidelity models for separate effects and system subcomponents

- Cementitious material degradation
- Corrosion
- Reactive chemistry

System models for deterministic and limited sensitivity analysis

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

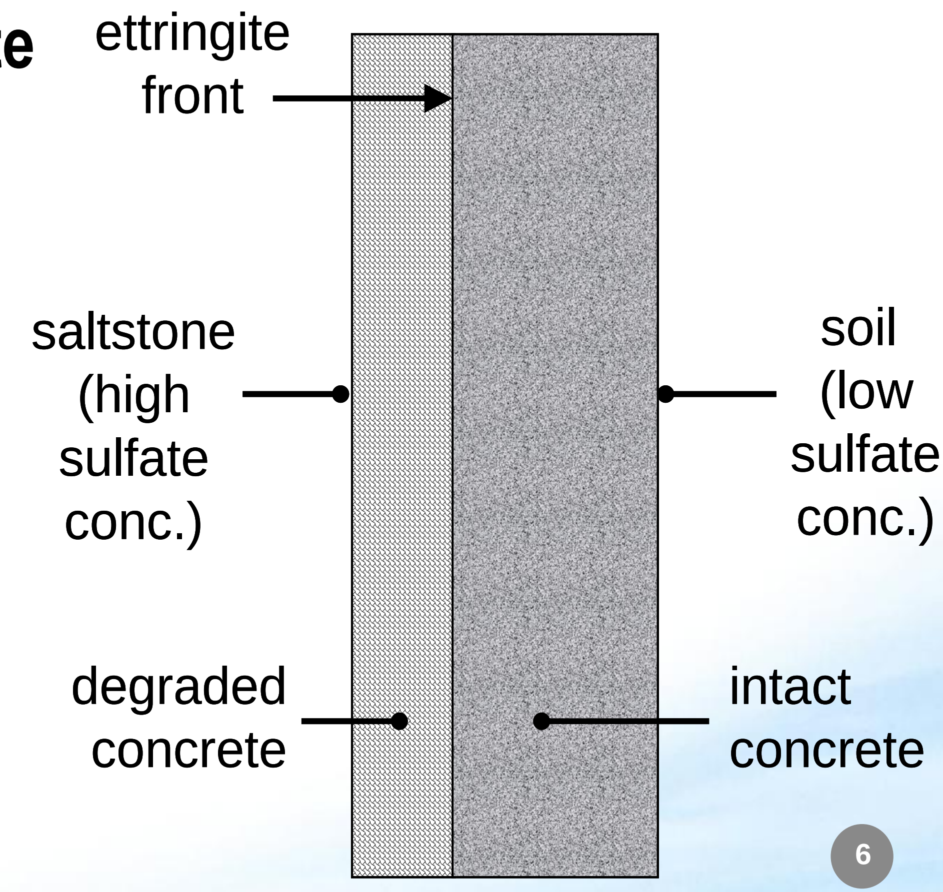
Probabilistic system model for Sensitivity Analysis (SA) and Uncertainty Quantification(UQ)

Chemical Degradation Abstraction Example

Physical abstraction:

$$\frac{\partial(wc_i)}{\partial t} - \mathrm{div}\left(D_i w\,\mathrm{grad}(c_i) + \frac{D_i z_i F}{RT} w c_i\,\mathrm{grad}(\psi) + D_i w c_i\,\mathrm{grad}(\ln\gamma_i) + \frac{D_i c_i \ln(\gamma_i c_i)}{T} w\,\mathrm{grad}(T) + c_i D_w\,\mathrm{grad}(w)\right) = 0$$

- **Extended Nernst-Planck equation implemented in STADIUM® code (coupled chemistry and transport)**
- **Used to predict formation of ettringite**
- **Simple damage model**
  - **Ettringite = physical damage (e.g. cracking, spalling)**
  - **Transport properties not affected by ettringite front**
- **Effective hydraulic properties by averaging**



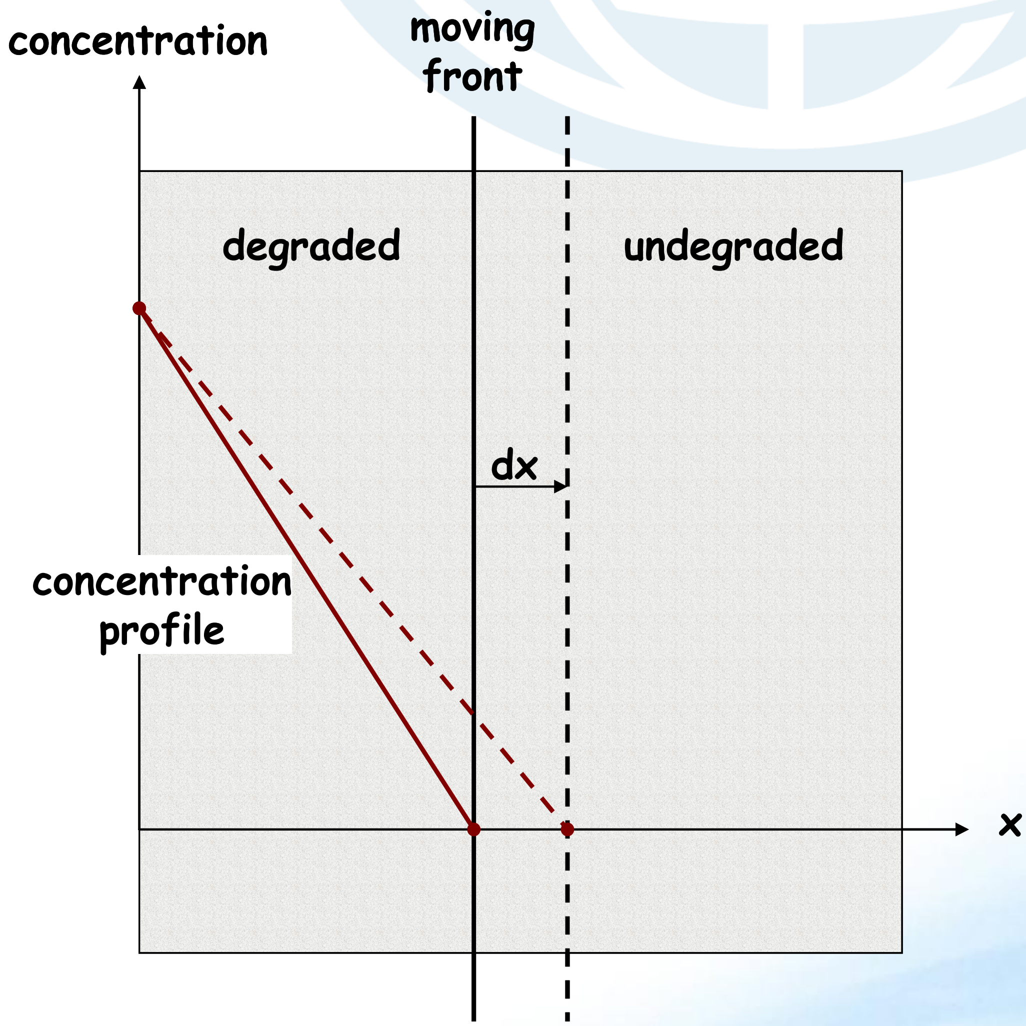
Chemical Degradation Abstraction Example

Model 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

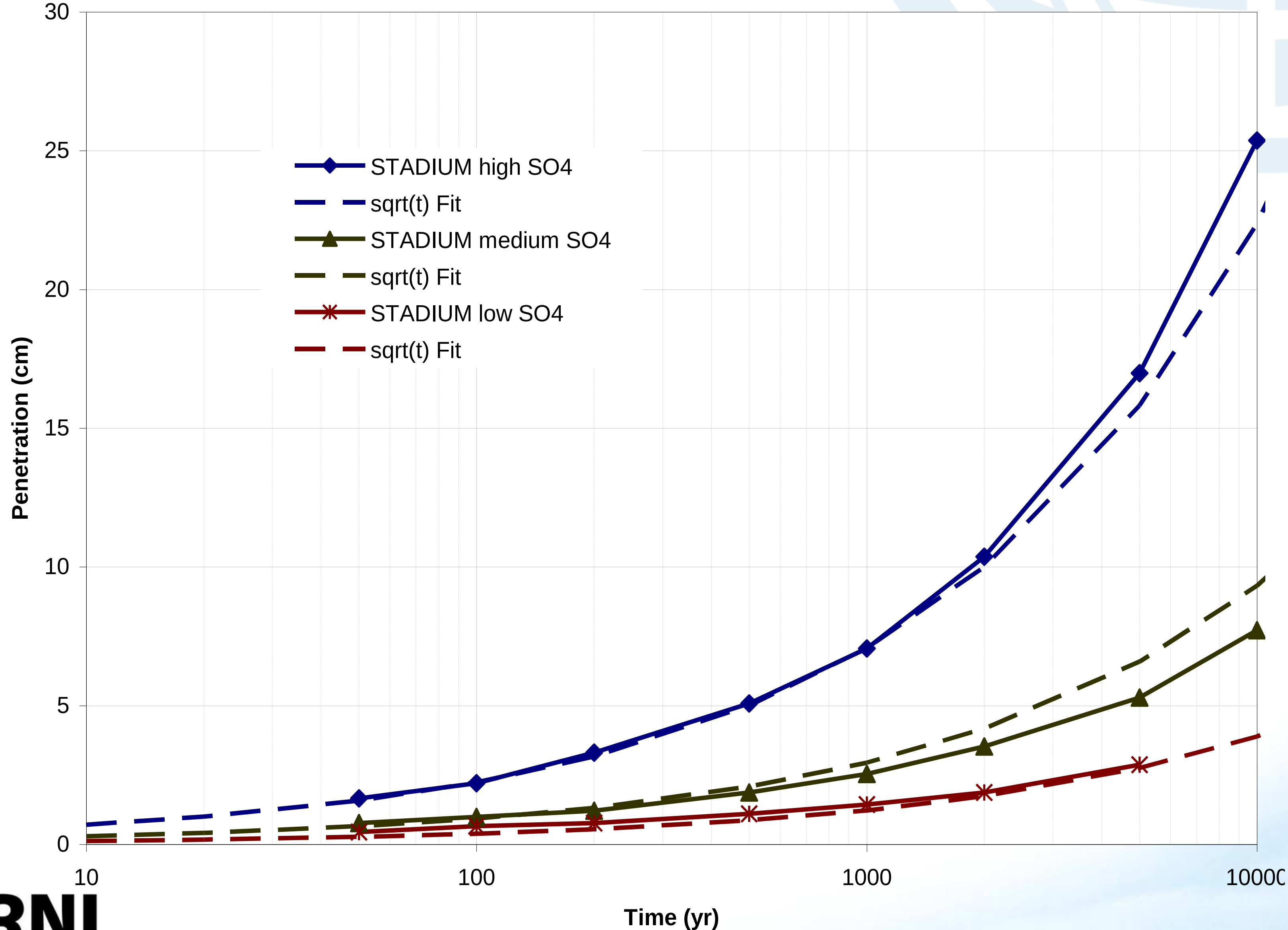


- **Analytic solution for ettringite front**

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

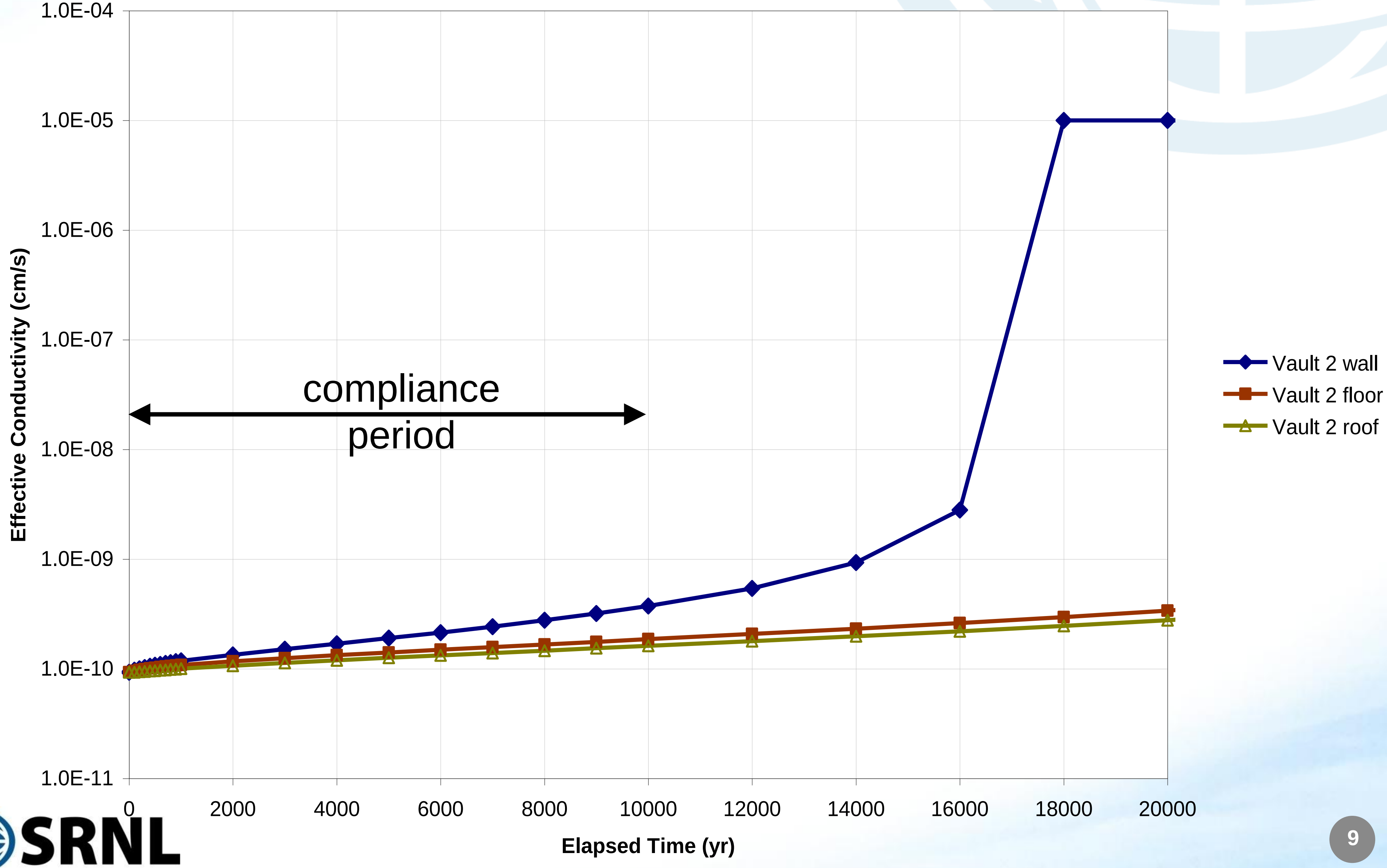
Chemical Degradation Abstraction Example

Calibration of reaction capacity to STADIUM®:

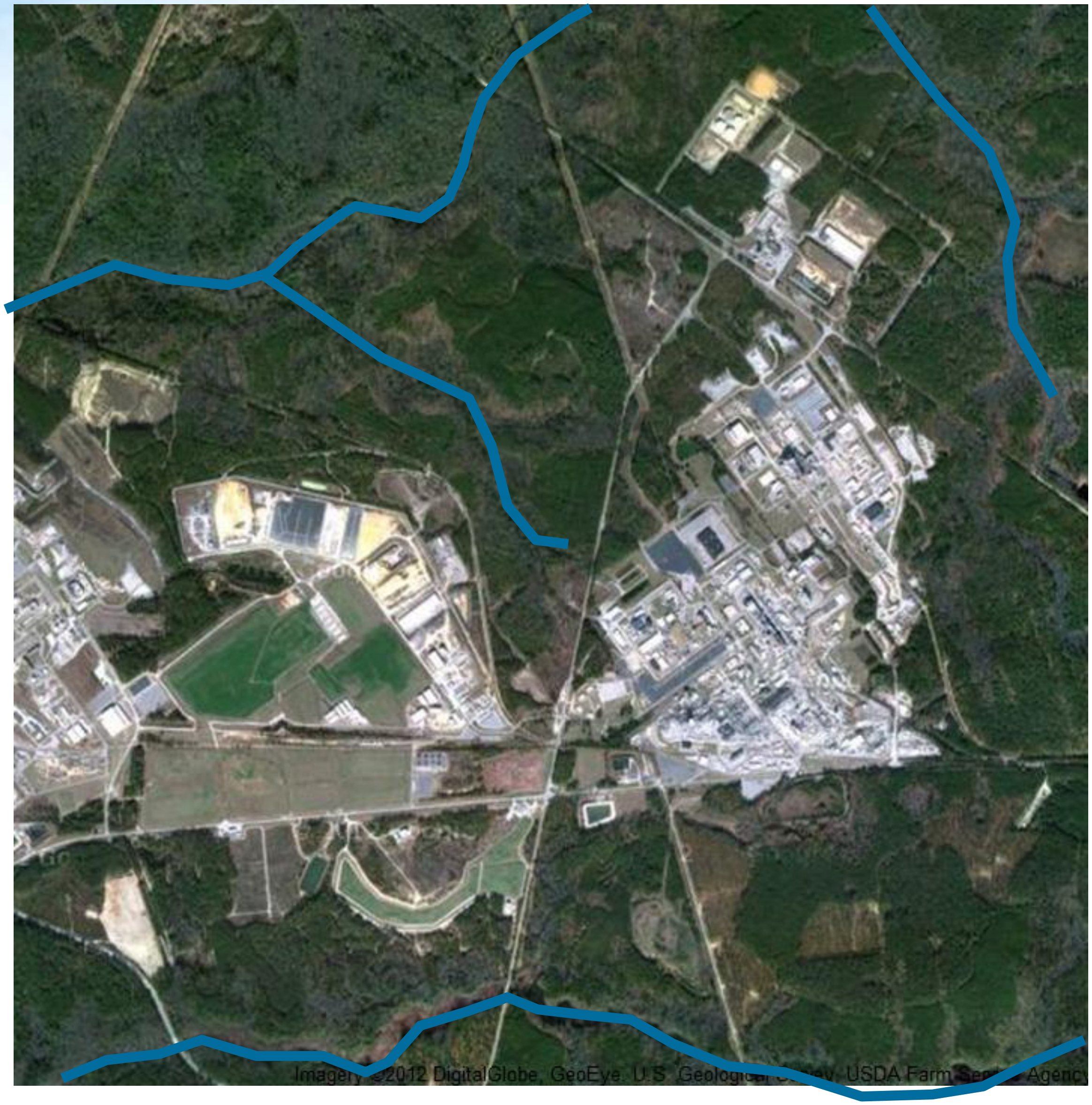


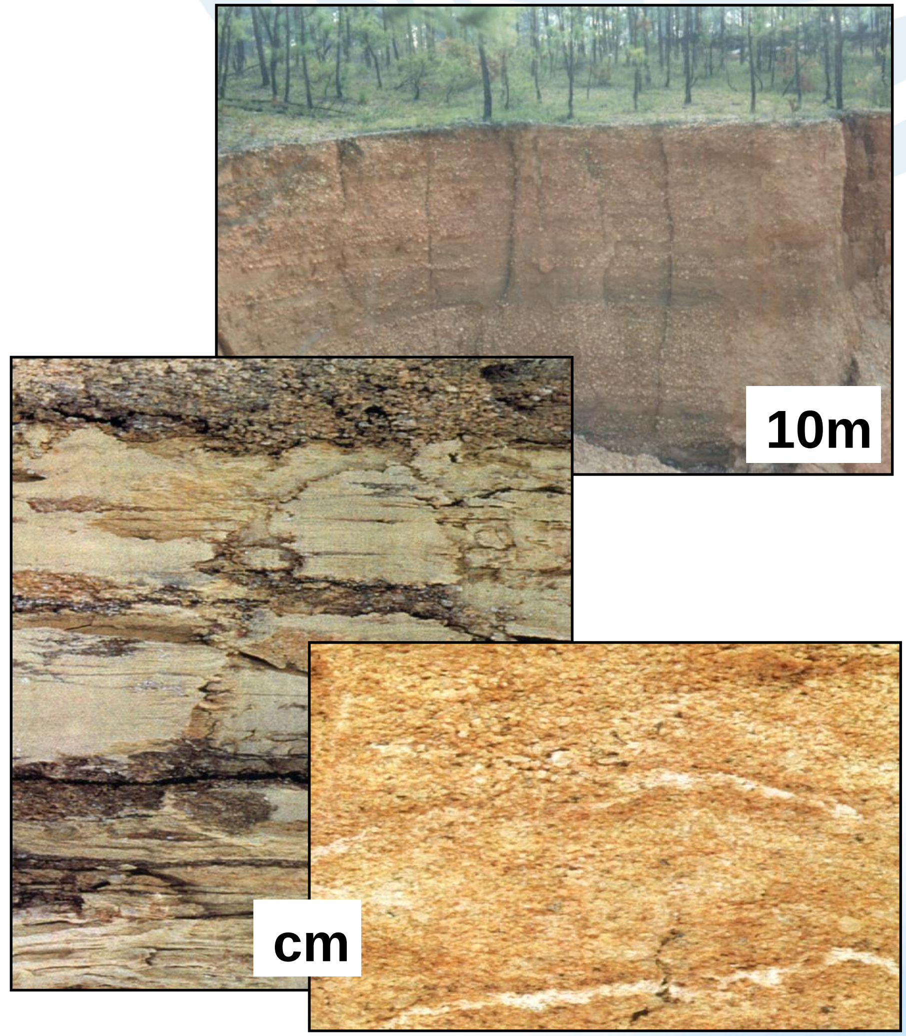
Chemical Degradation Abstraction Example

Effective hydraulic conductivity:

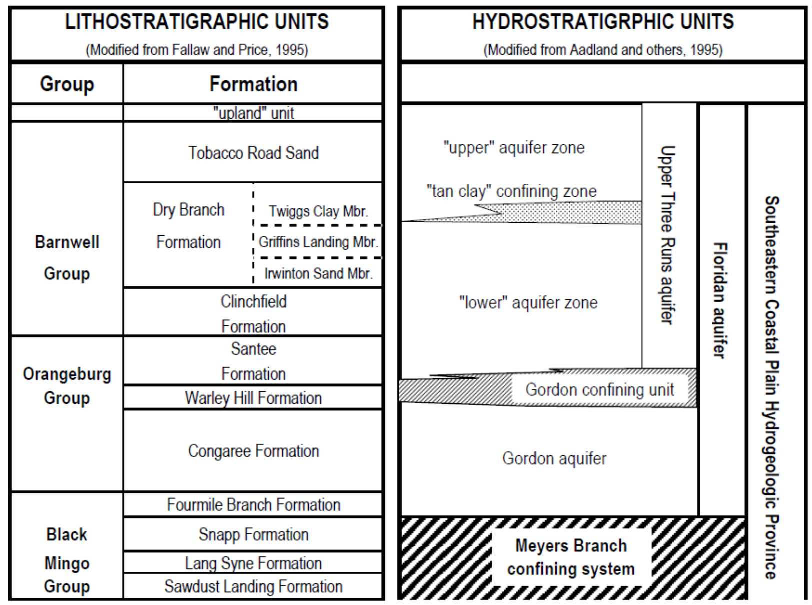


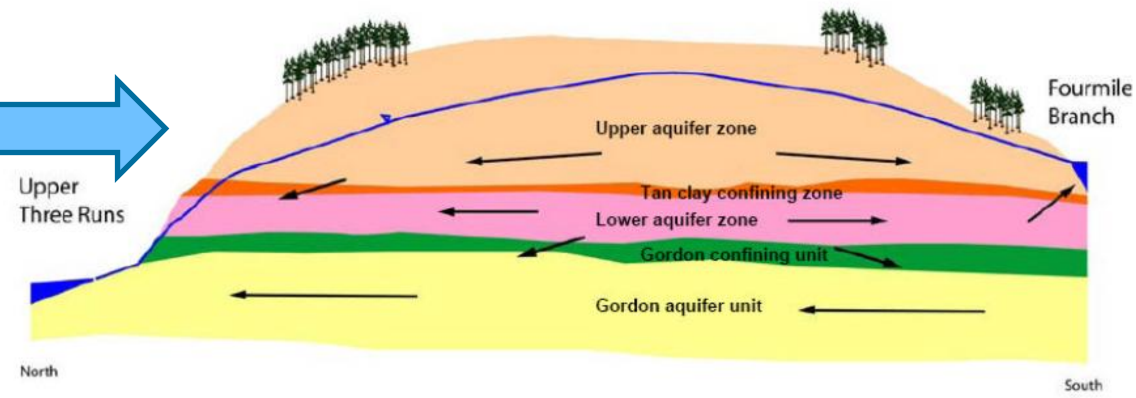
Groundwater Flow Physical System

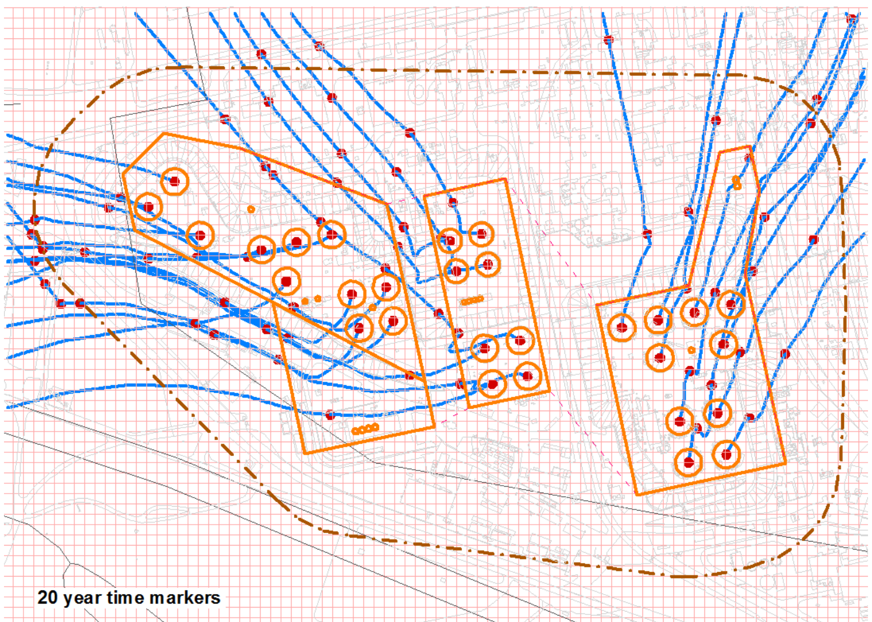


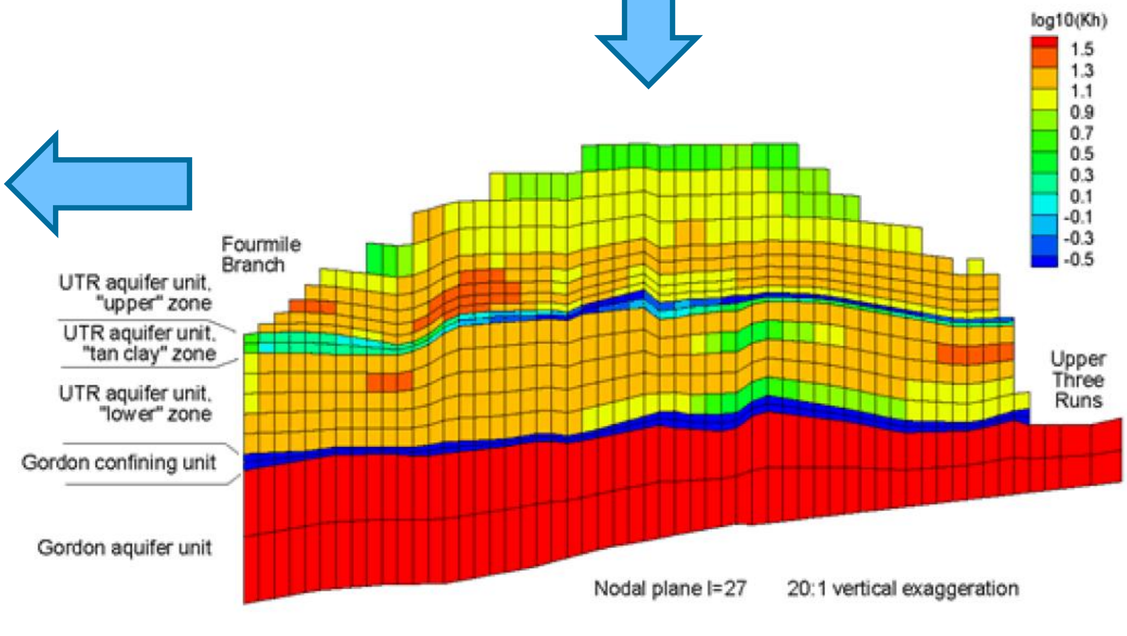


Groundwater Flow Physical Abstraction









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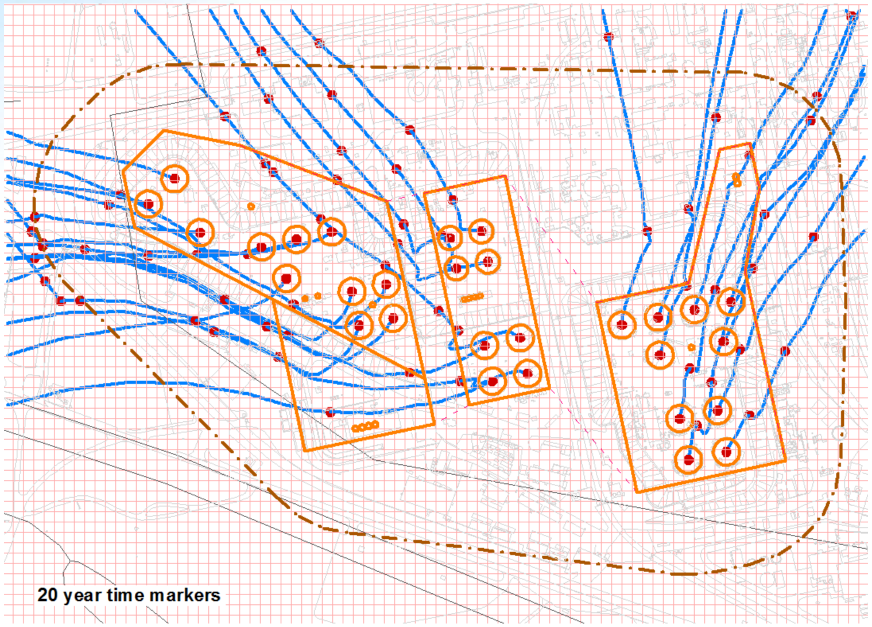
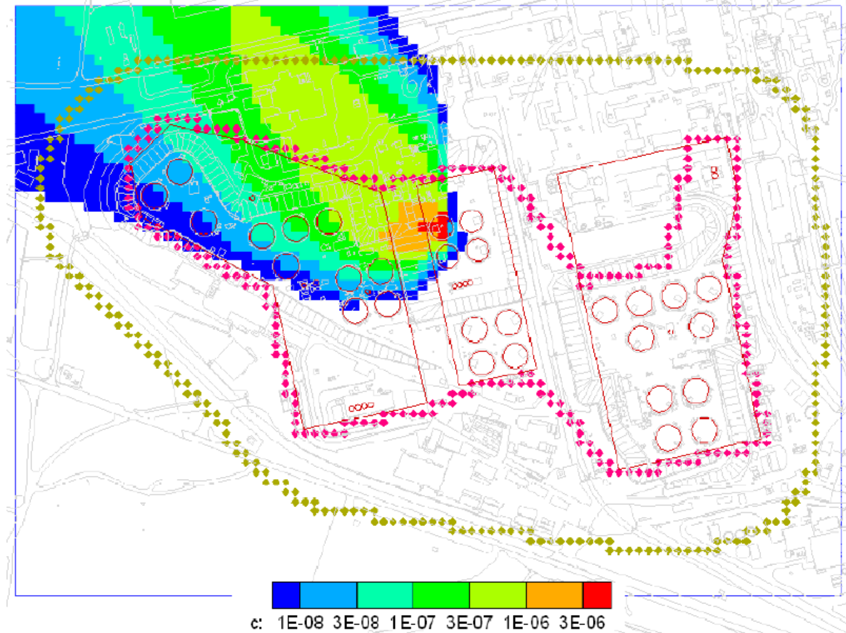
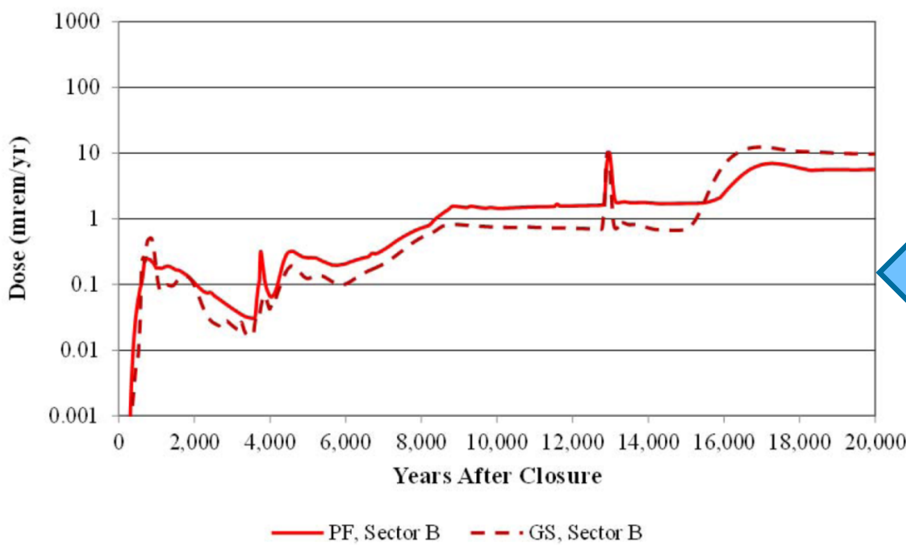
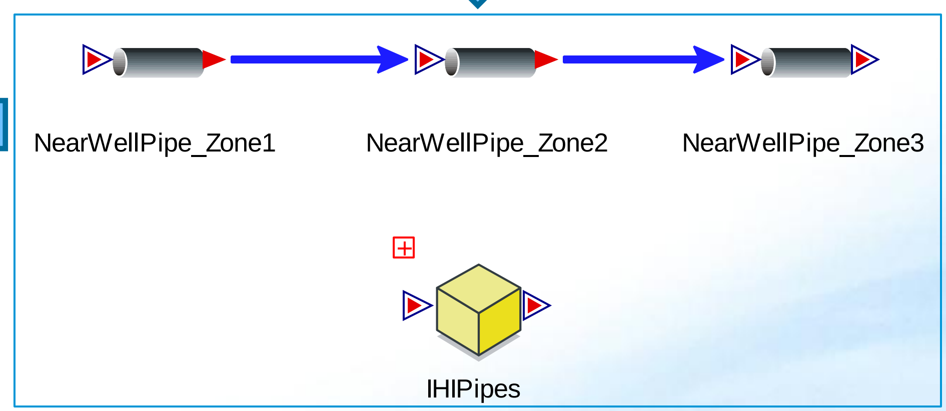
Groundwater Flow Model Abstraction









Significant Uncertainty

Sources of uncertainty

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

Uncertainties must be reduced and/or managed

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

Many modeling cases

Ambiguous / Multiple Objectives

Period of Performance?

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

"Reasonable" expectation / assurance?

- Subjective criterion
- Role of behavior (e.g. peaks) beyond period of performance

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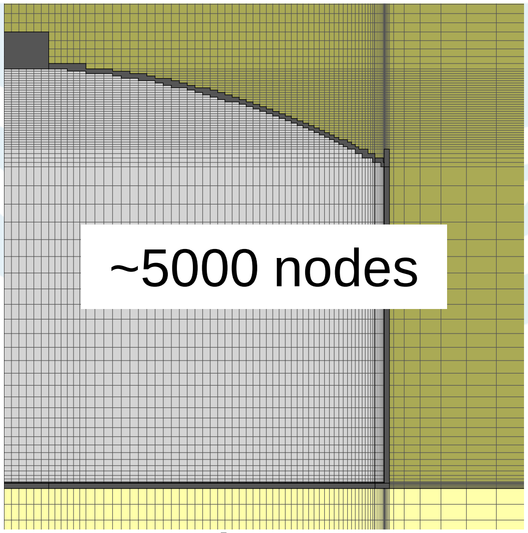
More modeling cases

Computing Demands: 14,400 simulations

Waste tank closure example



Vadose zone flow

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

Vadose zone transport

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

Aquifer transport

- 5200 simulations

Computing resource limitation

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Schedule Constraints

Performance Assessment

- Months to one year

Revisions

- Weeks to months

Comment response

- Days to weeks

Time and budget limitations

Software "Inertia"

Tendency to limit abstraction to that supported by current codes

- Familiarity = efficiency
- Procurement = time delay
- Habits

"Postulated" vs. "Predicted" Scenarios

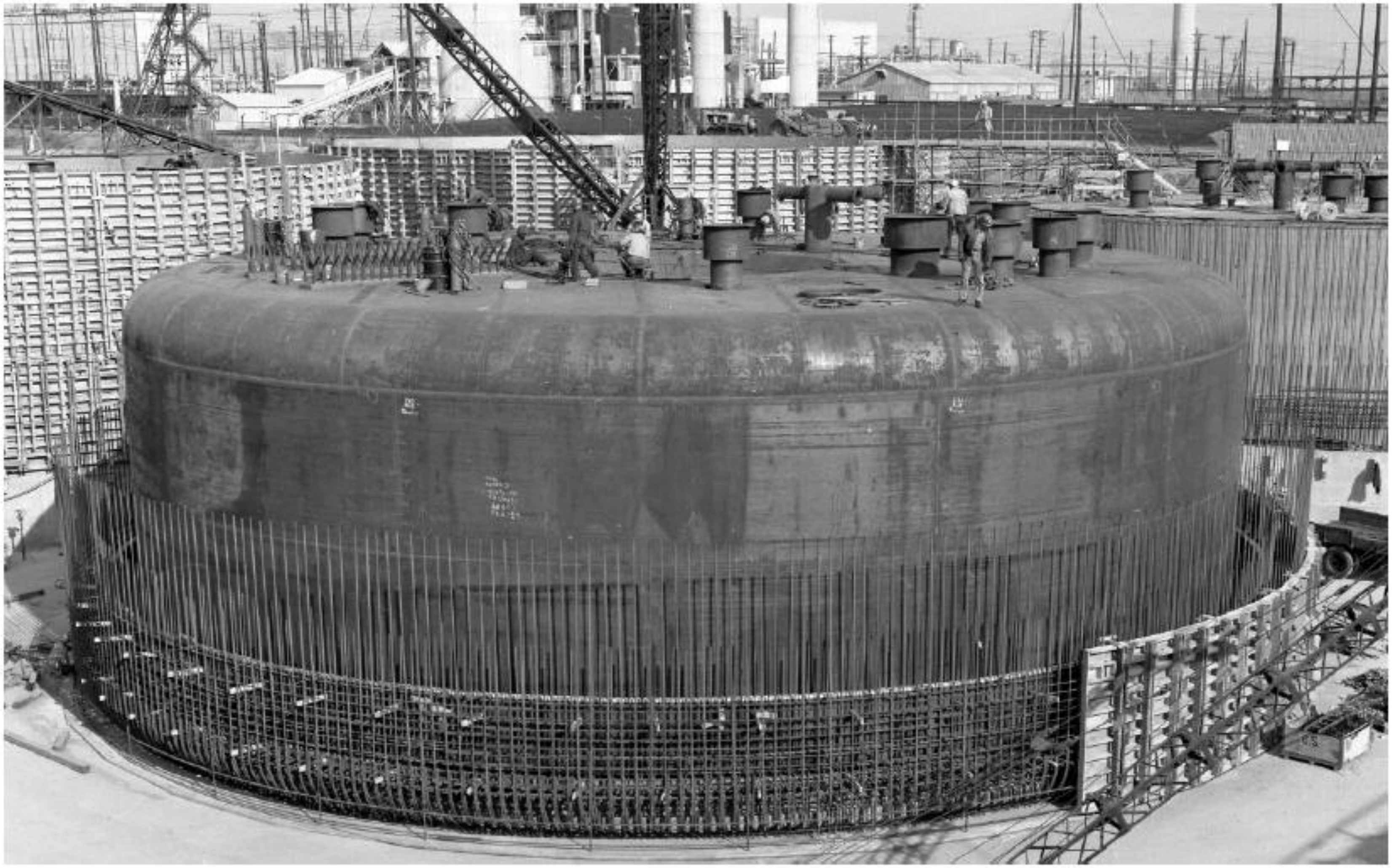
Definitions

- "Predicted" = derived from a first-principles (mechanistic) prediction of future conditions and system behavior
- "Postulated" = assumed without proof and accepted as potentially providing insight to future system behavior and consequences

Example motivations for postulated scenarios

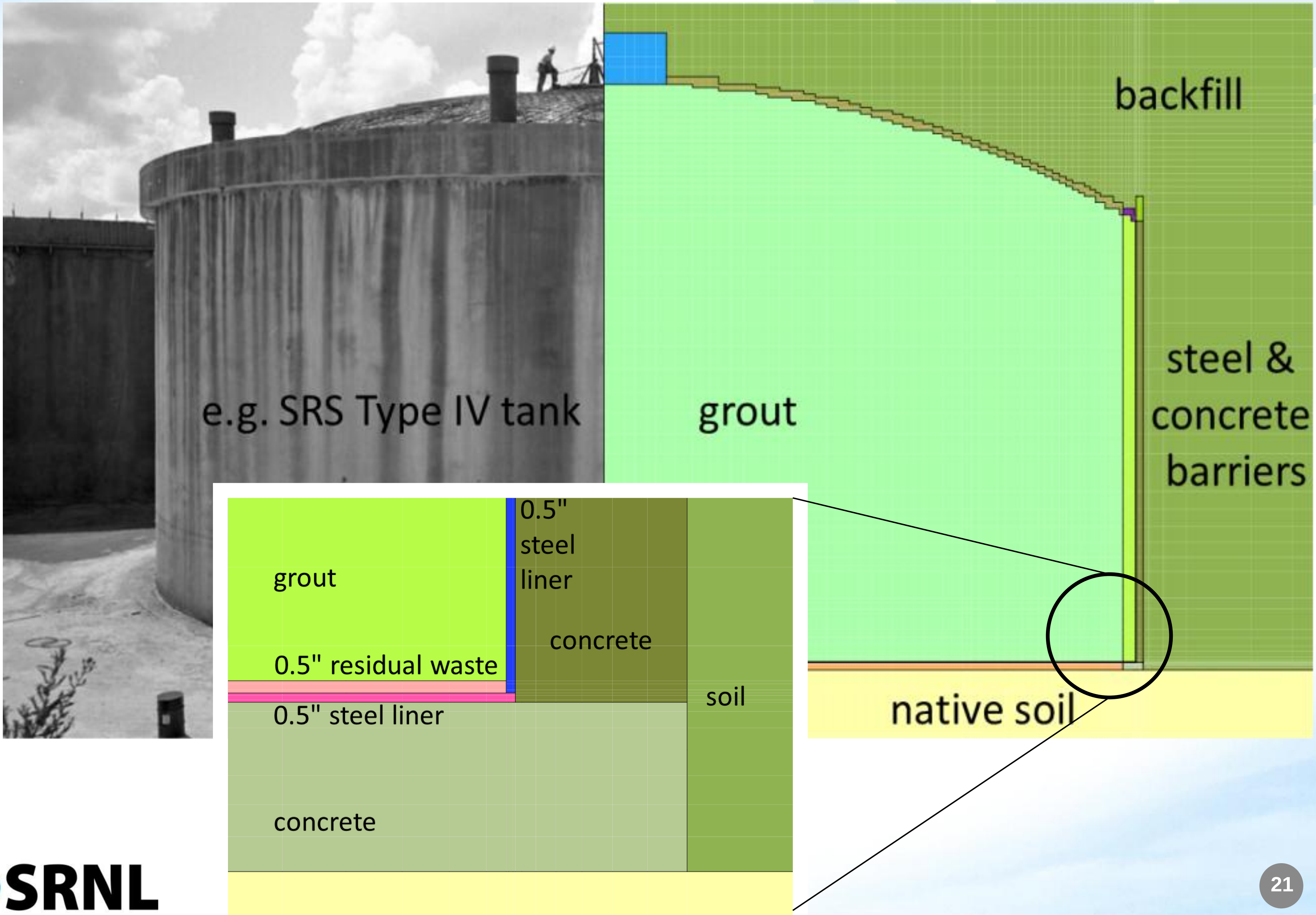
- Easy to describe and grasp by stakeholders
- Provide a point of reference, usually pessimistic / constraining
- Capture an alternative system behavior / performance

Waste Tank Construction – SRS Type II

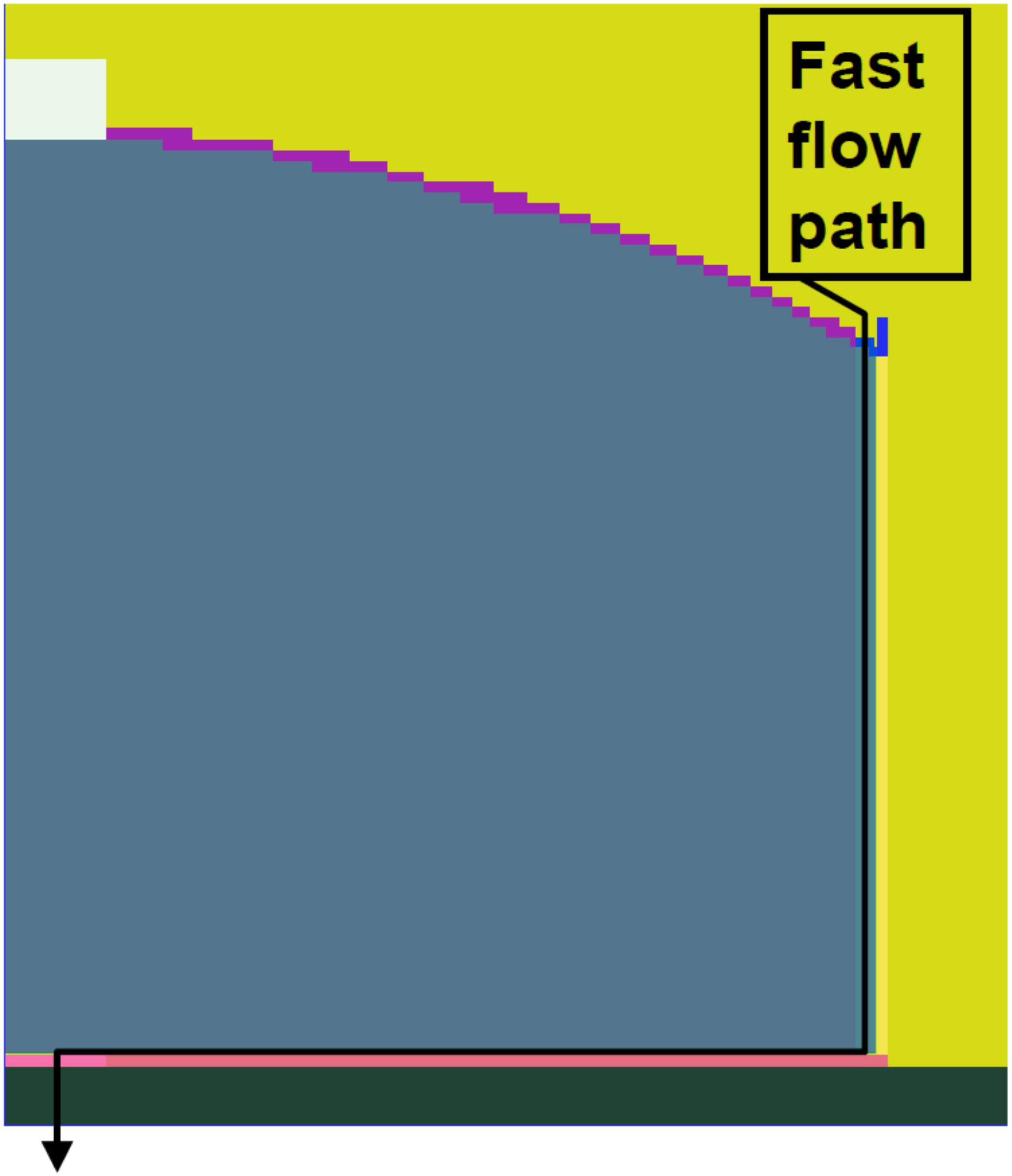


Waste Tank Construction – SRS Type IV

SRS Type IV Tank As Modeled



Postulated Case C and E Scenarios



Case A = Nominal

- As-designed performance
- Intact barriers

Case C

- Fast flow path
- Waste exposed to grout pore water

Case E

- Fast flow path
- Waste exposed to ground water chemistry

Validation of Model Abstraction?

Karl Popper

- Scientific theories (models) can only be invalidated

Bredehoeft and Konikow (Ground Water 1993, 2012)

- “Validation” and “verification” are not achievable in the sense understood by the public, and thus misleading
- Confidence bounds are helpful but do not account for model biases
- A model cannot be expected to reliably predict the future beyond the historical period for which the model has been vetted
- Critical decision is conceptual model selection

Conceptual Model (Abstraction) Errors

Mean square error: $\mathrm{MSE}(\hat{\theta}) = \mathrm{E}\left[(\hat{\theta} - \theta)^2\right].$

- Composed of variance + bias: $\mathrm{MSE}(\hat{\theta}) = \mathrm{Var}(\hat{\theta}) + \left(\mathrm{Bias}(\hat{\theta}, \theta)\right)^2.$
- Uncertainty quantification only addresses variance

Model abstraction bias

- Not addressed by probabilistic UQ and SA
- Most likely cause of a serious modeling deficiency

Most effective counter measures

- Multiple independent modeling efforts
- Multiple independent critical reviewers
- Formal report on model development

Lessons Learned / Best Practices

- **Postulated abstractions are useful for**
  - Understanding system behavior and performance limitations
  - Communicating with stakeholders
- **Conservatism is difficult to foresee in complex systems**
  - What is the conservative assumption?
- **Assigning significance to postulated cases is difficult**
- **Postulated tends to morph into predicted/expected with stakeholders**

Lessons Learned / Best Practices (cont'd)

- **Conceptual model deficiency is most significant vulnerability**
- **Multiple independent modelers and reviewers are most effective measures toward rooting out conceptual errors**
- **Need to document the process used to define abstracted modeling scenarios**
  - For communication to stakeholders
  - To ensure logical thought process
- **UQ and SA are more important than higher fidelity nominal simulations**

Key Points on Model Abstraction

- Driven in practice by both resource limitations and value gained from "postulated" rather than "predicted" scenarios
- Reducing physical reality to a mathematical concept is the greatest vulnerability, compared to simplification of an existing mathematical model
- Lessons-learned and best-practices reduce the chance of a serious Performance Assessment deficiency