Performance Assessment Insights on the Use of Cements in Waste Management

David Esh, Jacob Philip, Kenneth Snyder*

US Nuclear Regulatory Commission

*National Institute of Standards and Technology

david.esh@nrc.gov

AMP2010, Toronto Canada, November 10, 2010

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Overview

- Background
- Systems Evaluated and Model Description
- Analysis and Results
- Conclusions

Background

- Cementitious materials are used in a variety of applications.
- NRC performs independent modeling to develop risk insights.
- Desired performance can be much longer than engineering experience base.
- Risk insights can influence design and decision making.

Background – Performance Assessment

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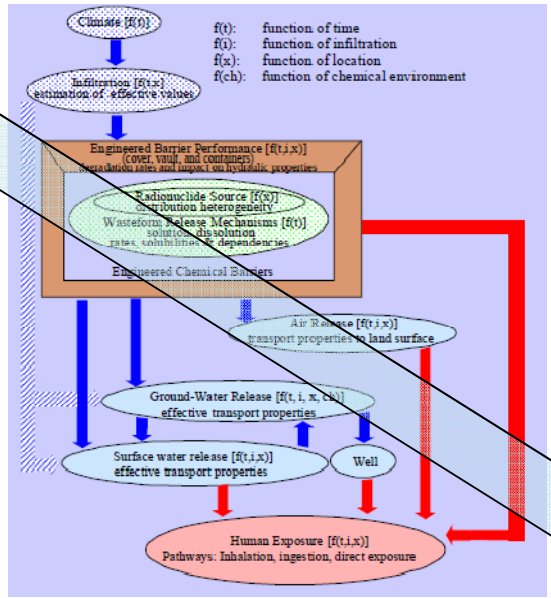
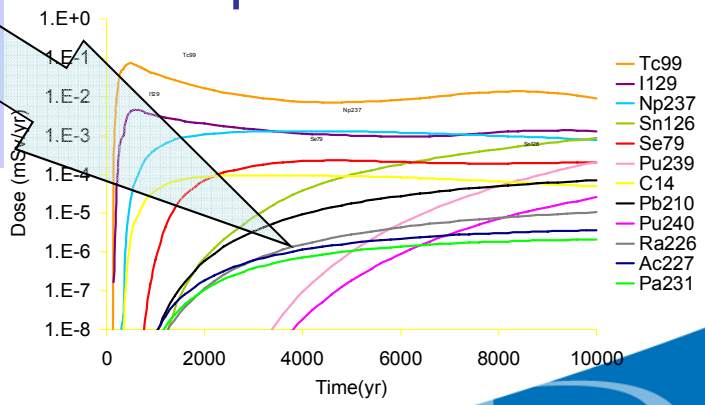
Real system

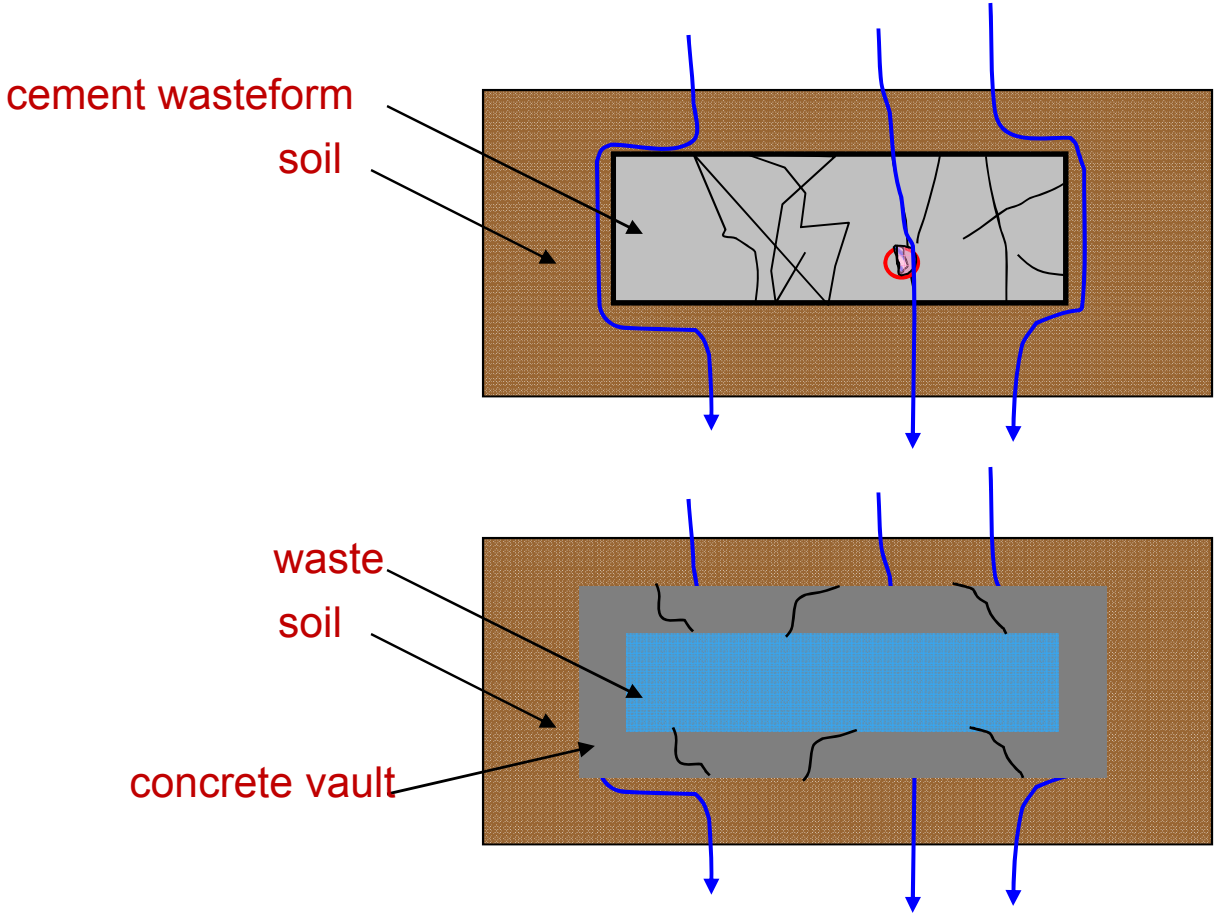


Mathematical model (abstraction)

Estimated future performance



Systems Evaluated



Wasteform – with and without cracks, inferior hydraulic properties, and degradation and oxidation

Vault – with and without cracks, inferior hydraulic properties

Model Development

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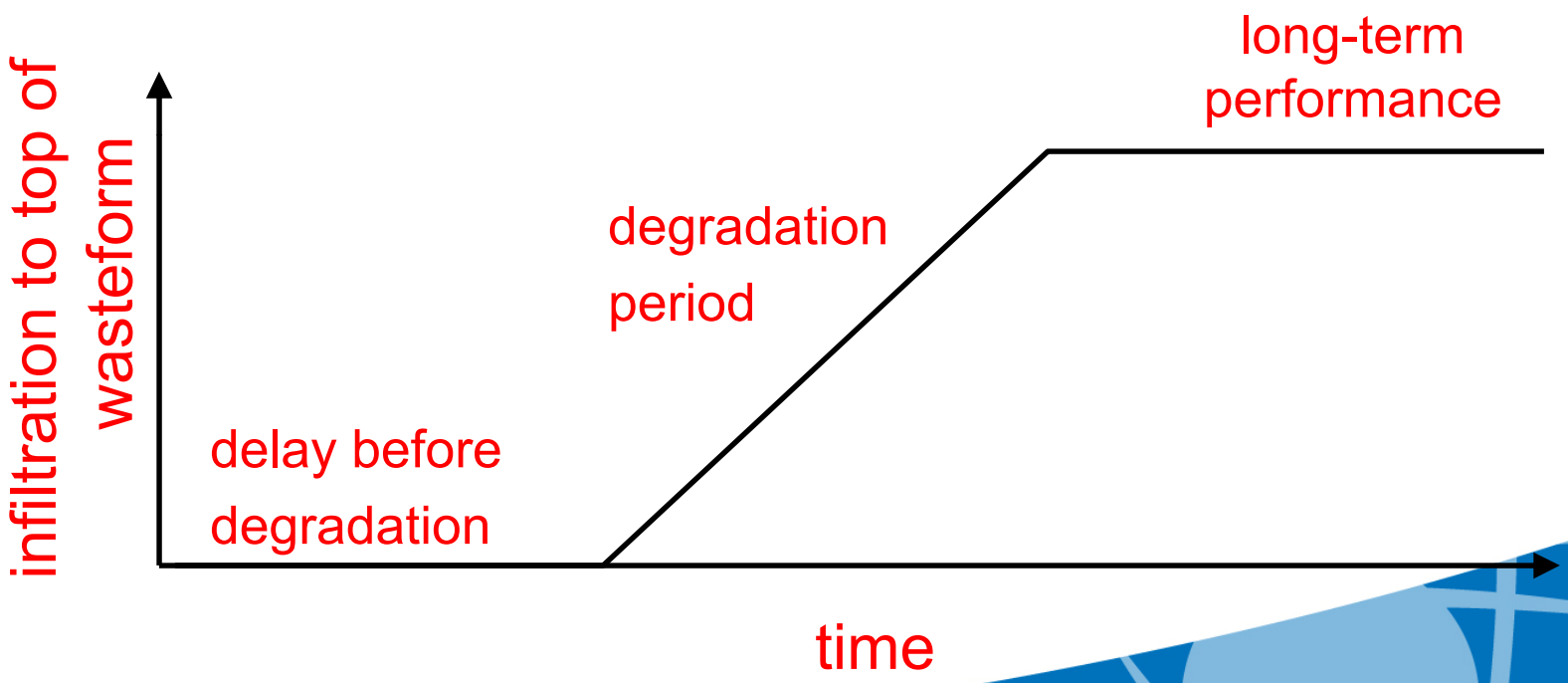
- GoldSim® software
- Probabilistic assessment
- Specialized elements facilitate radionuclide transport modeling
- 2,600 GoldSim elements, more than 300 stochastic elements
- Numerous submodels
  - Degradation of engineered cap
  - Oxidation of cementitious waste
  - Physical degradation of cementitious waste
  - Advective and diffusive releases
  - Transport in unsaturated and saturated zones
  - Dose assessment
- Modeling used abstractions

Engineered Cap Submodel

- Cap effectiveness implemented as factor that limits infiltration
- User specifies
  - Delay before degradation (constant)
  - Duration of degradation period (stochastic)
  - Long-term performance (stochastic)



Wasteform Degradation and Oxidation

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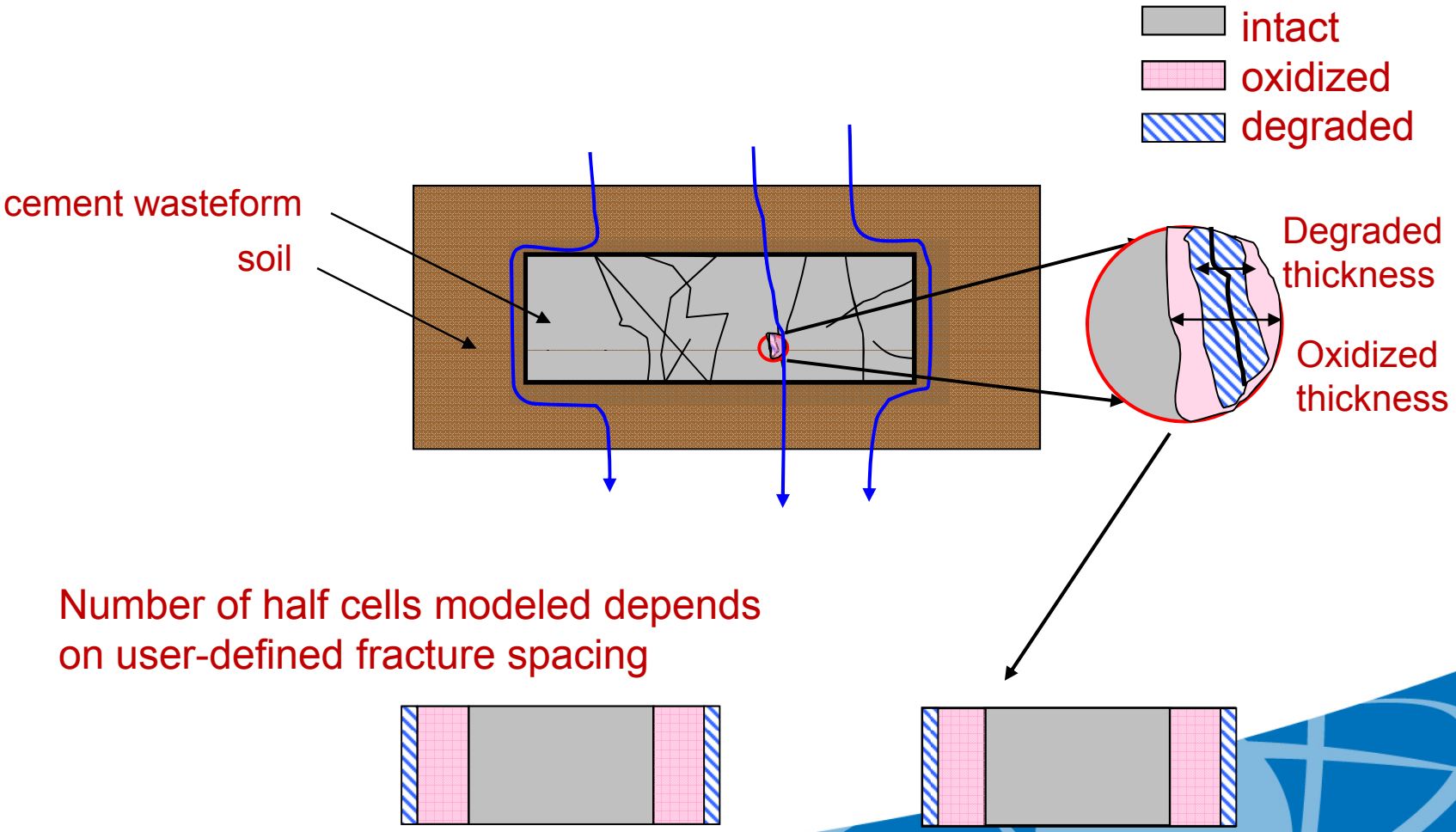
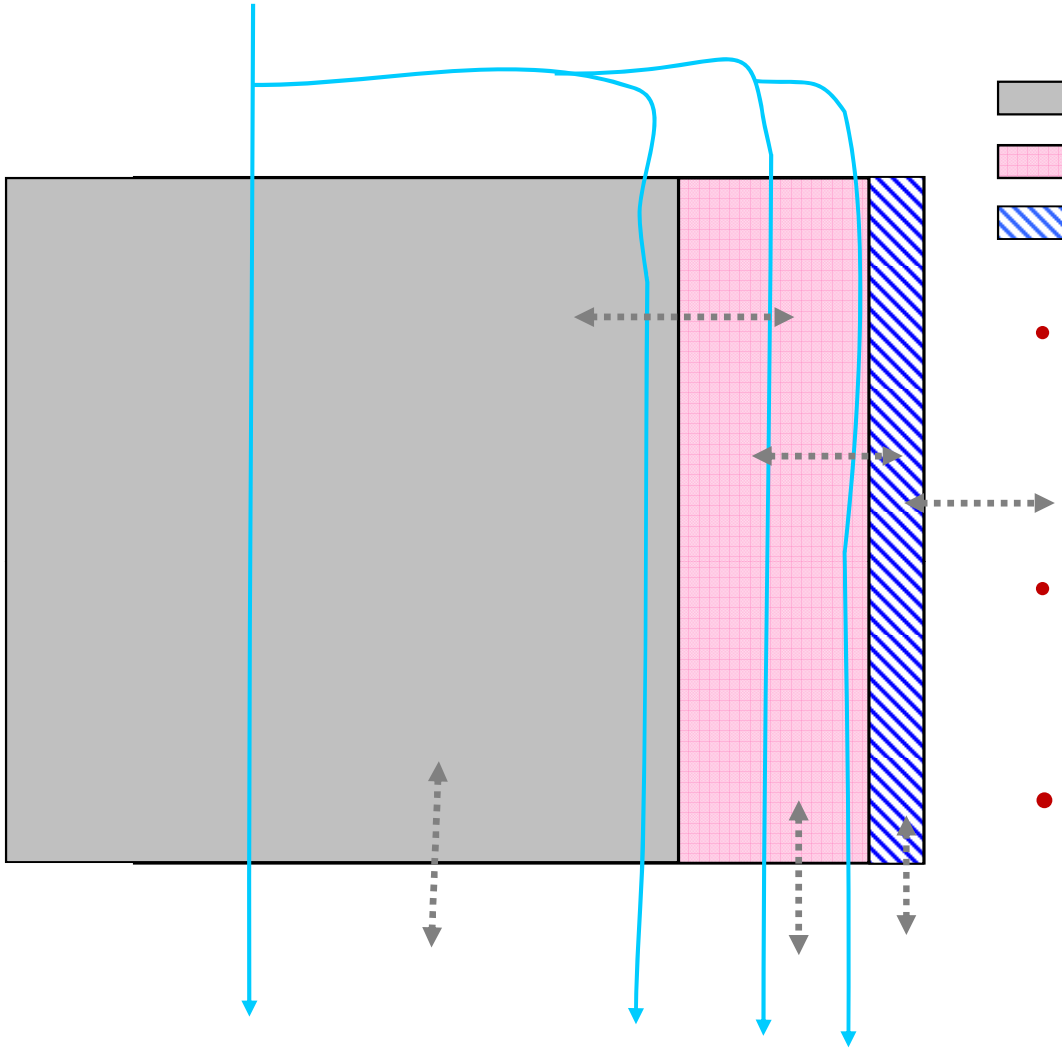


Number of half cells modeled depends on user-defined fracture spacing

Infiltration Thru Wasteform



intact
oxidized
degraded

- Flow diverted to next region as infiltration to region exceeds its saturated hydraulic conductivity
- Excess water is made available to fracture
- Diffusion and advection
  - between regions
  - between waste and the external environment

Degradation Representation

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$$DT(t) = 0.55\ C_c\ (C_m + C_s)\ t$$

DT(t) = degraded thickness (cm)
0.55 = empirical constant (cm · L)/(moles · yr)
C_c = weight percent of tricalcium aluminate in unhydrated cement
C_m = concentration of magnesium in the bulk solution (moles/L)
C_s = concentration of sulfate in the bulk solution (moles/L)
t = time (yr)

Atkinson, A., and Hearne, J.A. (1984), An Assessment of the Long-Term Durability of Concrete in Radioactive Waste Repositories, AERE-R11465. Harwell, U.K.

Oxidation Representation

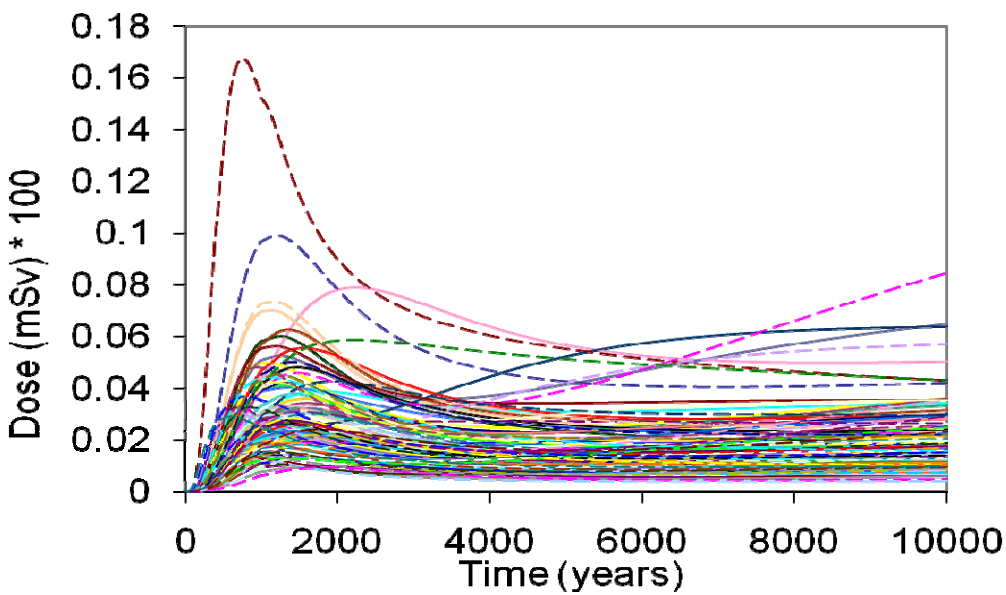
$$OT(t) = [\,(8D\theta\tau C_{O2}\,t) / \Xi\,]^{1/2}$$

OT(t) = penetration depth of the redox front (cm)
D = diffusion coefficient of oxygen in water (cm^2/s)
θ = volumetric water content
τ = tortuosity (geometry correction factor)
C_{O2} = concentration of oxygen outside the waste form ($moles/cm^3$)
Ξ = equivalents of reduced material per unit volume of the waste form ($equivalents/cm^3$)
t = time (s)

Smith, R.W. and J.C. Walton (1993), "The Role of Oxygen Diffusion in the Release of Technetium from Reducing Cementitious Waste Forms." Mat. Res. Soc. Symp. Proc.U ***294****: 247.*

Analysis Approach

- Run probabilistic base-case model (100 realizations, limit to ^{99}Tc and ^{226}Ra)
- Perform genetic analysis of base-case probabilistic results using Neuralworks Predict®
- Define and run alternative cases



Neuralware (2001), Neuralworks Predict® Product Version 2.40, Carnegie, PA.

Analysis Cases - Results

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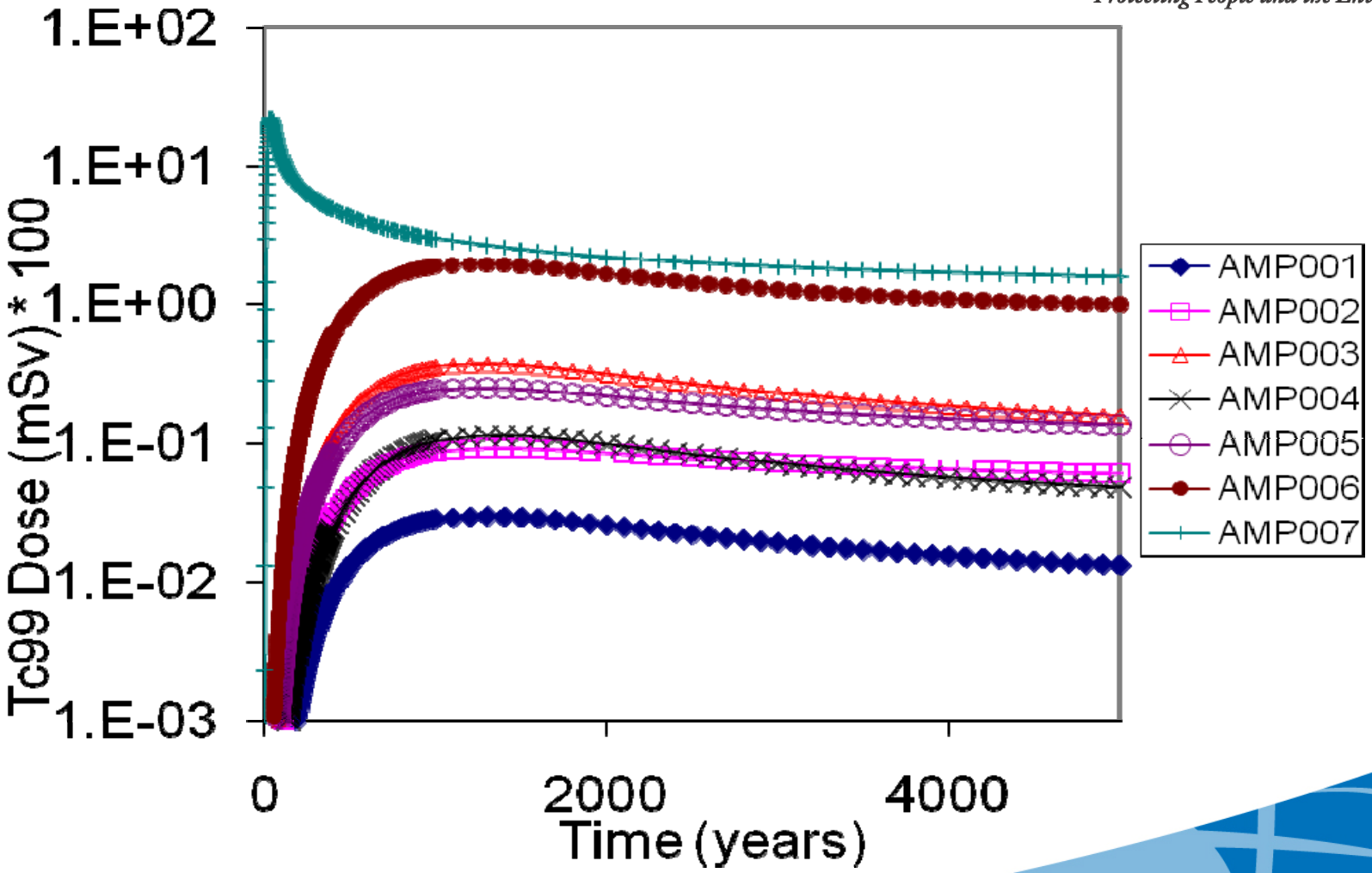
Case ID	Case Description	Description	^{99}Tc Ratio*	^{226}Ra Ratio*
A001	Ideal vault and wasteform	Idealized case - small-scale laboratory measurements of surrogate samples. No degradation. Parameterization described in the text.	1	1
A002	Field properties	100x larger Kh's (all regions) 100x larger De Waste porosity = [0.45-0.55] uniform	3	40
A003	Fractures	F = 10 m	10	10
A004	Degradation	DT = 5.3 cm, OT = 5.5 cm	4	1
A005	Field properties + Fractures	100x larger Kh's F = 10 m	8	60
A006	Field properties + Fractures + Degradation	100x larger Kh's F = 1 m DT = 5.3 cm, OT = 5.5 cm	70	80
A007	Case A006 + non-ideal cap	As indicated for A006 Infiltration increased to 10-15 cm/yr	700	30,000
B001	Ideal vault	Identical to case A001 but no credit for wasteform, only the vault.	1[a]	1[a]
B002	Field properties vault	10x larger Kh	9	10
B003	Fractures	Fractured vault	260	70

* - the ratios are calculated relative to the results for case A001. For example, the Ratio in the next to the last column for Case A002 is calculated as (peak Tc dose for A002/peak Tc dose for A001)

Analysis Cases - Results



Key Variables

	A003 (fractures)	A006 (fractures+degraded)	B002 (resistive)
Tc	Fracture width K_h (intact grout) Groundwater flow rate	Fracture width K_h (intact grout) Groundwater flow rate Nm (degradation) K_h (degraded grout)	K_h (vault floor) K_d Waste Groundwater flow rate
Ra	Fracture width Infiltration rate Groundwater flow rate K_d Ra UZ Fracture saturation	Fracture width Infiltration rate Groundwater flow rate K_d Ra UZ K_d Ra degraded grout	K_h (vault floor) Groundwater flow rate K_d Ra UZ

Conclusions

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- Uncertainties and coupling of processes can result in non-intuitive results with respect to barrier performance.
- Conservative modeling choices may be difficult to identify without detailed analysis.
- Initial fractures and processes that initiate fractures can be important to long-term performance.