REPRESENTATIVE PATHWAY LENGTH FOR CONTAMINANT TRANSPORT IN PERFORMANCE ASSESSMENT MODELS

Osvaldo Pensado,[1] *Stuart Stothoff,*[1] *Jin-Ping Gwo*[2]

[1]Center for Nuclear Waste Regulatory Analyses (CNWRA®)
Southwest Research Institute®
San Antonio, Texas, U.S.A

[2]U.S. Nuclear Regulatory Commission (NRC)
Office of Nuclear Material Safety and Safeguards
Division of High-Level Waste Repository Safety
Washington, DC, U.S.A

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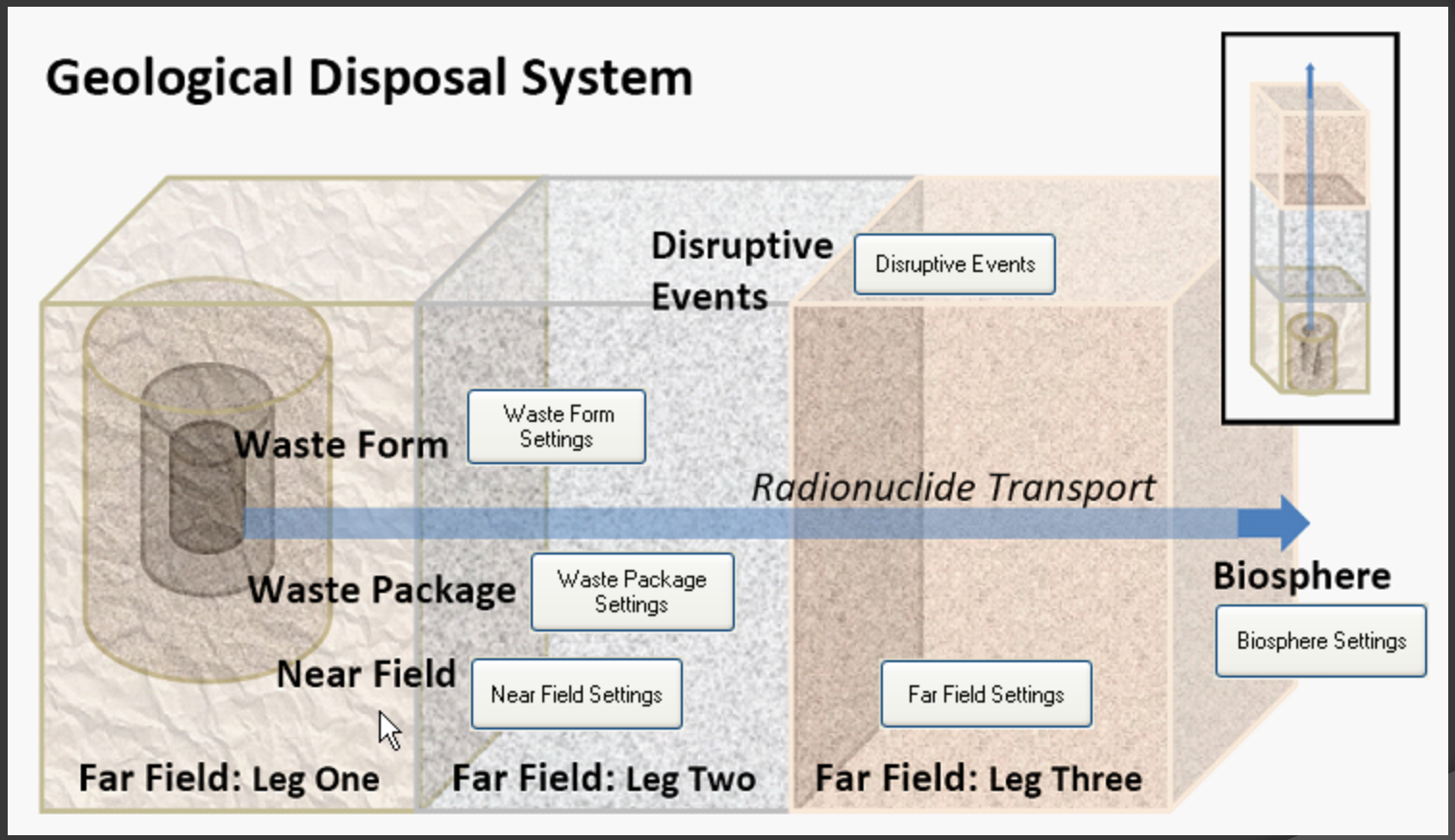
Outline

- Background
- Problem Statement
- Problem Analyzed with an Example
- Conclusions

Background


Geological Disposal System
Disruptive Events
Disruptive Events
Waste Form
Waste Form Settings
Radionuclide Transport
Waste Package
Waste Package Settings
Biosphere
Biosphere Settings
Near Field
Near Field Settings
Far Field Settings
Far Field: Leg One
Far Field: Leg Two
Far Field: Leg Three

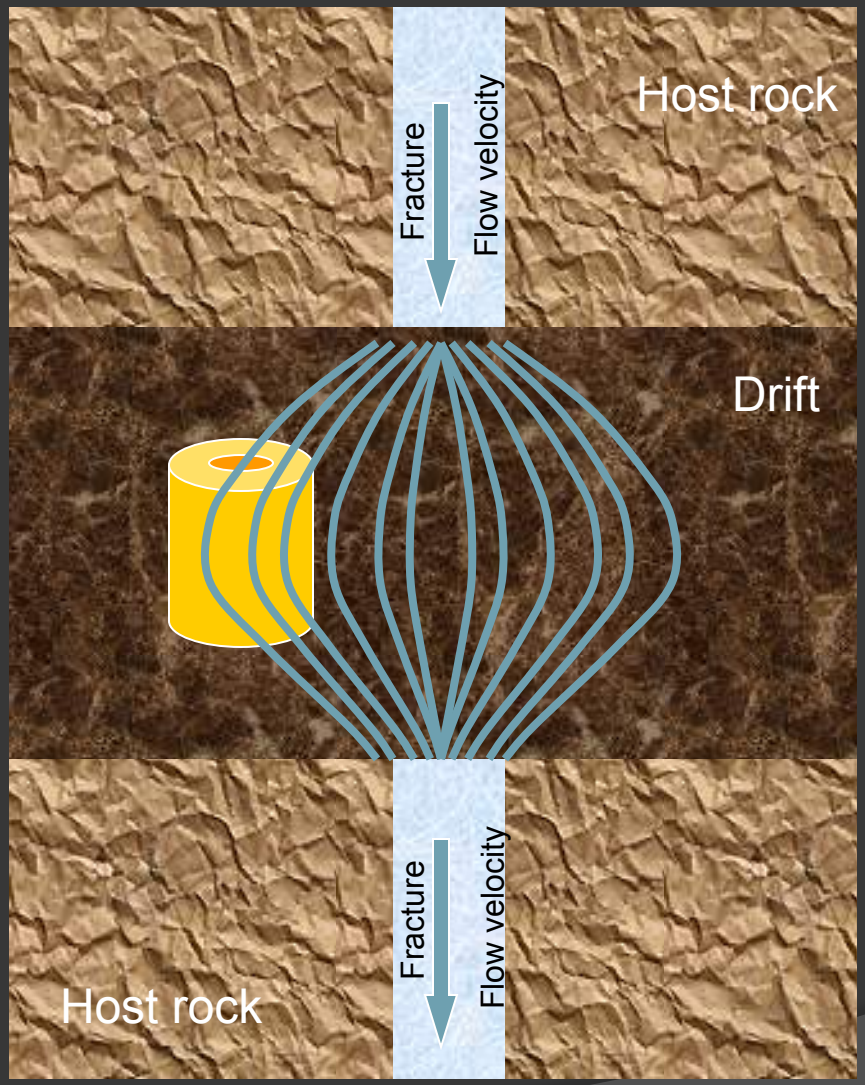
Simplicity in Performance Assessment Models

- Simplicity: desirable outcome
  - Clarity and legibility
  - Computational performance
  - Minimization of data input
  - Consistency with state of knowledge
  - Modeling appropriate for intended purpose (e.g., regulatory decision, scientific hypothesis testing)
- Working against simplicity
  - Researcher bias (background and interest of developer)
  - Stakeholder questions
  - Compliance requirements
  - Model needed to evaluate importance of physical aspect

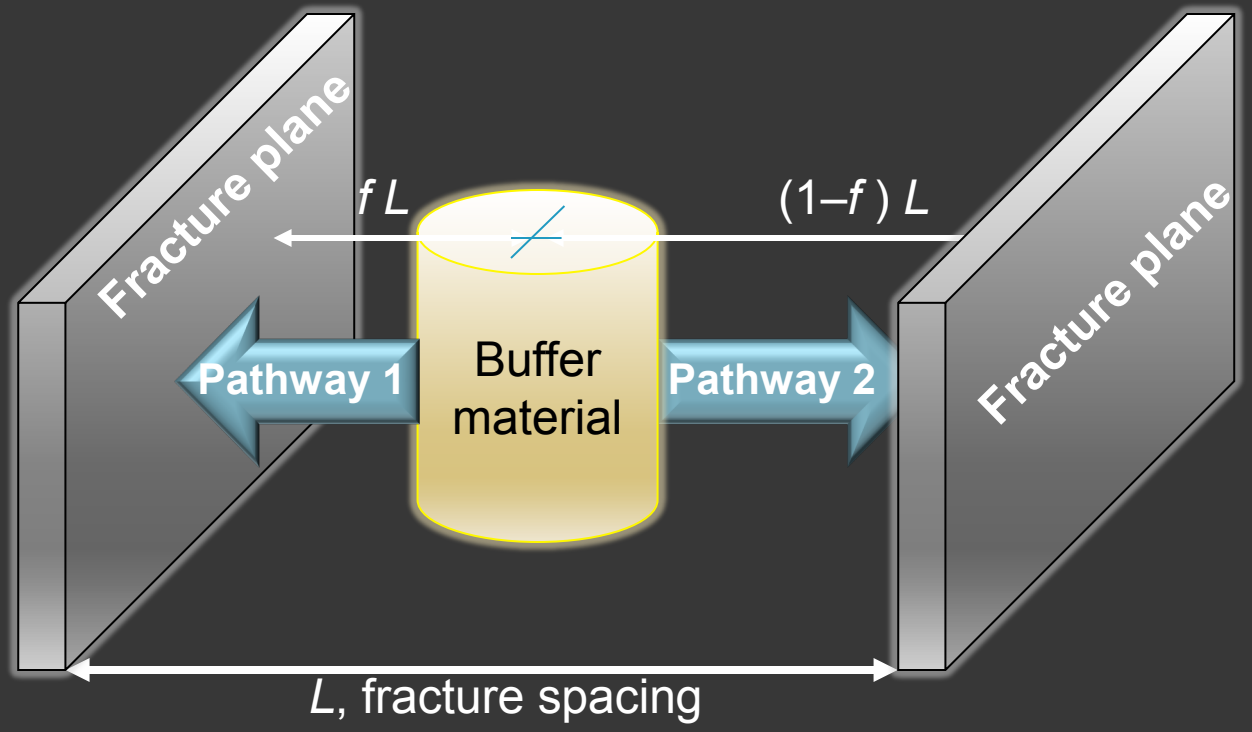
Question

- Can *simple models* be constructed *preserving attributes* of detailed or complex models?
- *Simple model* = single model component that disregards heterogeneity or variance in any single realization
- *Preserving attributes* = simple model yields similar output as detailed model

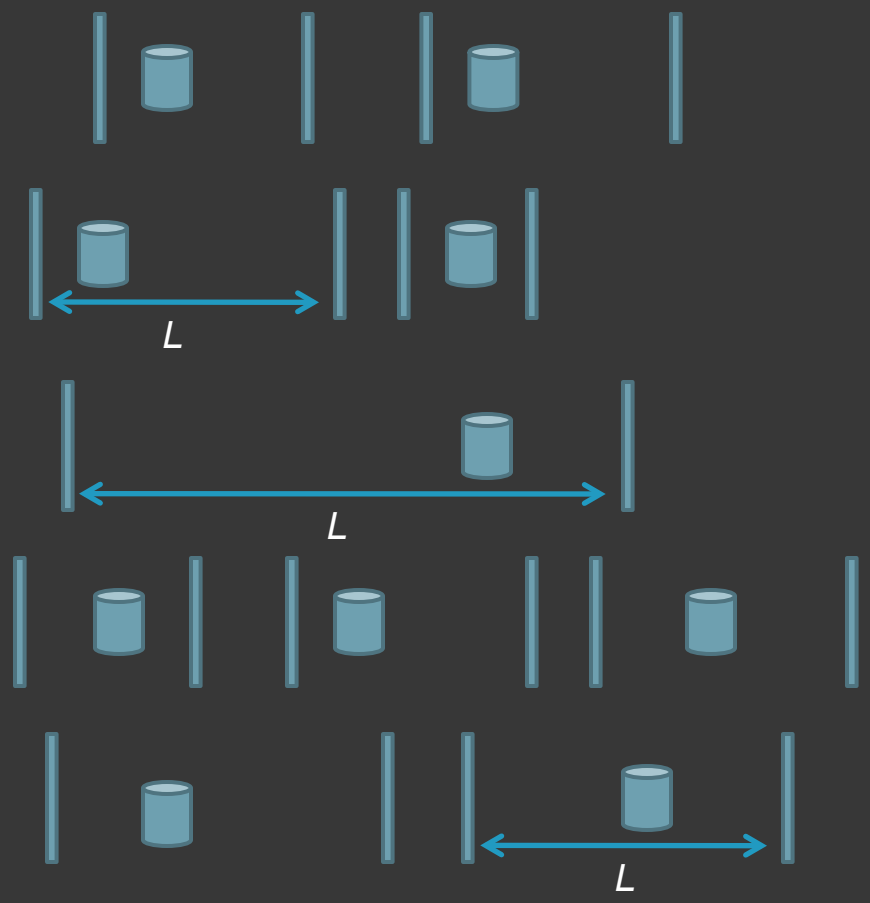
Description of Example Problem



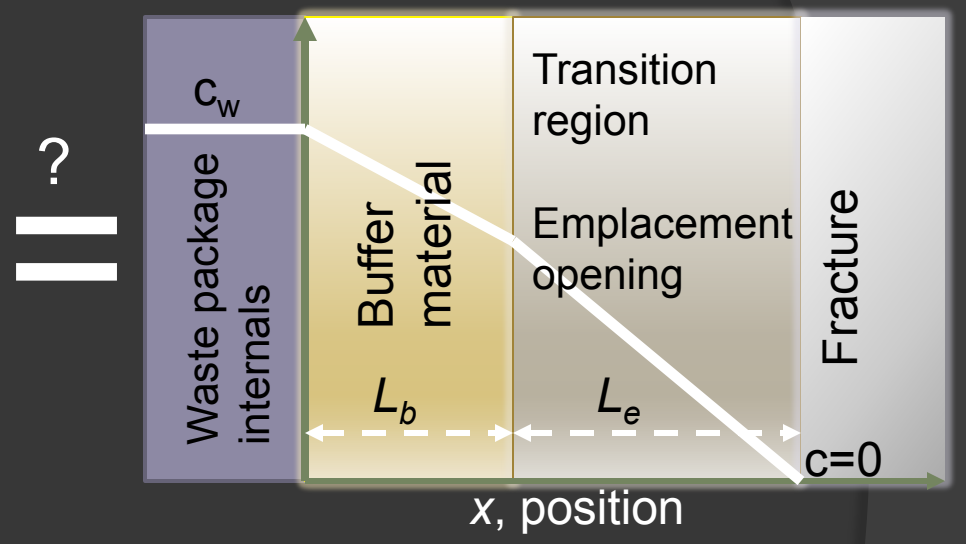
Abstraction



Ensemble (detailed model)



Representative (simple model)



L_e = ?

$$r = \int_0^\infty \rho(L) \int_0^1 F(L, f)\, df\, dL$$

$$r = \frac{1}{\alpha L_e + 1}$$

r = dimensionless release into fractures

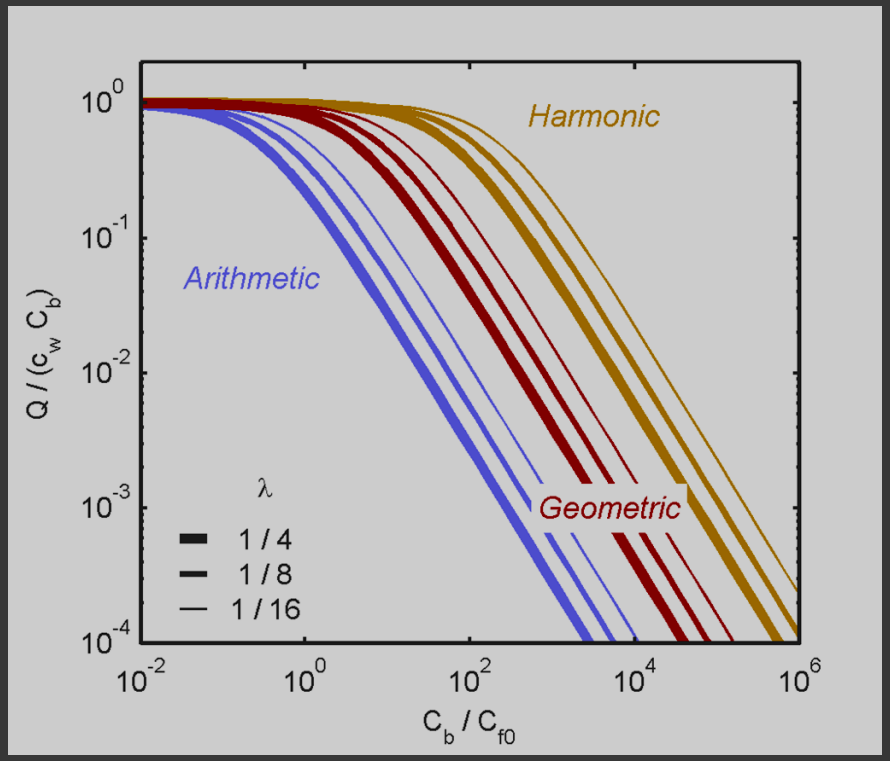
Approaches to Compute Parameters for the Representative Element

- Sample L_e
- Arithmetic average $$L_a = \int_0^\infty L\,\rho(L)dL$$
- Harmonic average $$L_h = \left[\int_0^\infty L^{-1}\,\rho(L)dL\right]^{-1}$$
- Geometric average $$L_g = \exp\left[\int_0^\infty \ln(L)\;\rho(L)dL\right]$$
- Find L_e as in a parameter estimation problem: fitting total release as a target

Results (Common Averages)

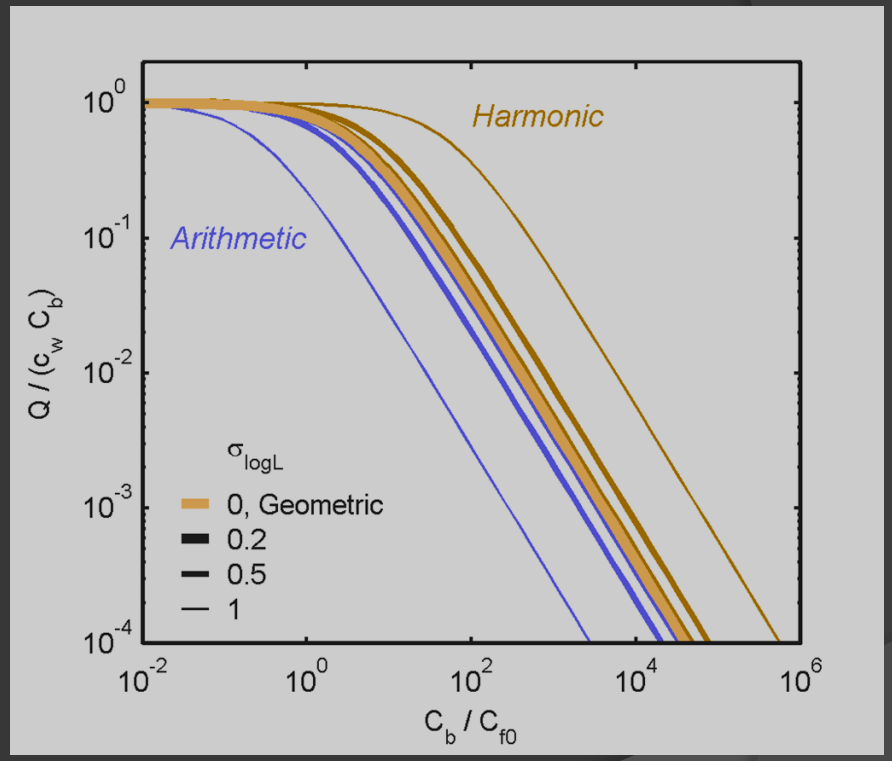
$$\frac{Q}{c_w C_b} = r = \frac{1}{\alpha \lambda L_{a,h,g} + 1}$$

λ = relative waste package location = 1/4



Buffer conductance/Transition region conductance

Dimensionless flux at fracture

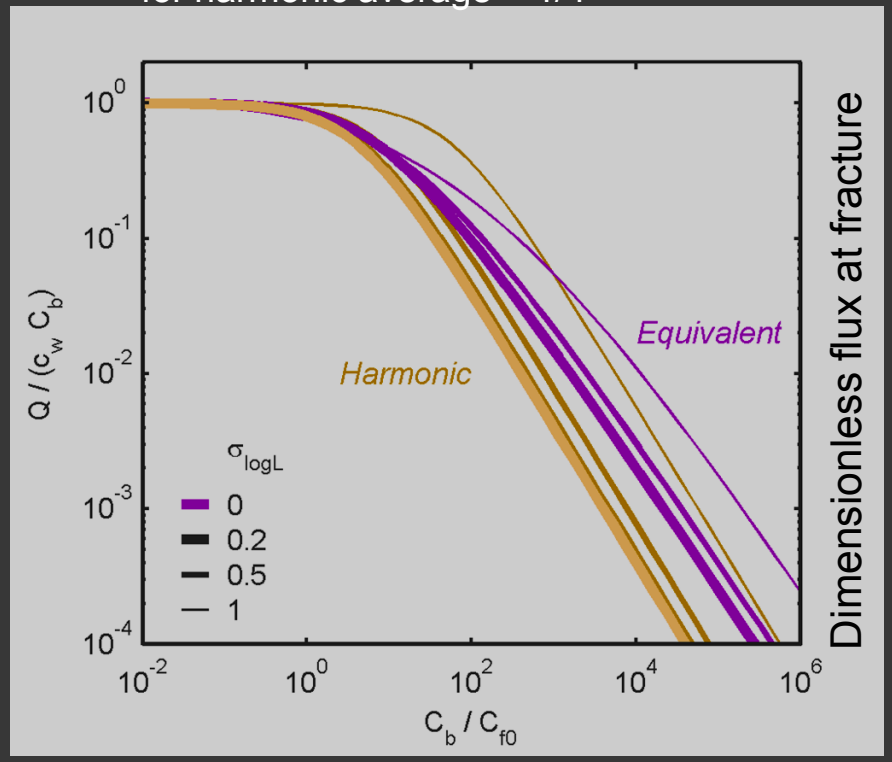


Buffer conductance/Transition region conductance

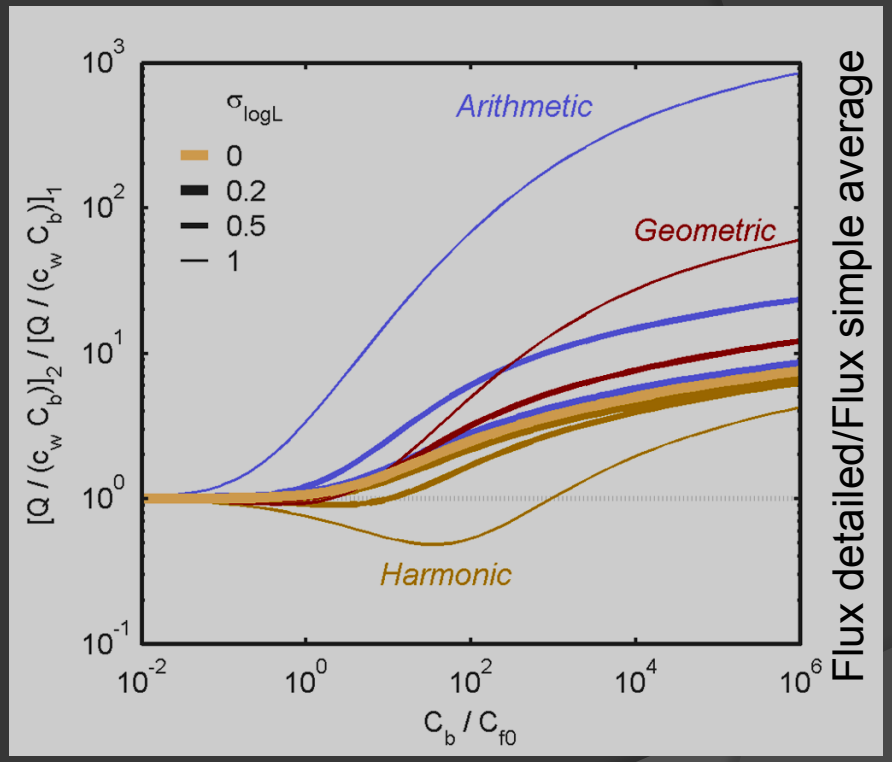
Results (Detailed Model)

$$\frac{Q}{c_w C_b} = r = \int_0^\infty \rho(L) \int_0^1 F(L, f)\, df\, dL$$

λ = relative waste package location for harmonic average = 1/4



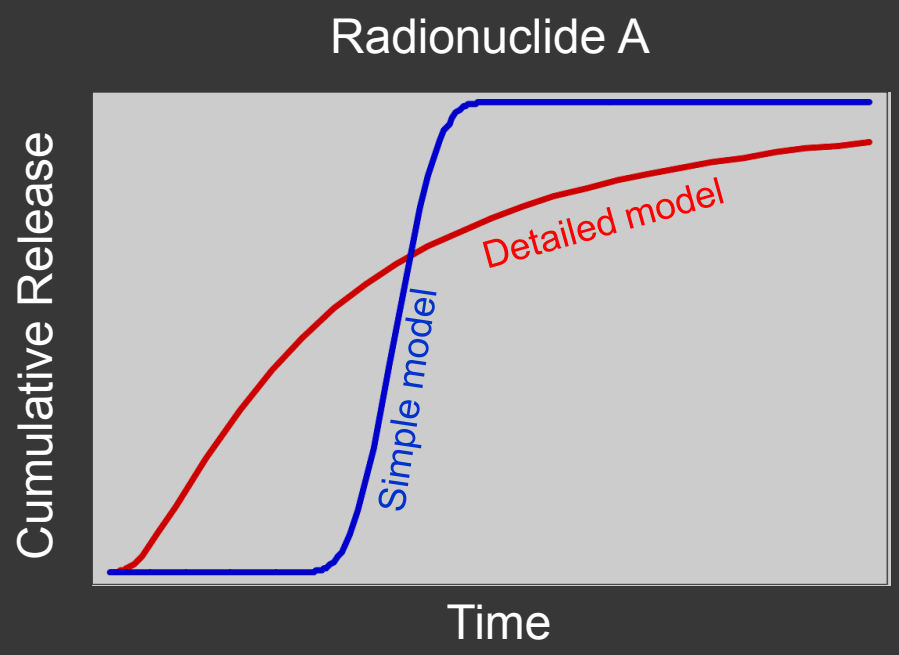
Buffer conductance/Transition region conductance

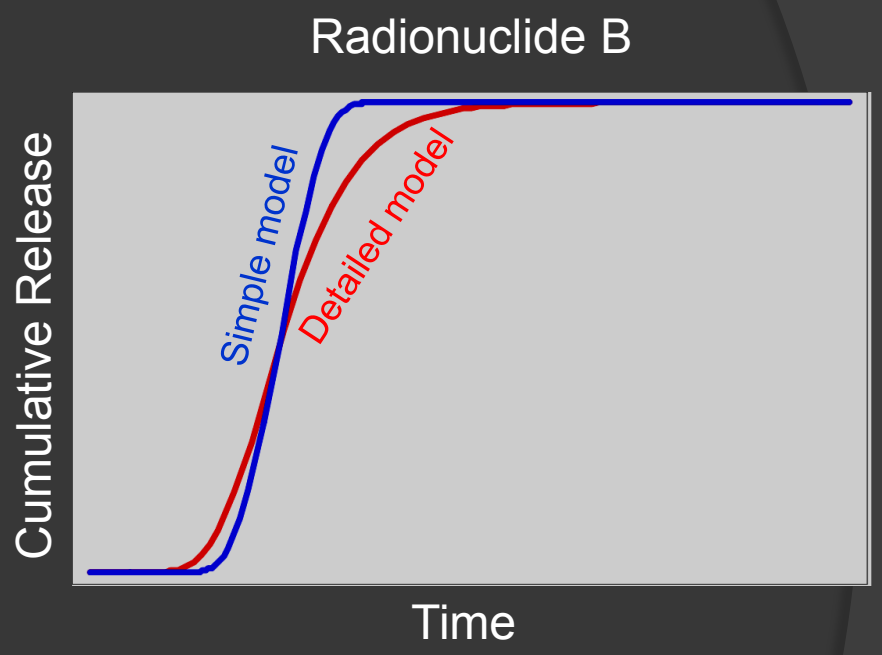


Buffer conductance/Transition region conductance

Observations

- Finding equivalent fracture spacing is possible (computing elaborated integrals needed)
- Other parameters can exhibit variance (e.g., diffusivity, distribution coefficients, solubility), be radionuclide dependent, or depend on other factors (e.g., temperature, water chemistry): difficult (or impossible) to define one accurate representative spacing for all radionuclides
- This example was steady state. Temporal variations bring additional complexity


Radionuclide A
Cumulative Release
Time
Simple model
Detailed model


Radionuclide B
Cumulative Release
Time
Simple model
Detailed model

Conclusions

- Problem of properly defining a representative element was examined with an example
- In general, a representative element can only approximate the ensemble behavior
- Depending on the purpose of the model, explicit representation of heterogeneity/variance may be needed

Acknowledgement

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