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Waste Form Modeling:

Status and Needs for Future Waste Forms

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Outline

- Context for Waste Form Modeling
  - Performance Assessment of Geologic Repositories
- Structure and Process for Performance Assessment
  - Examples from Yucca Mountain
- Challenge for Waste Form Models

Context for Waste Form Modeling : Performance Assessment of a Geologic Repository

For the Yucca Mountain Project:

Performance assessment means an analysis that:

(1) Identifies the features, events, processes (except human intrusion), and sequences of events and processes (except human intrusion) that might affect the Yucca Mountain disposal system and their probabilities of occurring during 10,000 years after disposal;

(2) Examines the effects of those features, events, processes, and sequences of events and processes upon the performance of the Yucca Mountain disposal system; and

(3) Estimates the dose incurred by the reasonably maximally exposed individual, including the associated uncertainties, as a result of releases caused by all significant features, events, processes, and sequences of events and processes, weighted by their probability of occurrence. (10 CFR 63.2)

Four Questions Underlying Performance Assessment

- **Q1: What can happen?**
- **Q2: How likely is it to happen?**
- **Q3: What are the consequences if it does happen?**
  - **Kaplan and Garrick "risk triplet"**
  - **Used to structure performance assessment for WIPP, Yucca Mountain Project, internationally**
- **Q4: What is the uncertainty in the answers to the first three questions?**

Treatment of Uncertainty

- Types of uncertainty
  - Aleatory: inherent uncertainty about the future
  - Epistemic: lack of knowledge about repository system
    - Parameter and model uncertainty

- Aleatory uncertainty
  - Set of scenarios (with probabilities of occurrence)
- Parameter uncertainty
  - Probability distributions on model inputs
- Model uncertainty
  - YMP approach: select a model, consider alternates, apply conservative and bounding criteria to justify selection

Iterative Performance Assessment Methodology

- **Identify features, events, processes (FEPs)**
- **Screen FEPs for inclusion or exclusion**
  - Process models may be developed for included and excluded FEPs
  - Uncertainty explicitly addressed in included FEPs
- **Incorporate included FEPs in system-level model**
  - Generally start with minimum acceptable detail
- **Conduct uncertainty and sensitivity analyses**
  - Estimate repository performance with uncertainty
  - Which uncertain inputs contribute to uncertainty in output?
  - Which FEPs contribute to magnitude of output?

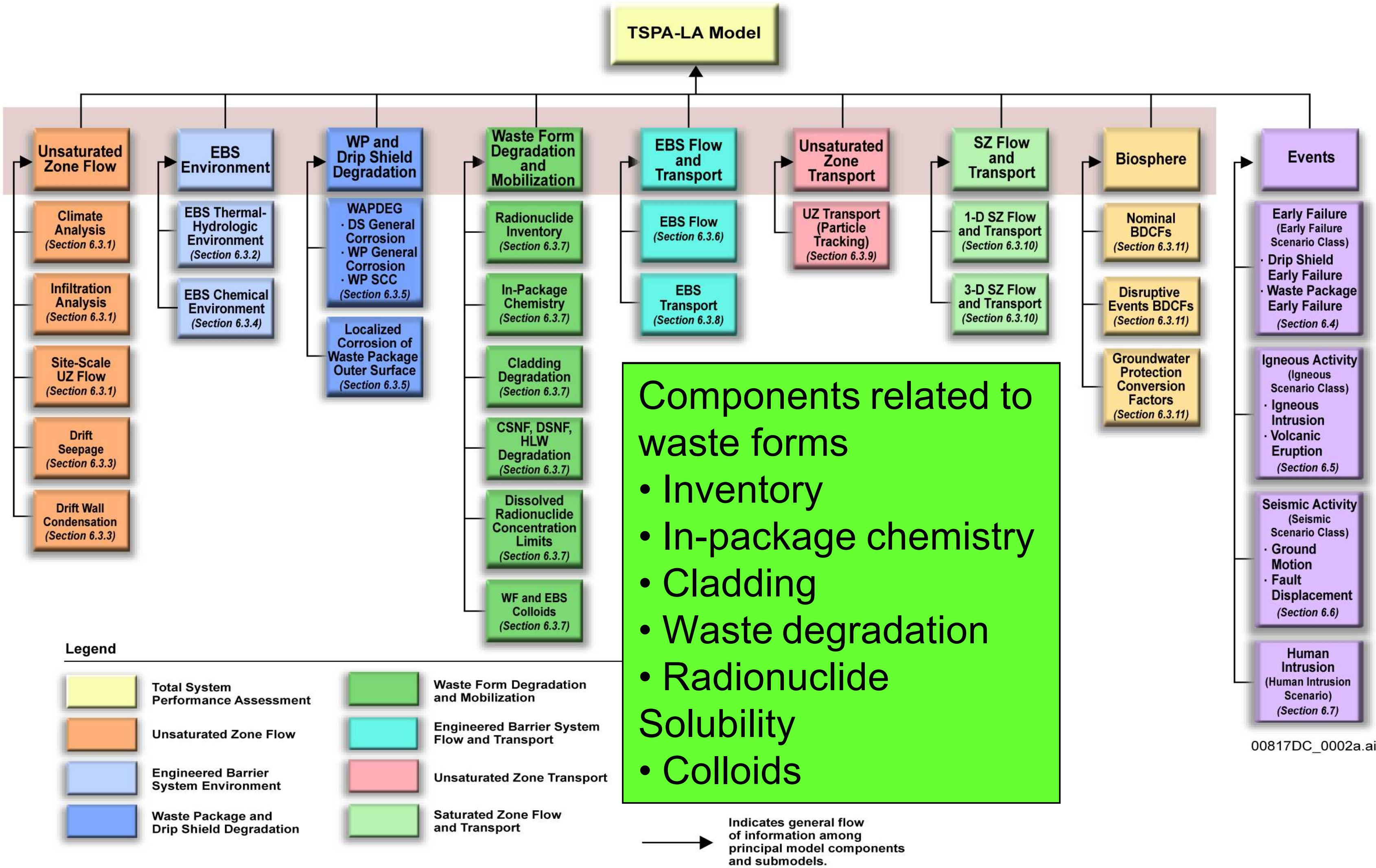
Iterative Performance Assessment Methodology (cont.)

- **Risk-informed iteration**
  - Ideally, adjust detail and uncertainty commensurate with process importance
    - Add detail where conservatism or bounding approach has undue effects
    - Remove detail and uncertainty that aren't significant
  - However, in reality, there are constraints
    - Maintain technical credibility
    - Building detail onto simple models can be problematic
    - Hard to justify resources for changing a model that is unimportant to performance
    - Regulatory inertia – hard to convince regulator to consider changing a model that has been deemed acceptable

Waste Form FEPs

- Probability and significance criteria for YM FEPs (10 CFR 63.114)
  - Events with occurrence exceeding 10^{-4} in 10kyr
  - Features and processes if "magnitude and time of resulting radiological exposures" would be "significantly changed by their omission"
- 374 FEPs evaluated (derived from NEA database with site specific FEPs added)
  - ~100 related to Waste Form
  - Half excluded due to low consequence, e.g.
    - Gas generation from waste form decay
    - Thermal expansion/stress of components within WP
    - Advection through stress-corrosion cracks in WP outer barrier
  - Half included in system model
    - HLW glass degradation (alteration, dissolution and radionuclide release)
    - Chemical characteristics of water in the waste package
    - General corrosion of the WP outer barrier
- Criticality (an event) is excluded in the basis of low probability

System Model for Yucca Mountain



Components related to waste forms

- Inventory
- In-package chemistry
- Cladding
- Waste degradation
- Radionuclide Solubility
- Colloids

ries

Representation of Waste in Yucca Mountain PA

Three generic waste forms:

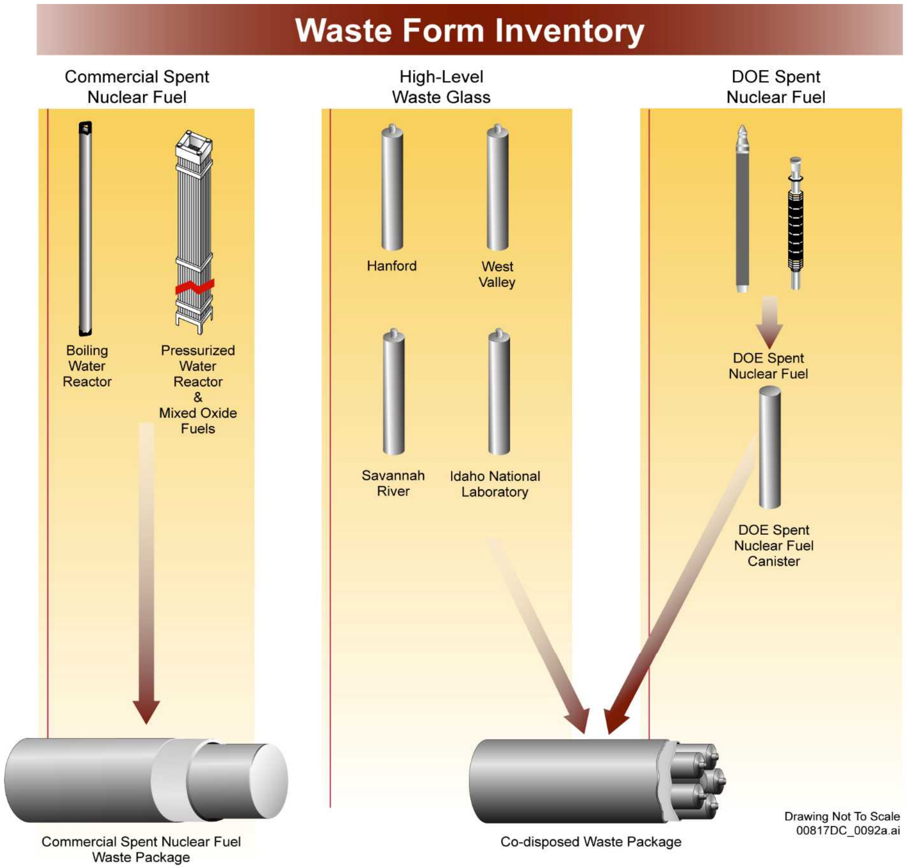
1. Commercial SNF
2. DOE SNF
3. HLW glass + MOX + LABS glass

In two generic waste packages

Aggregation tends to use conservative assumptions and analogs rather than average properties

Inventory limited to radionuclides judged to be potentially important

Acceptable compromise between level of detail, computational burden, and transparency of analysis



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In-Package Chemistry
Abstraction from large set of EQ3/6 results

Key inputs to abstraction

- Waste Package Relative Humidity (RH)
- Waste Package Liquid Flux Rate (Q)
- Waste Package Temperature (T)
- Time Since Waste Package Failure (time)
- Chemistry in the Drift (P_{O_2}, P_{CO_2})

CSNF Cell 1

pH
- Non-Dripping: Calculate and sample distributions as *f*(I, P_{CO_2})
- Dripping: Calculate and sample distributions as *f*(I, P_{CO_2})

I
- Non-Dripping: Calculate and sample distributions as *f*(RH)
- Dripping: Calculate and sample distributions as *f*(Q, time)

ΣCO_3 Calculate *f*(pH, P_{CO_2}, T)

CDSP Cell 1A and Cell 1B

pH
- Non-Dripping: Calculate and sample distributions as *f*(I, P_{CO_2})
- Dripping: Calculate and sample distributions as *f*(I, P_{CO_2})

I
- Non-Dripping: Calculate and sample distributions as *f*(RH)
- Dripping: Calculate and sample distributions as *f*(Q, time)

P_{O_2}: Equilibrium with the Drift
P_{CO_2}: Equilibrium with the Drift

Choose Dripping or Non-Dripping Results

Submodels using Output:
CSNF Waste Form Degradation
HLW Waste Form Degradation
Dissolved Concentration Limits
Colloid Stability

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Determine pH, Ionic Strength (I) and ΣCO_3 in a failed waste package

Key outputs from abstraction

Must consider 10^X in ranges of these environmental variables

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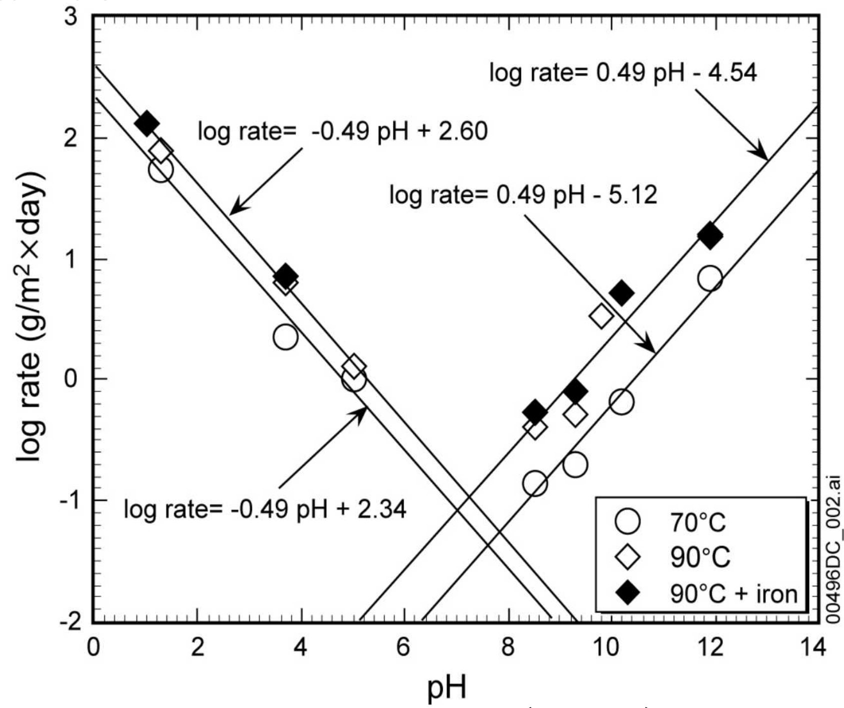
DSNF and HLW(+MOX+LABS) Degradation

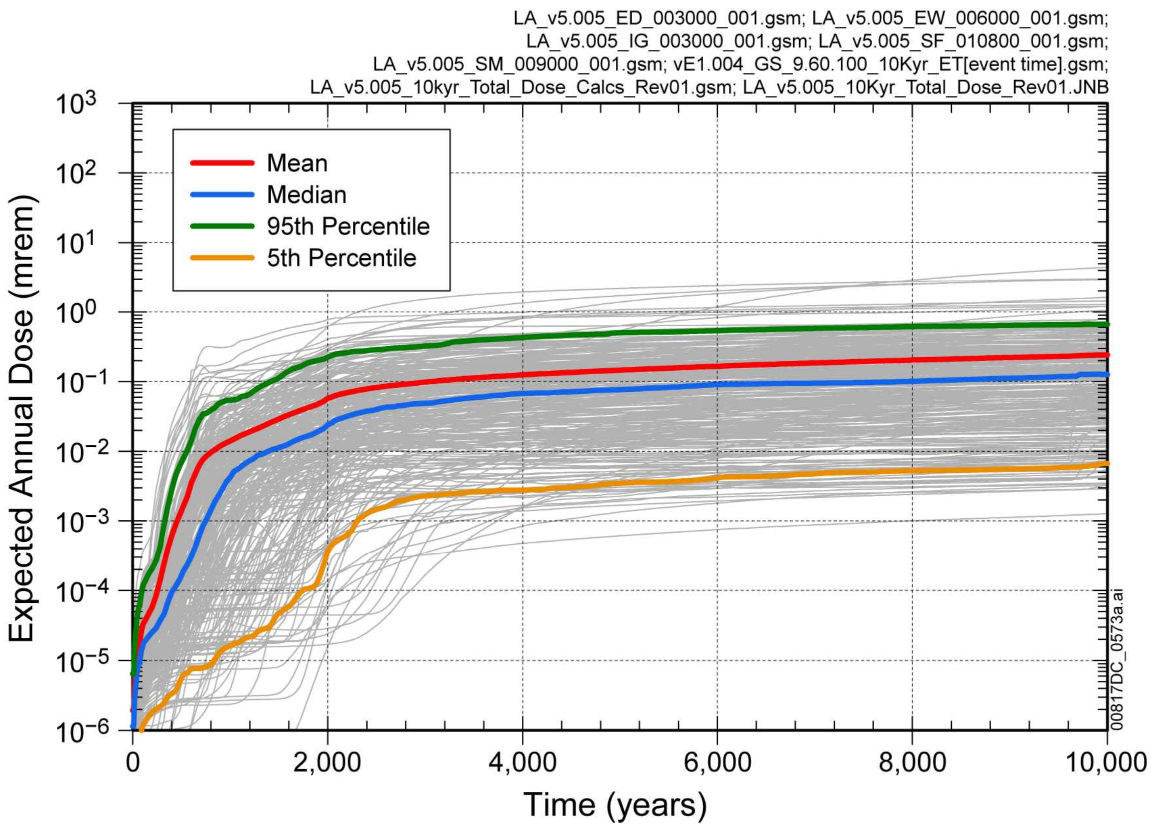
- **DSNF: Bounding degradation rate (instantaneous)**
  - **Appropriate for N-Reactor uranium metal fuel**
  - **Conservative for other DOE SNF**

- **HLW**
  - **Based on reference West Valley, Hanford, and Savannah River glasses which meet the waste acceptance criteria that they are more degradation resistant than "Environmental Assessment" glass**
  - **Degradation rate ($g/m^2/d$)**
  - **RH ≤ 44% (T ≥ 125 °C) 0**
  - **100°C ≤ T ≤ 125°C r(pH=10,T)**
  - **20°C ≤ T ≤ 100°C r(pH, T)**
  - **Instantaneous degradation if igneous intrusion occurs**



$$r = k_E 10^{\eta \times pH} \exp\left(\frac{-E_a}{RT}\right)$$

Total System Performance Assessment Results
Individual Protection Standard: 10,000 yr



MDL-WIS-PA-000005 REV 00 AD 01, Figure 8.1-1[a]

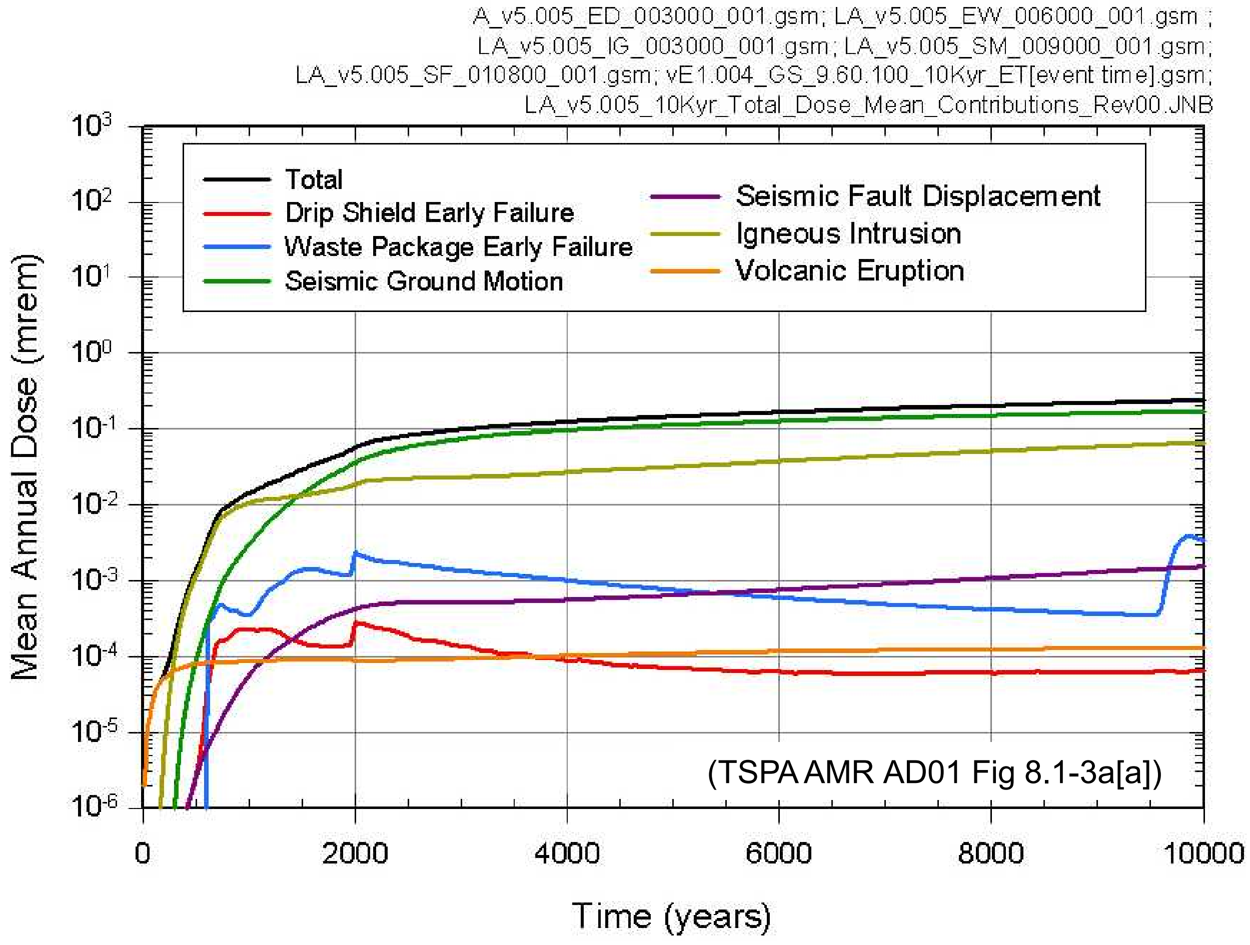
Key questions:

1. What determines the <u>magnitude</u> of total mean dose?

2. What determines the <u>uncertainty</u> in total expected dose?

Analysis decomposes the bottom-line

Total Mean Dose Contributions By Modeling Case



Note: Contribution from Nominal Modeling Case is zero within 10,000 years

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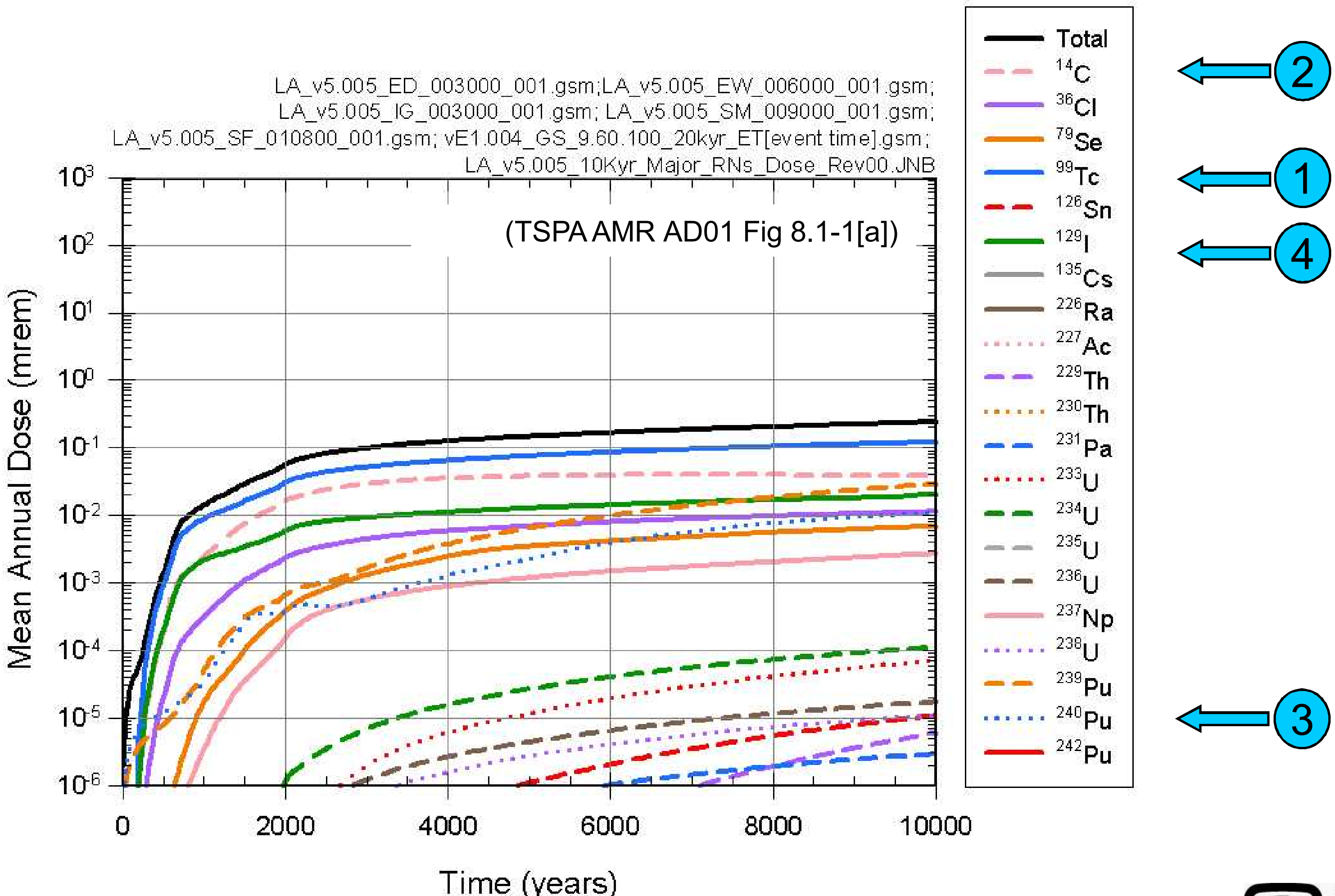
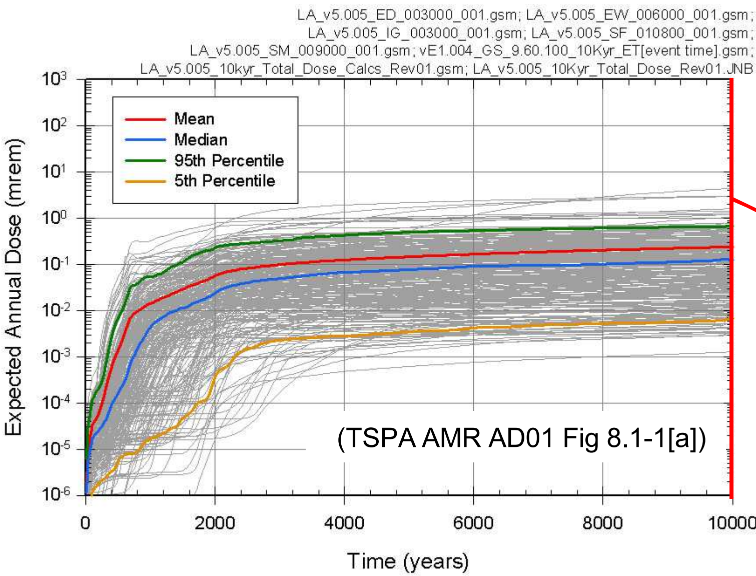
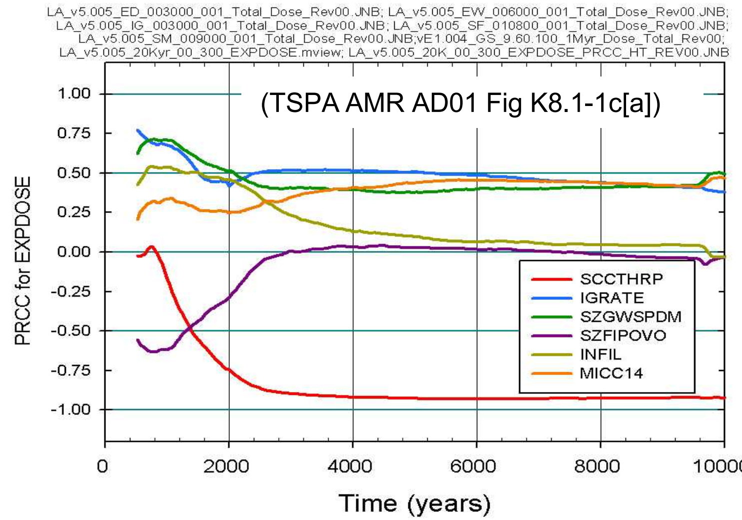
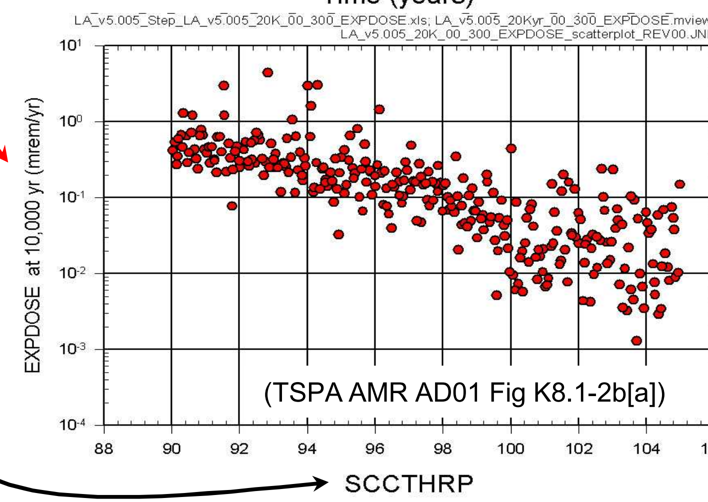
Radionuclides Contributing to Total Mean Dose at 10,000 Years



Uncertainty in Total Expected Dose







SCCTHRP – stress threshold for SCC initiation (90 to 105% of yield strength)
IGRATE – frequency of igneous events
SZGWSPDM – logarithm of uncertainty factor in groundwater specific discharge
SZFIPOVO – flowing interval porosity in volcanic units INFIL – infiltration case
MICC14 – biosphere dose conversion factor for C14

Modeling "Wishes"

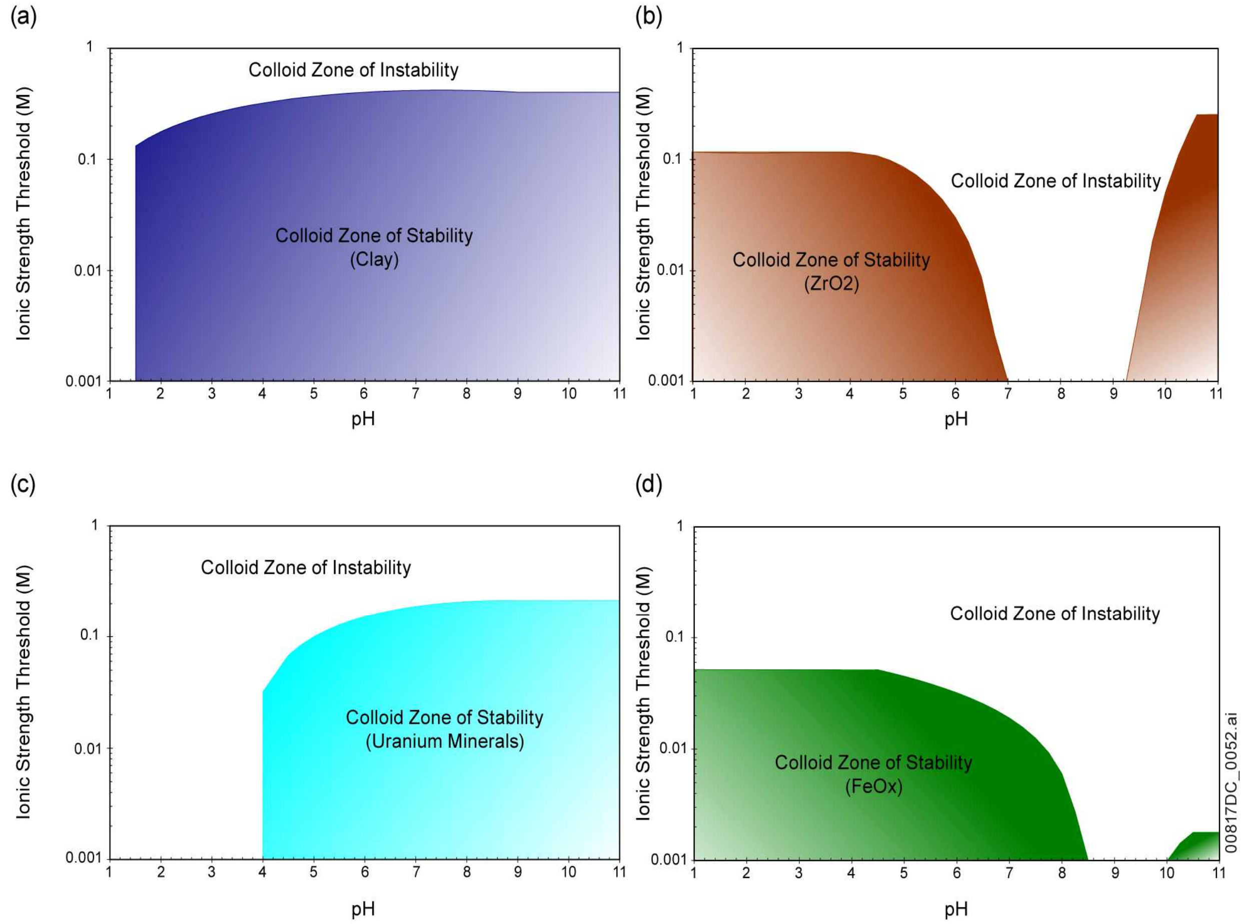
- Scalable modeling solutions
  - Level of detail and dimension of uncertainty
  - Enable changes within PA iterations
  - Accommodate regulatory and programmatic "inertia"
- Standardize interfaces with environmental models
  - Range of environmental conditions
  - Spatial variability
  - Units

Backup

Model for Stability of Colloids

Different colloid types for each of three waste forms

Colloid stability is a function of pH and ionic strength



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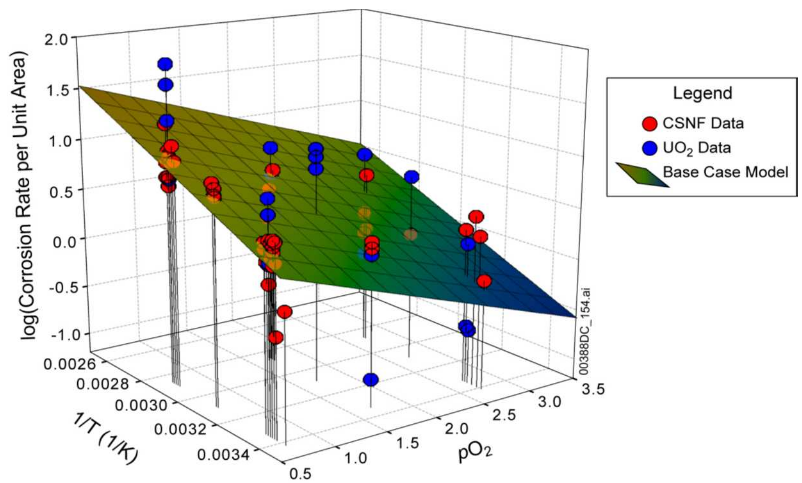
Model for CSNF Degradation

- Based on regression of data from single pass flow through experiments
- No degradation before waste package breach
- Oxidative dissolution rate after waste package breach
  - T ≥100°C instantaneous degradation
  - T< 100°C

$$\log_{10} F = \log_{10}(SA) + a_0 + a_1 \frac{1}{T} + a_2(-\log_{10} \Sigma CO_3) + a_3(-\log_{10} P_{O_2}) + a_4 pH$$



  - Parameter values depend on acidic or basic conditions
- Gap fraction for Cs, I, Sr, Tc

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