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Fuel Cycle Technologies

Performance Assessment Models for Geologic Media and Potential Application to Site Screening, Selection, and Characterization

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**Nuclear Waste Technical Review Board
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■ Introduction to generic performance assessment

- *The need: a full range of repository design options and media are available for consideration*
- *What it is: simplified system-level analyses of representative disposal concepts suitable for evaluating concept viability and R&D needs*
- *What it isn't: detailed performance assessments comparable to those used for licensing*

■ The approach

- *Representative repository designs based on international experience*
- *Repository inventories based on available projections*
- *Material properties for media based on international experience*
- *Simple models that focus on key properties and processes*

■ Examples from current “Generic Disposal System Modeling” (GDSM) work

- Generic analyses of Features, Events, and Processes (FEPs)
- Deep borehole
- Salt

■ The path forward: improving generic performance assessment models and applying insights to support concept evaluation and site screening, selection, and characterization

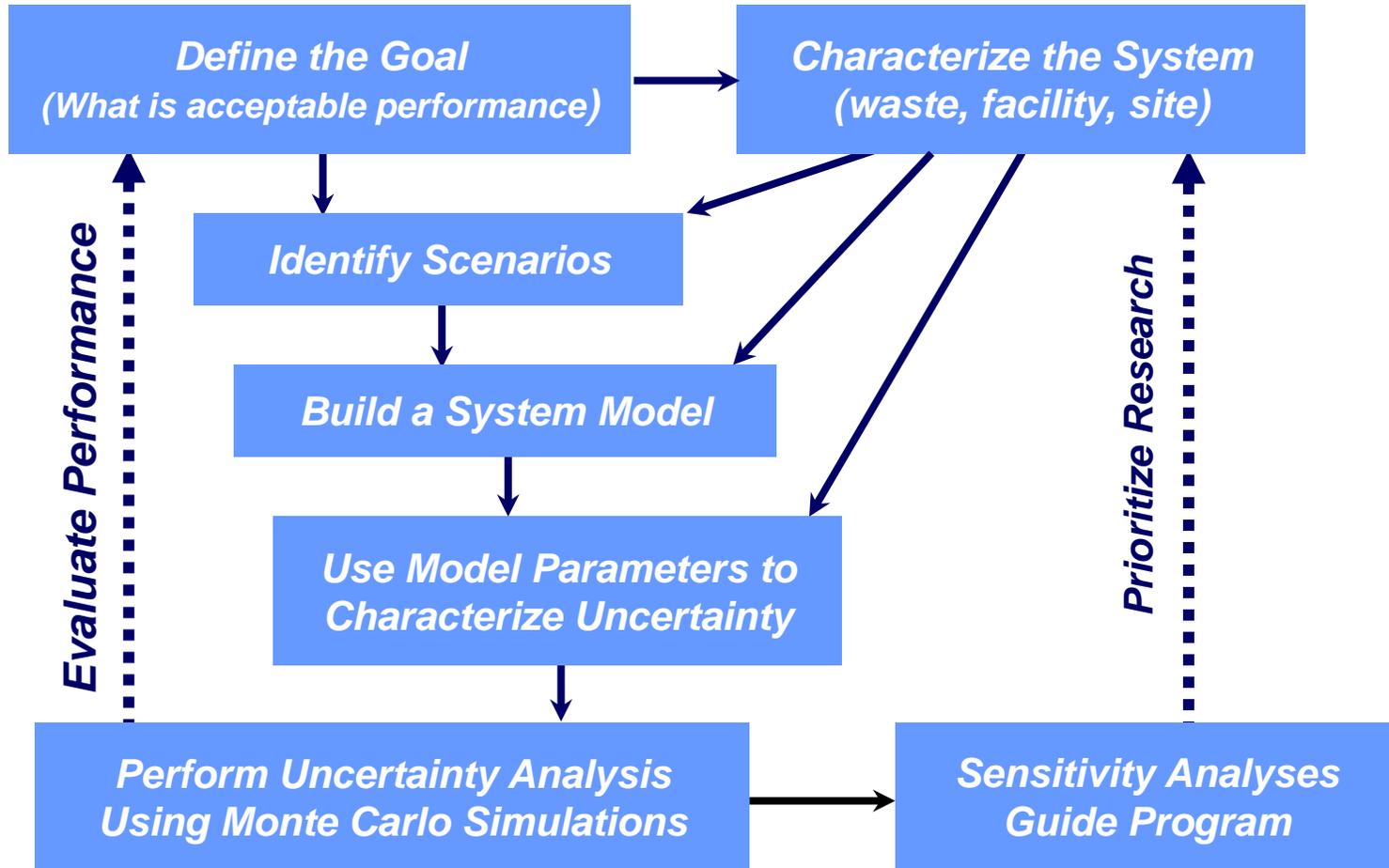


What is Performance Assessment?

- **Performance assessment (PA) is a method for estimating how a disposal system will perform over geologic time**
- **Defined by the U.S. Environmental Protection Agency (EPA) at 40 CFR 191.12 (Environmental Radiation Protection Standards for Management and Disposal of Spent Nuclear Fuel, High-Level and Transuranic Radioactive Wastes)**
 - *Performance assessment* means an analysis that
 - (1) Identifies the process and events that might affect the disposal system;
 - (2) examines the effects of those processes and events on the performance of the disposal system; and
 - (3) estimates the cumulative releases of radionuclides, considering the associated uncertainties, caused by all significant processes and events. These estimates shall be incorporated into an overall probability distribution of cumulative release to the extent practicable.
- **Yucca Mountain Standards (40 CFR 197) define PA in terms of annual dose**
- **The International Atomic Energy Agency (IAEA) defines the analogous term “safety assessment”**



Implementing Disposal System Performance Assessment



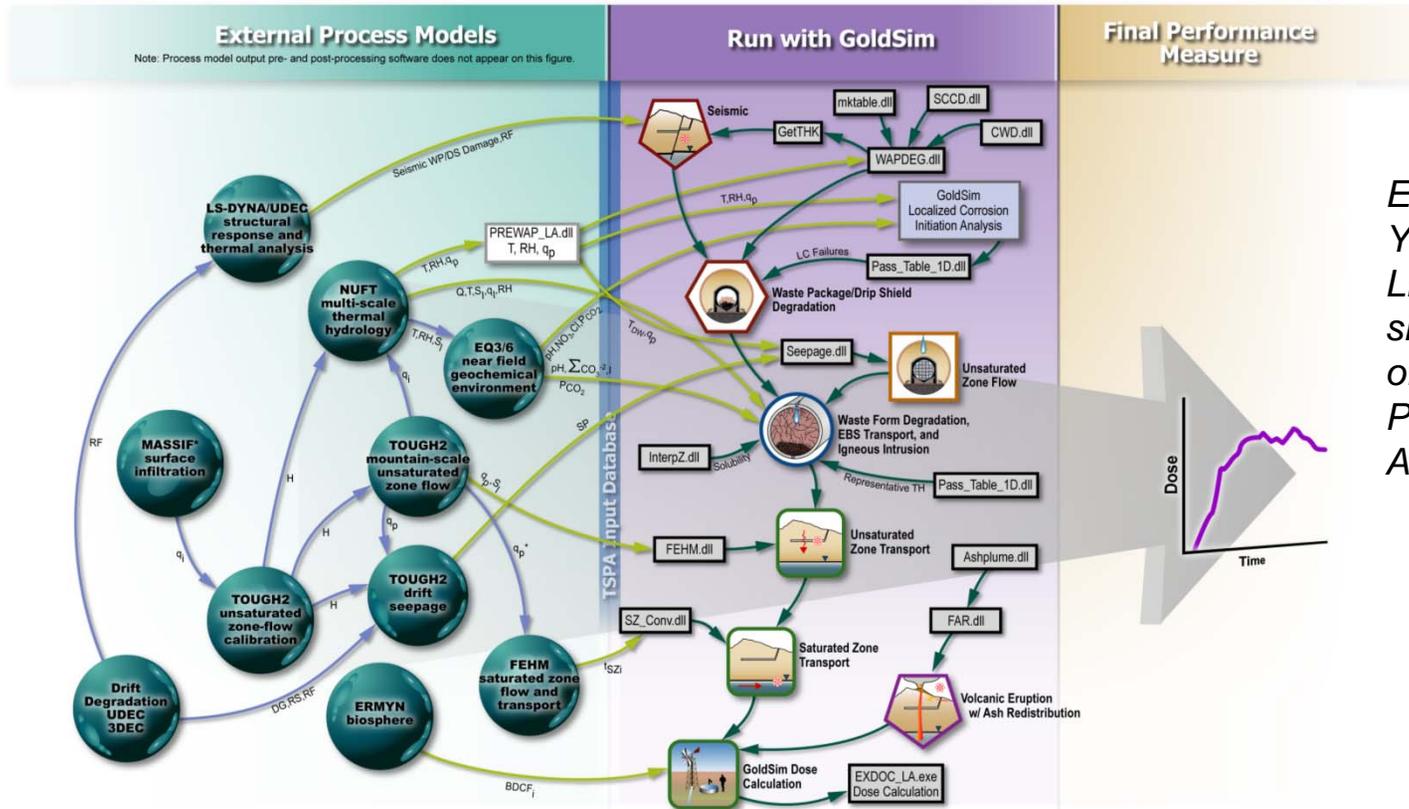


Applying Performance Assessment to Generic Disposal Concepts

- **Steps in PA as applied to Yucca Mountain and WIPP, with observations on generic applicability**
 - **Identify and screen potentially relevant Features, Events, and Processes (FEPs) and develop scenarios for modeling**
 - *Final FEP screening is site-specific, but many questions can be addressed usefully at the generic level*
 - **Develop models and abstractions, along with their scientific basis, for logical groupings of FEPs within scenario**
 - *The final “scientific basis” will be site specific*
 - **Evaluate uncertainty in model inputs**
 - *Uncertainty is both generic and site specific*
 - **Construct integrated PA model using all retained FEPs and perform calculations for scenarios**
 - *Models must be stylized for those aspects of the system that are site-specific (e.g., far-field transport in the geologic system, biosphere pathways)*
 - **Evaluate total system performance, incorporating uncertainty through Monte Carlo simulation**
 - *Generic uncertainty analysis is only relevant for those aspects of the system that are generic (e.g., inventory, host rock properties)*



What a Generic PA is not: Comprehensive Modeling of All Potentially Relevant Processes



Example from the Yucca Mountain License Application showing the structure of the Total System Performance Assessment (TSPA)

Output Parameters

f_S	Fraction of WPs with Seeps	q_p	Percolation Flux	q_i	Infiltration Flux	H	Hydrologic Properties
EBS	Engineered Barrier System	NO_3	Nitrate Concentration	DG	Drift Geometry	SP	Seepage Parameters
Q_S	Seep Flow Rate	T	Temperature	Cl	Chloride Concentration	RS	Rock Strength
Q	Evaporation Rate	RH	Relative Humidity	I	Ionic Strength	RF	Rockfall Size and Number
pH		S_l	Liquid Saturation	t_{szi}	Saturated Zone Transport Time		
ΣCO_3^{-2}	Carbonate Concentration	X_a	Air Mass Fraction	BDCF ₁	Biosphere Dose Conversion Factor		
P_{CO_2}	Partial Pressure of CO ₂	q_l	Liquid Flux	q_g	Gas Flux		

* Note: q_p derived from INFIL model

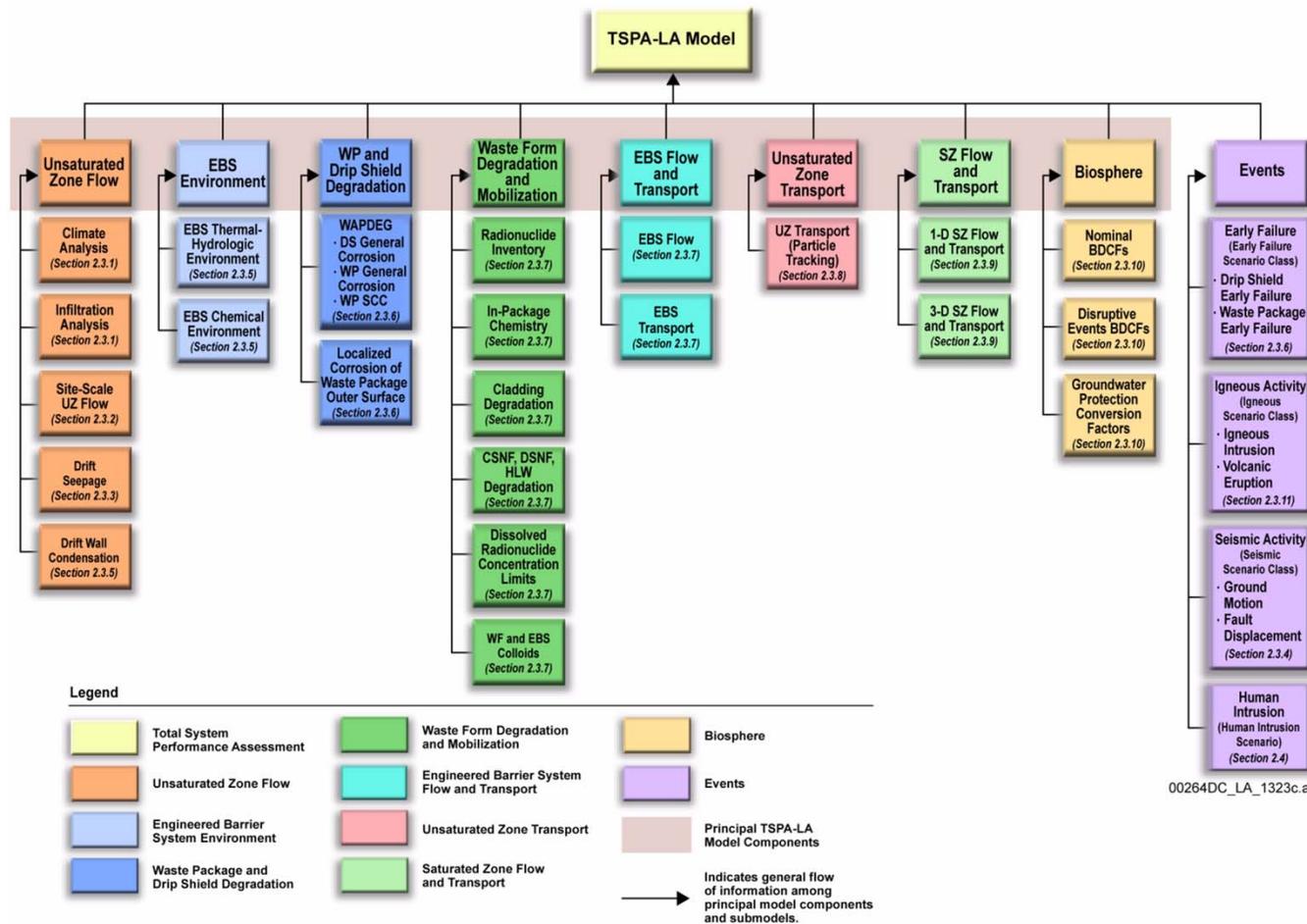
Legend

- Response Surface between Process Models
- Response Surface from Process Model to GoldSim
- Connection in GoldSim
- Preprocessor
- TSPA Model DLL

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What a Generic PA is not: Thousands of Pages of Documentation to Support a License Application



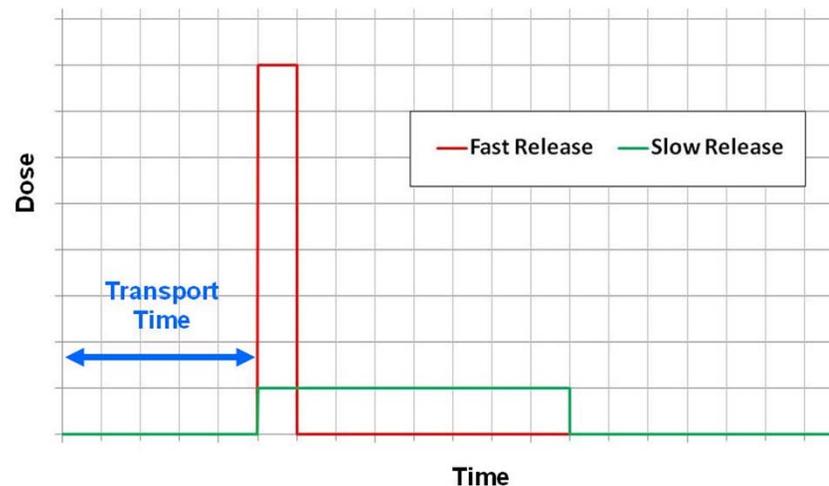
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DOE/RW-0573, Rev 1, figure 2.4.2



Insights from Simple Generic PAs

- **Dose estimates in most long-term repository PAs are controlled by a few key processes/parameters**
 - Initial mass (inventory) of dose-contributing radionuclides (or parents)
 - Rate of radionuclide releases from waste packages (WPs) (fast vs. slow)
 - *Waste form (WF) and WP degradation rates, radionuclide solubility*
 - Transport processes/residence time in the engineered barrier system (EBS) and in the natural system / geosphere
 - *Mass spreading: advection, dispersion, diffusion,*
 - *Mass retention/loss: sorption, decay*

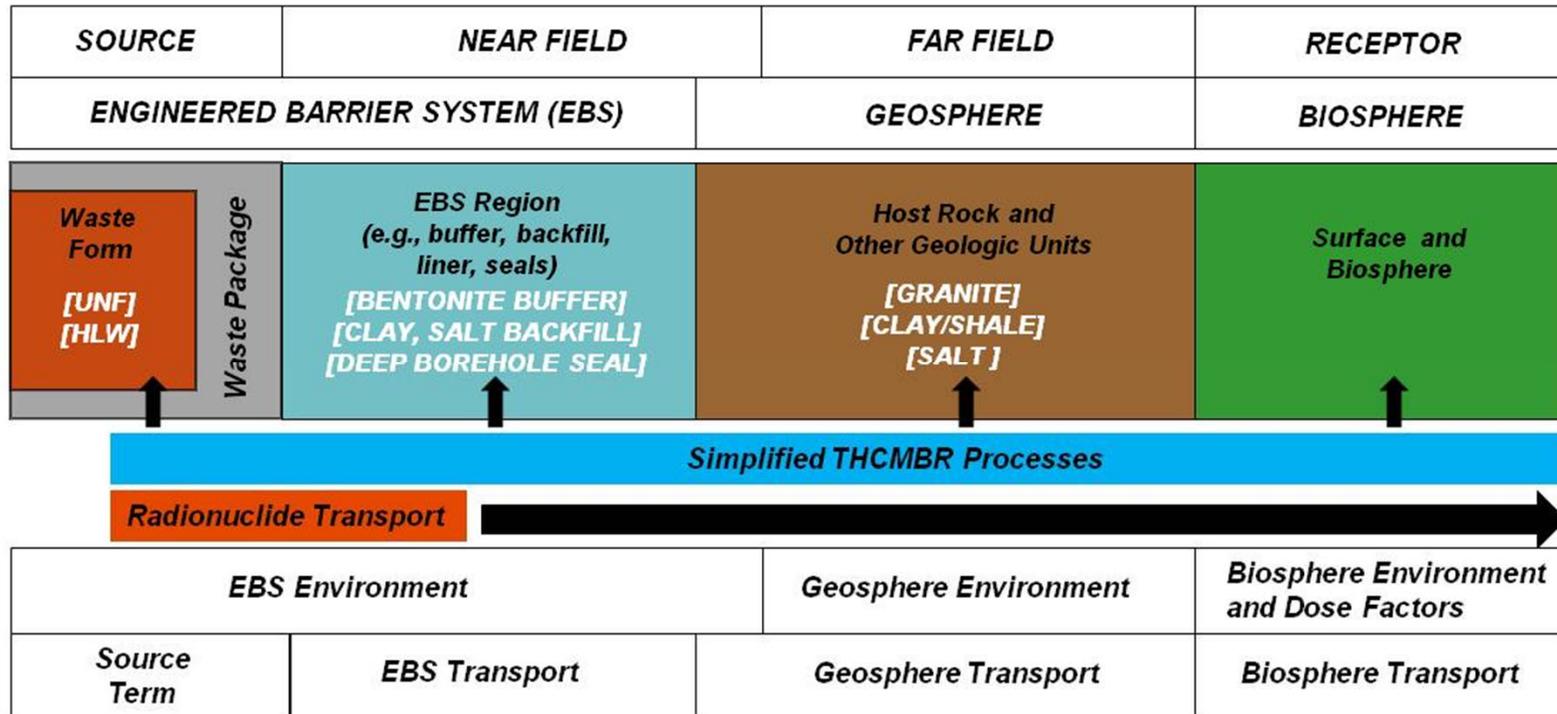


Freeze and Lee, 2011



Generic Disposal System Conceptual Model

1-D schematic representation of generic system domains and phenomena common to most disposal system alternatives



Freeze and Lee, 2011



Example PA for Clay/Shale Disposal: ANDRA Dossier 2005

■ Source

- 13,500 UNF WPs
- WP failure time = 10,000 yrs
- WF degradation rate = $2 \times 10^{-5} \text{ yr}^{-1}$,
(gradual releases over 50,000 yrs)
- Radionuclide specific solubilities
- Diffusive releases from WPs

■ Near Field

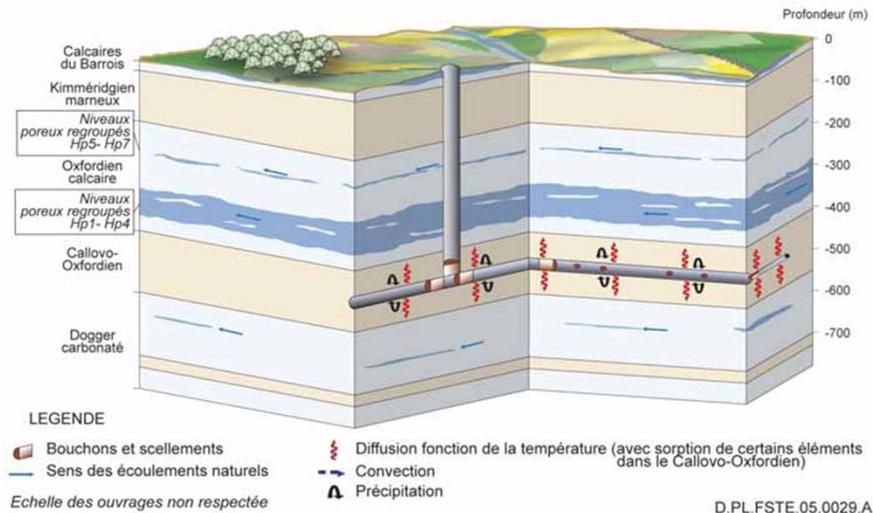
- Bentonite / disturbed argillite (5 m)
- Diffusion-dominated transport
- Radionuclide specific diffusion coefficients and retardation factors

■ Far Field

- Callovo-Oxfordian (COX) argillite (60 m)
- Diffusion-dominated transport
- Radionuclide specific diffusion coefficients and retardation factors

■ Biosphere

- Pumping well in the permeable formation overlying the Callovo-Oxfordian discharges to the Saulx Valley
- Pumping rate = 100 L/min
- Biosphere dose conversion factors (BDCFs) representative of a farming community

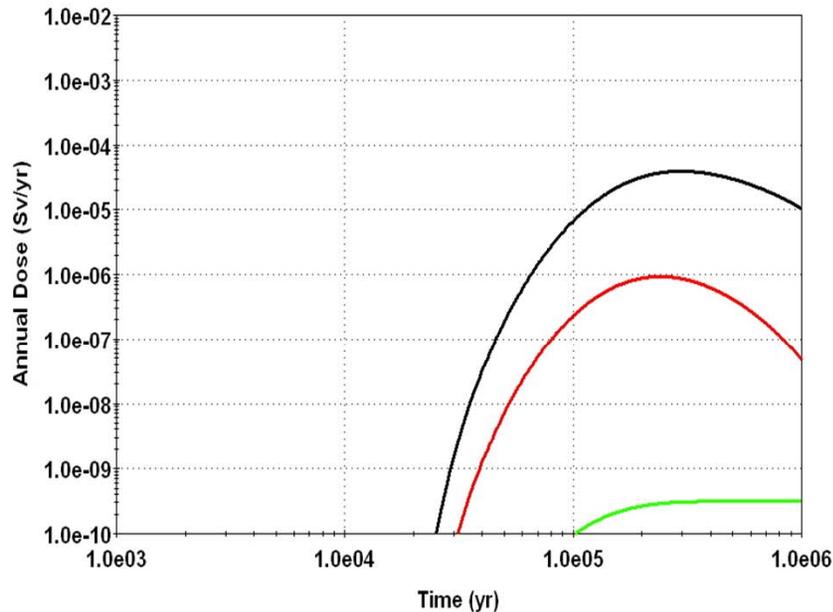
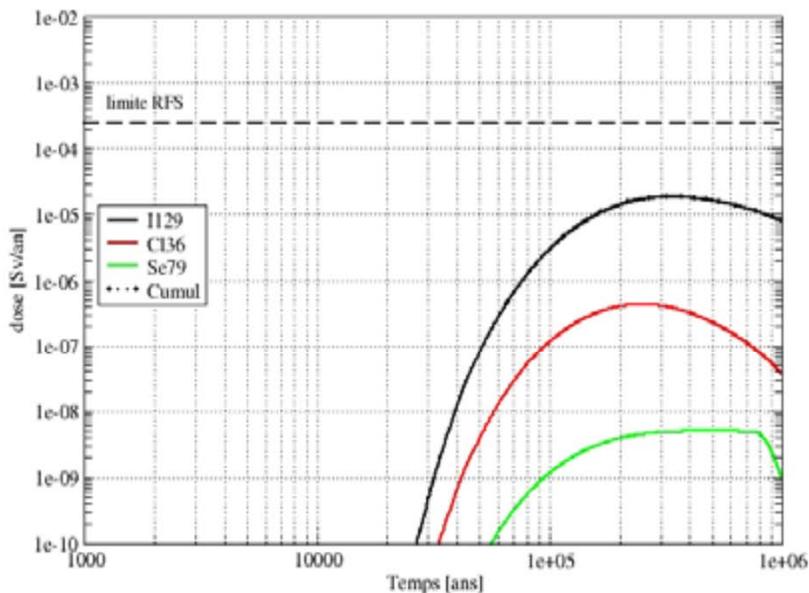


ANDRA Dossier 2005, Figure 5.3-11



Extremely Simplified PA Model Results: Clay/Shale, Comparison to ANDRA 2005

Annual Dose (at Saulx Outlet)



[Cl36] [I129] [Se79]

ANDRA Dossier 2005, Figure 5.5-18
Scenario S2: UOx spent fuel)

Simplified PA Model (Freeze and Lee, 2011)
1-D diffusion, key radionuclides only; waste, buffer, disturbed zone, and far field properties from Andra 2005



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Generic Analyses of Features, Events, and Processes (FEPs)



■ Objectives for Generic FEP analyses

- Identify FEPs that are potentially relevant to multiple disposal options
 - *E.g., “Microbial Activity in the Engineered Barrier System”, 207 others*
- Support demonstration of completeness
 - *“Have we thought of everything?”*
- Use generic FEP analyses to focus R&D on important phenomena
 - *Initial list of 208 generic FEPs used as input to the Disposal R&D Roadmap work*
 - *Is current understanding sufficient to evaluate the importance of each FEP for each disposal option?*
 - *Will improved understanding be needed for future decision points?*

■ Site-specific FEP screening, as done for WIPP and YM, is not an objective at this stage

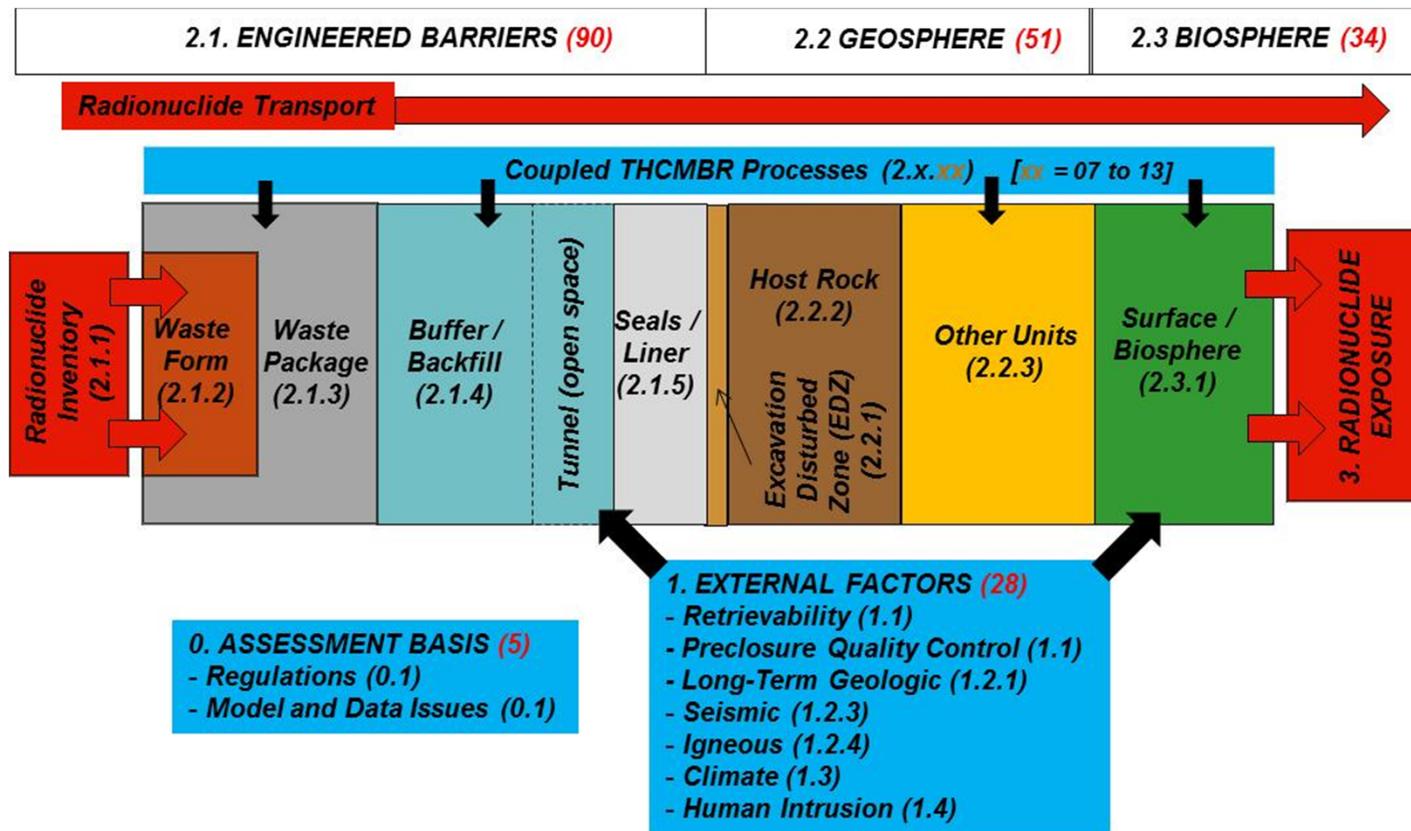
- Requires regulatory criteria and site- and design-specific information

■ FEPs related to external factors (e.g., disruptive events) are generally site specific, and are not a focus area for generic work



Generic FEP Identification and Categorization

- 208 preliminary FEPs mapped to repository features





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Generic PA Modeling: Deep Borehole Disposal



Generic Concept for Deep Borehole Disposal

Nominal 5 km borehole

45 cm bottom hole diameter

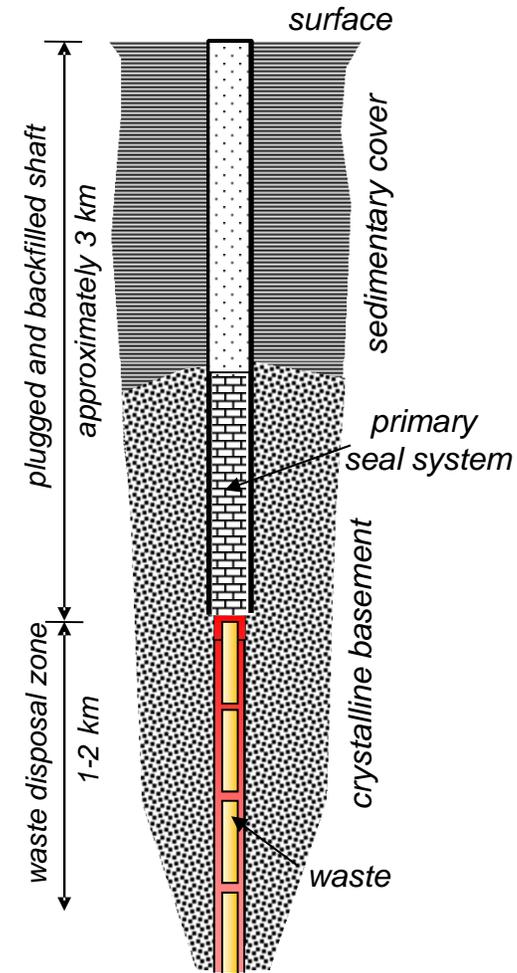
***1 PWR assembly or 3 BWR
assemblies without
consolidation***

***Lower 3 km in crystalline
basement***

2 km emplacement zone

1 km minimum of robust plugs

***Yucca Mountain spent fuel
inventory could be emplaced in
~ 600 holes***



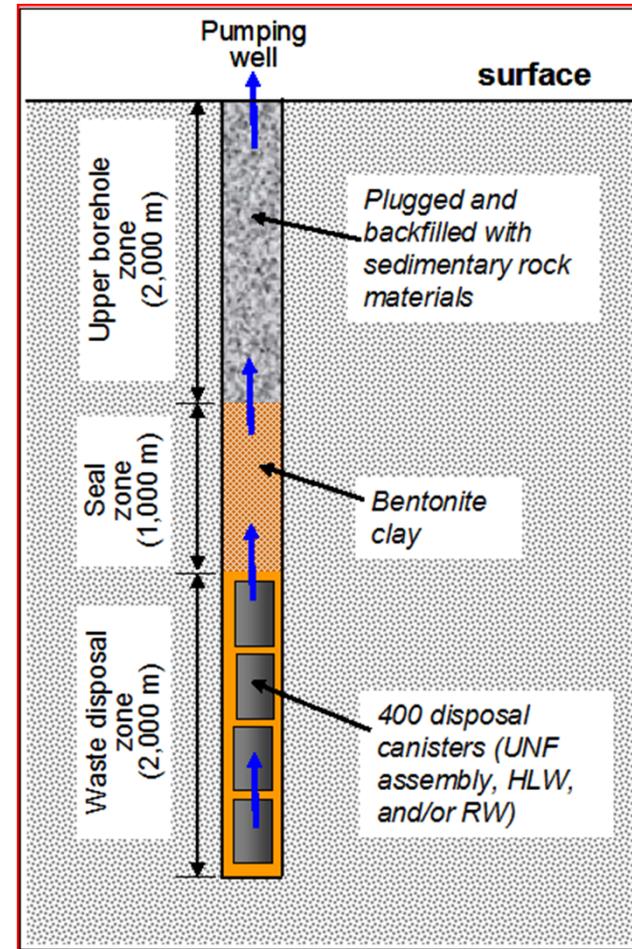
modified from Brady et al., 2009

(not to scale)



Generic PA Model for a Single Disposal Borehole

- Model domain consists of three components:
 - Waste-disposal zone
 - Seal zone
 - Upper-borehole zone and aquifer
- Groundwater flow driven by thermal-hydrologic effects (thermal expansion and thermal buoyancy) – no ambient gradient in fluid potential (Arnold et al., 2009)
- Groundwater flow in the upper-borehole zone driven by 3D radial flow to a water supply well (Brady et al., 2009)
- Flow and radionuclide transport in waste-disposal and seal zones occurs in 1 m² cross-sectional area consisting of the borehole, borehole seals or canisters plus grout, and disturbed rock zone (DRZ) surrounding borehole



Swift et al. 2011



Generic PA Model for a Single Disposal Borehole (cont.)

- Waste canister failure occurs immediately after emplacement
- Constant fractional waste-form degradation rate
- Radionuclide solubility limits representative of reducing conditions in brine (Brady et al., 2009)
- Linear sorption coefficients representative of reducing conditions are used for radionuclide retardation (Brady et al., 2009)
- Radionuclide transport processes of advection, dispersion, diffusion, sorption, decay and ingrowth are included
- Groundwater flow rates vary with depth and time in the waste-disposal and seal zones (derived from separate 3D thermal-hydrologic modeling of a 9-borehole array, Arnold et al. 2011)
- Groundwater flow rates are constant in the upper borehole zone and surrounding aquifer
- Radionuclide releases to the biosphere diluted in 10,000 m³/year water supply (IAEA 2003, Example Reference Biosphere 1B)
- Numerical model is implemented with the GoldSim software code



Generic PA Model for a Single Disposal Borehole: Cases and Parameters

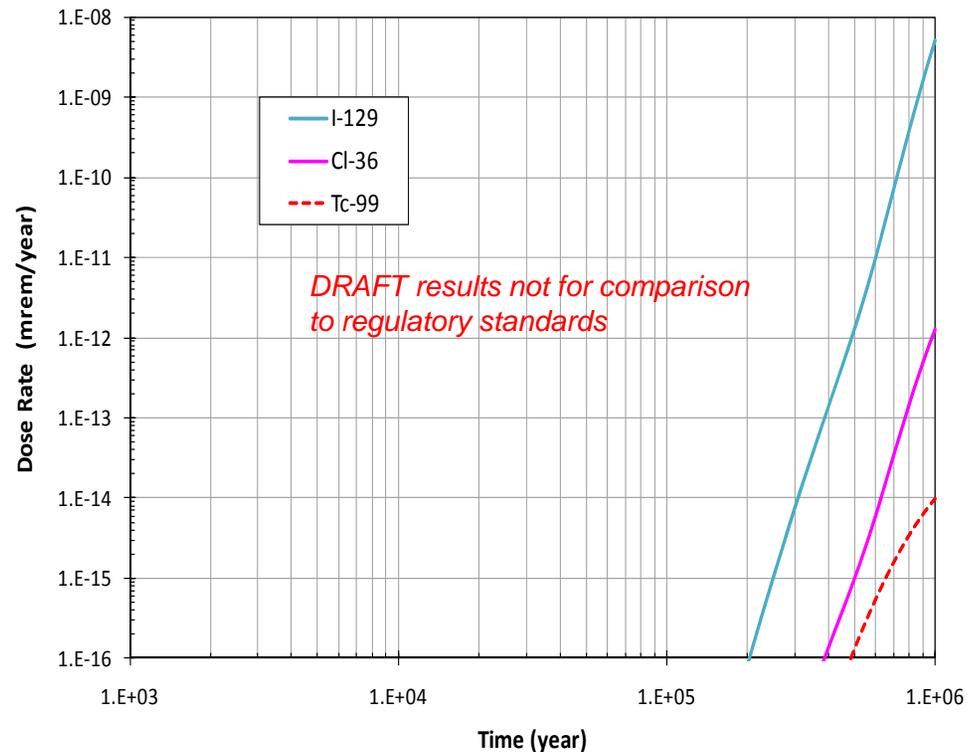
- **Direct disposal of US Commercial Used Nuclear Fuel (UNF)**
- **Radionuclide inventory and thermal output based on PWR (pressurized water reactor) fuel**
 - 60 GWd/MTHM burnup, 30 year cooling period after reactor discharge
- **Sampled values for UNF fractional dissolution rate**
 - log triangular: min = $10^{-8}/\text{yr}$, mode = $10^{-7}/\text{yr}$, max = $10^{-6}/\text{yr}$
 - *“Instantaneous” release of gap fraction not modeled*
- **Radionuclide solubility limits and sorption coefficients from Brady et al., 2009**
 - Essentially unlimited solubility and no sorption for I-129 and Cl-36
- **Three flow cases considered from Arnold et al., 2011**
 - Base case: rock permeability = 10^{-19} m^2 and borehole/DRZ permeability = 10^{-16} m^2
 - Low permeability case: rock permeability = 10^{-19} m^2 and borehole/DRZ permeability = 10^{-19} m^2 (corresponds conceptually to a highly-effective seal system)
 - High permeability case: rock permeability = 10^{-16} m^2 and borehole/DRZ permeability = 10^{-12} m^2 (equivalent to fine sand, conceptually intended to provide a conservative representation of a fully-failed seal system)



Generic PA Model for Deep Borehole Disposal: Preliminary Estimate of Mean Annual Dose

- Low permeability seal case not illustrated: estimated million-year dose is zero
- Base case permeability results in an estimated peak mean annual dose less than 10^{-10} mSv/yr
 - I-129 is primary contributor, lesser contributions from Cl-36 and Tc-99

Results shown for a single borehole, direct disposal of 60 GWd/MTHM burnup PWR UNF, 30 year cooling period after reactor discharge



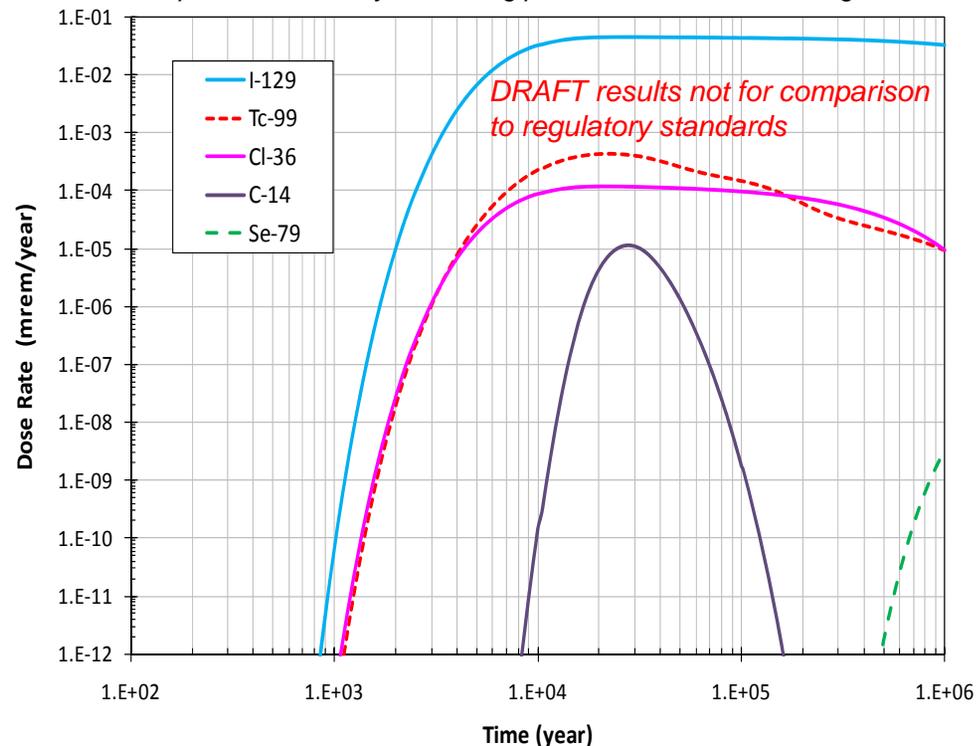
Base case: rock permeability = $10^{-19} m^2$ and
borehole/DRZ permeability = $10^{-16} m^2$



Generic PA Model for Deep Borehole Disposal: Preliminary Estimate of Mean Annual Dose (cont.)

- **High permeability case (fully degraded seals) results in an estimated peak mean annual dose less than 0.001 mSv/yr**
 - I-129 is primary contributor, lesser contributions from Cl-36, Tc-99, C-14, and Se-79
 - Peak dose rate limited by the fractional dissolution of the used fuel
- **Relatively higher (but still small) estimated doses for high permeability case indicate the importance of a robust seal design**

Results shown for a single borehole, direct disposal of 60 GWd/MTHM burnup PWR UNF, 30 year cooling period after reactor discharge



High permeability case: rock permeability = 10^{-16} m^2 and borehole/DRZ permeability = 10^{-12} m^2 (equivalent to fine sand, conceptually intended to provide a conservative representation of a fully-failed seal system)



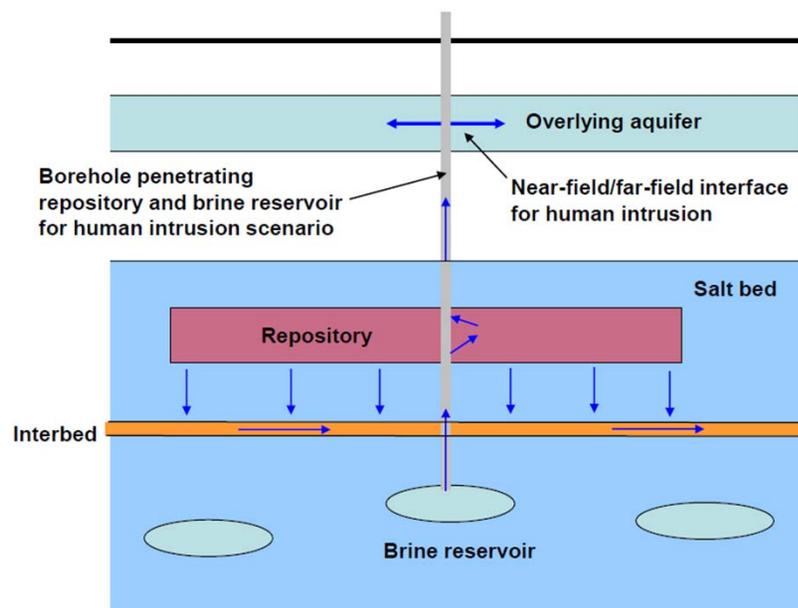
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Generic PA Modeling: Salt



Generic Conceptual Model for Disposal in Salt



Lee et al. 2011

- Repository in bedded salt below an aquifer
- Disposal environment is water-saturated and reducing
- Isothermal conditions (25° C)
- Undisturbed (or Reference) Scenario
 - Radionuclides released into and transported in a 1-m-thick interbed below repository
 - Time-dependent two-phase interbed flow calculated as a function of pressure, gas generation
- Disturbed Scenario
 - Single borehole penetration at 1,000 yr
 - Sampled number of affected waste packages (between 1 and 5)
 - Radionuclides released directly to overlying aquifer by steady-state flow from underlying brine reservoirs
 - Does not include potential dose impacts of waste brought to surface by drilling activities



Generic PA Model for Salt: Model Parameters

- **Commercial used nuclear fuel (UNF) (140,000 MTU)**
 - Convert the total inventory to equivalent pressurized water reactor (PWR) inventory
 - *60 GWd/MTHM burn-up, 4.73% enrichment 30 yrs after discharge from reactor*
 - 32,154 UNF WPs (10 assemblies per WP)
- **Square repository footprint**
 - Spacing between emplacement tunnels: 25 m
 - Spacing between WPs: 6 m
- **No WP containment barrier performance**
 - Waste form degradation and RN release at the beginning of simulation
- **Fractional degradation rate model for waste form degradation**
 - Commercial UNF: log-triangular: min = $10^{-8}/\text{yr}$, mode = $10^{-7}/\text{yr}$, max = $10^{-6}/\text{yr}$
- **Disposal area modeled as a mixing cell**
 - No radionuclide sorption on corrosion products and geologic materials
- **Radio-element solubility for two redox conditions**
 - Near-field brines (reducing condition)
 - Far-field brines (less reducing or slightly oxidizing condition)



Generic PA Model for Salt: Model Parameters (cont.)

- **Radionuclide sorption in near-field and far-field transport**
 - Linear equilibrium sorption (K_d) model for interbed and overlying aquifer
- **Pore flow velocity in interbed**
 - 100 realizations of time-dependent pore velocity in interbed generated with BRAGFLO code, range from $<10^{-16}$ m/yr to $\sim 10^{-6}$ m/yr
- **Steady-state borehole flow upward from a brine reservoir into overlying aquifer**
 - 0.1 to 5.0 m^3/yr , uniform
- **Pore flow velocity in overlying aquifer (consistent with WIPP modeling)**
 - Log-uniform (3.15×10^{-3} m/yr to 31.5 m/yr)
- **Performance measure**
 - Mean dose at hypothetical accessible environment
 - 5 km down-gradient from the edge of repository
 - IAEA BIOMASS Example Reference Biosphere 1B (ERB1B) dose model
 - Dilution rate of 1×10^4 m^3/yr in aquifer
 - Individual water consumption rate of 1.2 m^3/yr

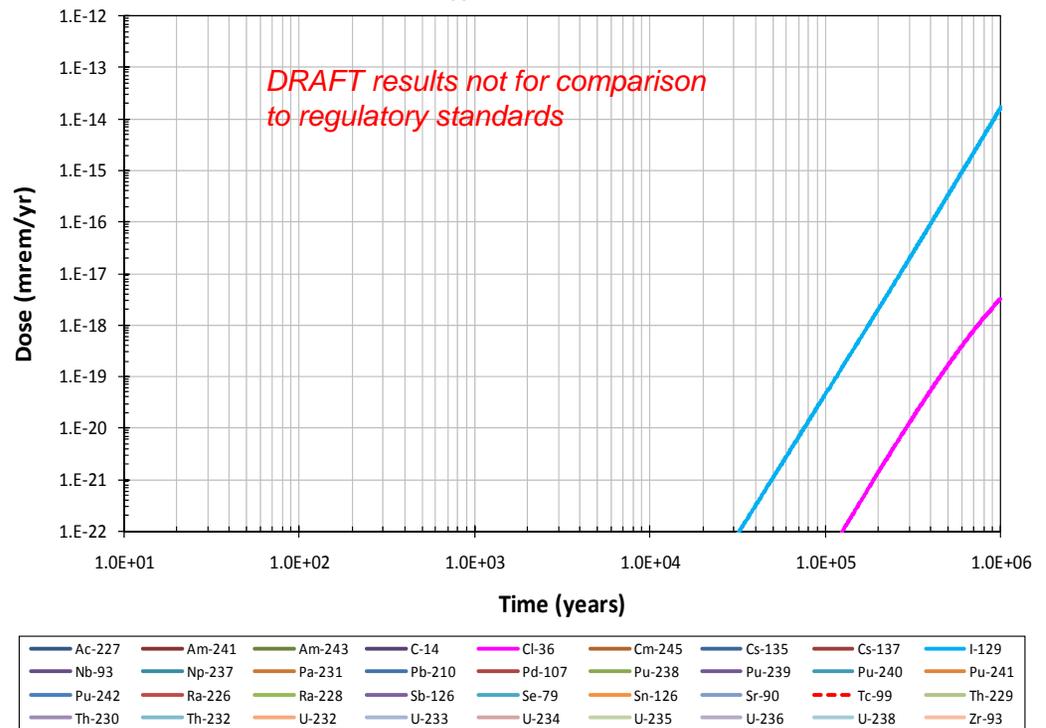


Generic PA Model for Salt: Preliminary Results for Undisturbed Case

Results shown for direct disposal of 60 GWd/MTHM burnup UNF, 30 year cooling period after reactor discharge

- **Slow, diffusion-dominated transport in interbeds due to low flow velocities**
- **RN transport further retarded in the interbed by sorption**
- **Non-sorbing or weakly sorbing RNs (I-129, Cl-36) with a significant inventory are released from the far-field interbed**
- **I-129 is the dominant long-term dose contributor**
 - Unconstrained solubility
 - Extremely long half-life (~16 M yr)
 - Significant inventory in the waste

Mean Dose at Hypothetical Accessible Environment



Clayton et al. 2011, Fig. 3.1-8



Generic PA Model for Salt: Preliminary Results for Human Intrusion Case

Higher dose estimates than for undisturbed scenario

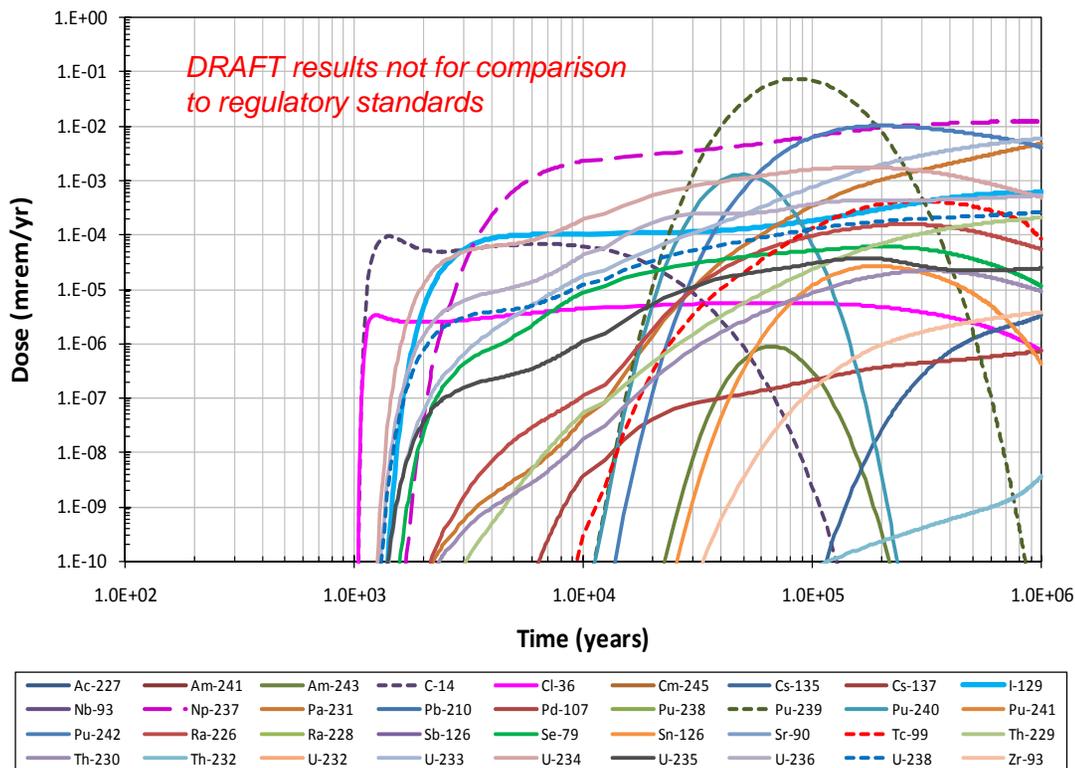
- RNs transported at much higher rates in the overlying aquifer than in the interbed

Actinides contribute due to direct release into the overlying aquifer with higher water flow rates and higher solubility limits

Np-237, Pu-239, and Pu-242 are the dominant contributors

Results shown for direct disposal of 60 GWd/MTHM burnup UNF, 30 year cooling period after reactor discharge

Mean Dose at Hypothetical Accessible Environment



Clayton et al. 2011, Fig. 3.1-15



Path Forward for Generic Disposal System Modeling

- **Generic performance assessment model development will proceed in parallel with the Used Fuel Campaign mission and the national repository program**
- **Five-year goal**
 - Have in place the system architecture and computational environment to support full uncertainty analyses of long-term performance for site-specific disposal concepts
 - Maintain flexibility to support evolving programmatic needs
 - *Disposal options viability*
 - *Site selection and screening*
 - *Identification and prioritization of research and characterization needs.*
 - *Support licensing*
- **Continue development of scientific models and databases**
 - E.g., see Engineered Barrier Systems presentation by Jové Colón
- **Develop performance assessment computational framework tool**
 - Link scientific models in a common environment
 - *Pre- and post-processing, meshing, uncertainty and sensitivity analysis tools, built-in quality assurance and reproducibility*
 - *Allow analysis at multiple levels of detail: deterministic or probabilistic, system or sub-system, desk-top to high-performance computing*



Conclusions

- **Generic disposal system modeling provides first-order insights**
 - Processes and parameters with the greatest impact on performance in different disposal concepts
 - *Relative importance of engineered and natural barriers; release rates and transport times*
 - *Relative importance of assuring low-permeability release pathways, diffusive transport*
 - *Relative importance of redox state*
 - Thermal load management strategies
- **Generic disposal system models help prioritize R&D needs**
 - Focus on the processes and parameters that will have the greatest impact for different disposal concepts and alternative fuel cycle options
 - *E.g., seal system properties for deep boreholes*
 - Identify processes that are targets for further R&D to develop advanced data and models
- **Generic disposal system models help confirm viability of concepts**
- **Generic disposal system models will mature into site-specific models suitable to help guide site characterization and eventually support licensing**
- **Generic disposal system models do not identify “the best concept”: results are preliminary, not suitable for direct comparison to each other or regulatory standards**



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- **ANDRA (Agence nationale pour la gestion des déchets radioactifs), 2005, *Dossier 2005: Argile. Tome: Safety Evaluation of a Geological Repository.***
- **Arnold, B.W., T. Hadgu, D. Clayton, and C. Herrick, 2011, *Thermal-Hydrologic-Chemical-Mechanical Modeling of Deep Borehole Disposal*, proceedings of the 2011 International High-Level Radioactive Waste Management Conference, April 10-14, 2011, Albuquerque, NM.**
- **Brady, P.V., B.W. Arnold, G.A. Freeze, P.N. Swift, S.J. Bauer, J.L. Kanney, R.P. Rechar, J.S. Stein, 2009, *Deep Borehole Disposal of High-Level Radioactive Waste*, SAND2009-4401, Sandia National Laboratories, Albuquerque, NM.**
- **Clayton, D., G. Freeze, T. Hadgu, E. Hardin, J. Lee, J. Prouty, R. Rogers, W.M. Nutt, J. Birkholzer, H.H. Liu, L. Zheng, S. Chu, 2011, *Generic Disposal System Modeling—Fiscal Year 2011 Progress Report*, FCRD-USED-2011-000184, SAND2011-5828P, Sandia National Laboratories, Albuquerque, NM.**
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- **IAEA, 2003, *“Reference Biospheres” for solid radioactive waste disposal*, International Atomic Energy Agency, IAEA-BIOMASS-6.**
- **Lee, J.H, M. Siegel, C. Jove-Colon, Y. Wang, 2011, *A Performance Assessment Model for Generic Repository in Salt Formation*, proceedings of the 2011 International High-Level Radioactive Waste Management Conference, April 10-14, 2011, Albuquerque, NM.**
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- **US DOE (United States Department of Energy), 2008, *Yucca Mountain Repository License Application*, DOE/RW-0573, Rev. 1.**