SAND2007-6502P

Nuclide Transport Modeling in WIPP Performance Assessment

KHNP Training Program
Module 6: Assembly of a Safety Case

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Outline

I. **Introduction to nuclide transport modeling**

II. Description of Conceptual Model

III. Numerical Implementation

IV. PABC Results

Introduction to nuclide transport modeling

- **To ensure compliance with regulations, we need to show that releases of radioactive materials falls under prescribed probabilistic limits**
- **How do we track evolution of radioactive species?**
  - **Transport of nuclides**
  - **Decay to daughter species**

Introduction to nuclide transport modeling

- **Other concerns:**
  - How much radioactive material will dissolve into brine?
  - Where does the radioactive material leave the Land Withdrawal Boundaries?
  - What are the effects of changing intrusion time on releases?
  - What species dominate releases?

Introduction to nuclide transport modeling

- There are two codes used in PA to address various aspects of the modeling of the movement of radioactive species in the repository (also known as nuclide transport)
  - NUTS
  - PANEL
- We will discuss the basic ideas underlying the use of these codes, and what they tell us about nuclide transport at WIPP

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Conceptual models for nuclide transport

- Several conceptual models play a role in NUTS and PANEL
  - Multiple Intrusions
  - Actinide Source Term
  - Chemical Conditions
  - Castile and Brine Reservoir
  - Actinide Transport

Multiple Intrusions Model

- Waste panels are treated as independent units
- Long-term releases to environment are negligible
  - Only affects spallings and direct brine releases
- Pressure in the repository will be different for each intrusion

Actinide Source Term

- Actinide concentrations in solution are predicted using information gathered from
  - The inventory of radionuclides and other chemical species in the waste
  - Brine chemistry for undisturbed and intrusion scenarios
- Colloidal actinide concentrations come from radionuclides that are:
  - Sorbed on microbes or mineral fragments
  - Condensed into polymerized clusters
  - Adsorbed onto large organic molecules (humics)

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Chemical Conditions Model

- Determines the choice of several chemical parameters:
  - pH in the repository
  - Selection of actinide oxidation states
  - Major ion composition of brines and wastes
- The WIPP repository is assumed to be:
  - Basic with respect to pH (pH > 9)
  - Strongly reducing
  - Largely anoxic (no free oxygen)
- MgO backfill plays large role in governing chemical conditions

Castile and Brine Reservoirs Model

- Smaller reservoirs are more significant in causing direct brine releases than larger reservoirs
- Intrusions that intersect Castile brine reservoirs are assumed not to release radioactive material to surface (except as cuttings or cavings)

Actinide transport model

- Brines entering repository interact with waste
- Waste containers will be breached by corrosion or broken by pressure from creep closure
- Waste is transported only by advection
- No credit taken for elimination of radionuclides via sorption onto surfaces

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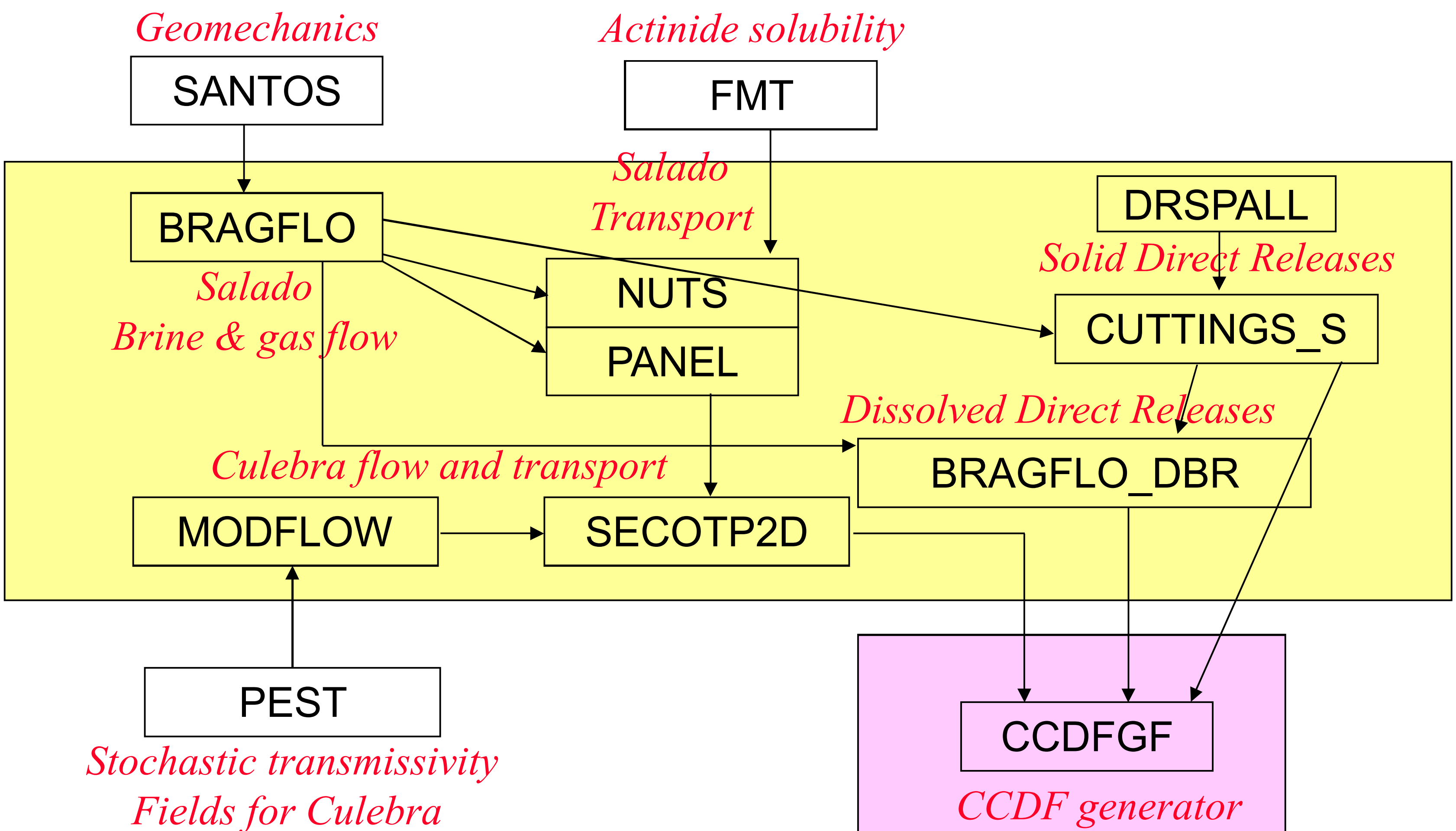
Numerical implementation

- WIPP PA uses two different codes to implement numerical modeling of transport:
  - PANEL
  - NUTS
- NUTS requires input from PANEL
- Both PANEL and NUTS requires fluid flow information from BRAGFLO

Interdependence of PA codes



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Role of PANEL in PA

- PANEL operates in four different “modes”:
  - SOURCE TERM: Determines the amount of radionuclides available for transport via brine pathways
  - DECAY: Performs nuclide decay over the 10,000-year operating horizon
  - CONCENTRATION: Uses source term to compute amount of radioactive nuclides mobilized
  - STANDARD: Uses source term and fluid flow information to compute amount of radionuclides removed from a panel

Role of NUTS in PA

- **NUTS runs in multiple modes:**
  - **SCREEN: Determines which vectors in PA require a full analysis**
  - **ISOTOPE: Determines the amount of radionuclide transport through boreholes, marker beds, and the Culebra**
  - **TIME INTRUSION: Like ISOTOPE, but shifts fluid flow profiles to various times to model intrusions earlier and later than the ISOTOPE scenarios**

Chemical processes modeled

- **Radioactive decay**
- **Advective transport**
- **Precipitation**
- **Interior sources**
- **Solubility limits**

- **Dispersion *not* modeled**

Simplified decay chains (NUTS)

- **PANEL explicitly models all radioactive decays**
- **NUTS code is more "expensive" computationally**
  - **Handling all decay reactions would slow down the code ~10x**
  - **3-5 days of run time would become 1-2 months!**
- **Solution: Reduce number of decay reactions**
  - **What criteria do we use to determine which reactions to keep?**

Conceptual model: Intrusion scenarios

- **Six scenarios tested**

- **Two different intrusion types:**
  - **E1 intrusions penetrate both borehole *and* pressurized brine reservoir in Castile formation below repository**
  - **E2 intrusions only penetrate borehole**

Summary of intrusion scenarios

Scenario	# of Drilling Intrusions	Time of Intrusion (Years)	Castile Brine Pocket encountered	Intrusion Type
S1	0 (Undisturbed)	NA	NA	NA
S2	1	350	Yes	E1
S3	1	1,000	Yes	E1
S4	1	350	No	E2
S5	1	1,000	No	E2
S6	2	1,000 and 2,000	Only at 2,000	E2 and E1

NUTS models Scenarios 1-5; PANEL models Scenario 6

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Cumulative releases

Releases are normalized by radionuclide and by the total inventory:

$$R = \sum \frac{Q_i}{L_i}\left(\frac{1\times10^6 curies}{C}\right)$$

R **= Normalized release in "EPA units"**
Q_i = 10,000-year cumulative release (in curies) of radionuclide *i*
L_i = Release limit for radionuclide *i*
C **= the total transuranic inventory (in curies) of α-emitters w/half-lives > 20 years)**

Methodology for selecting decay reactions

- **"Lumped" decay sequences chosen so that:**
  - **Isotopes with similar decay patterns are combined**
  - **Isotopes with similar transport characteristics are combined**
  - **Total magnitude of EPA units is conserved**
- **Result of analysis (Stockman *et al.*, 1996) shows that only *one* decay chain, with *five* isotopes, is needed to model successfully all of the decay chains occurring in the WIPP repository!**

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Lumped decay chain

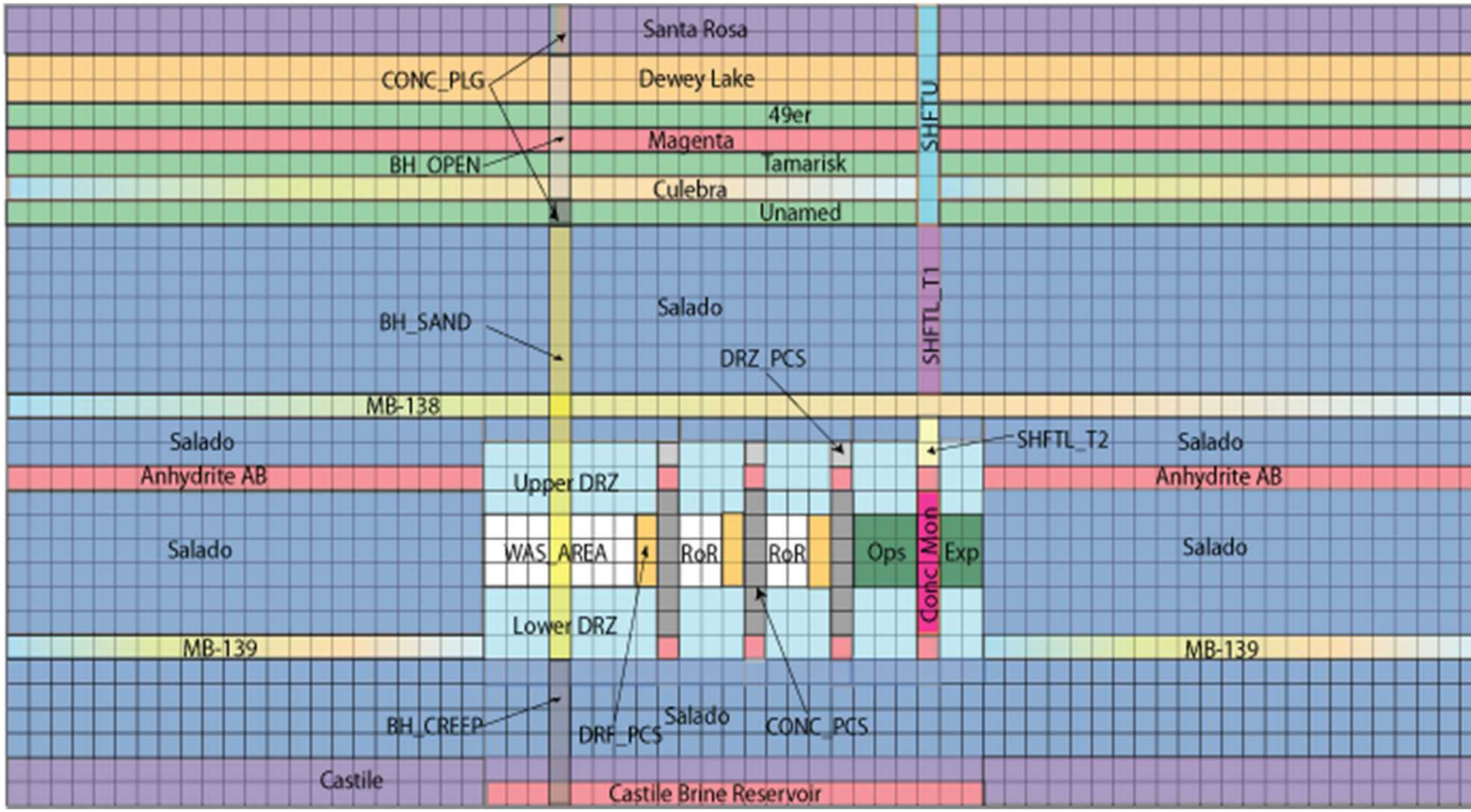
$$\left.\begin{array}{r} {}^{241}\mathrm{Am} \\ {}^{238}\mathrm{Pu} \\ {}^{239}\mathrm{Pu} \end{array}\right\} \rightarrow {}^{234}\mathrm{U} \rightarrow {}^{230}\mathrm{Th}$$

- **Of these isotopes, ^{238}U has a half-life of 87.7 y; it will decay almost completely within 1000 y!**
- **Analysis in NUTS focuses on remaining isotopes: ^{241}Am, ^{239}Pu, ^{234}U, and ^{230}Th**

Mathematical method

- **Both NUTS and PANEL are *finite element codes***
  - **A continuous region is divided into a large number of individual cells, each with its own properties**
  - **The equations which describe the evolution of the system are also discretized**
  - **Derivatives become differences between cells**
  - **Results from the simulations are analyzed using post-processing codes**

WIPP Repository



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NUTS and PANEL: basic features

- **Model solubilities**
  - **Includes colloids (humic, microbial, mineral fragment, and actinide-intrinisic)**
  - **Assumes actinides always in equilibrium**
  - **All dissolution occurs instantaneously**
- **Uses BRAGFLO results to provide fluid flow patterns in the repository**

NUTS: Screening runs

- A generic "tracer" is modeled
  - Placed in all cells containing waste
  - Initial concentration: 1 kg/m^3
- Concentration tracked as a function of time
- Vector "screened in" if concentration at any time exceeds 10^{-7} kg/m^3:
  - At surface
  - In Culebra at Land Withdrawal Boundary
  - In marker beds at Land Withdrawal Boundary

NUTS: Isotope runs

- Explicitly considers inventory in repository
- Tests undisturbed and disturbed scenarios
- Releases to Culebra, Borehole, and Markerbeds are accumulated over time in curies
- Conversion to EPA units made after simulations are complete

NUTS: Time-intrusion runs

- Fluid-flow profiles from BRAGFLO are time-shifted to other times
- Decay processes allowed to occur before fluid flow begins
- Same analysis process used as in isotope runs
- Time shifts to 100, 3000, 5000, 7000, or 9000 years
- As time increases, fewer vectors show significant releases

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PANEL: Mobilization calculations

- Calculates the exit rates of isotopes from the repository, which depends on
  - Flow rates and volume of brine (from BRAGFLO)
  - Concentration of isotopes and size of inventory
- Studies all isotopes (versus 5 in PANEL)
- Initial concentrations assumed to be uniform within a panel
- Supersaturation is not allowed
- Used for multiple intrusion scenario (S6)

PANEL: Contaminants in Brine Releases

- In addition to S6 scenario, PANEL is also used to determine the activity of actinides in brine releases caused by a blowout
- Determined by
  - Volume of brine present in repository
  - Rate of brine flow out of repository

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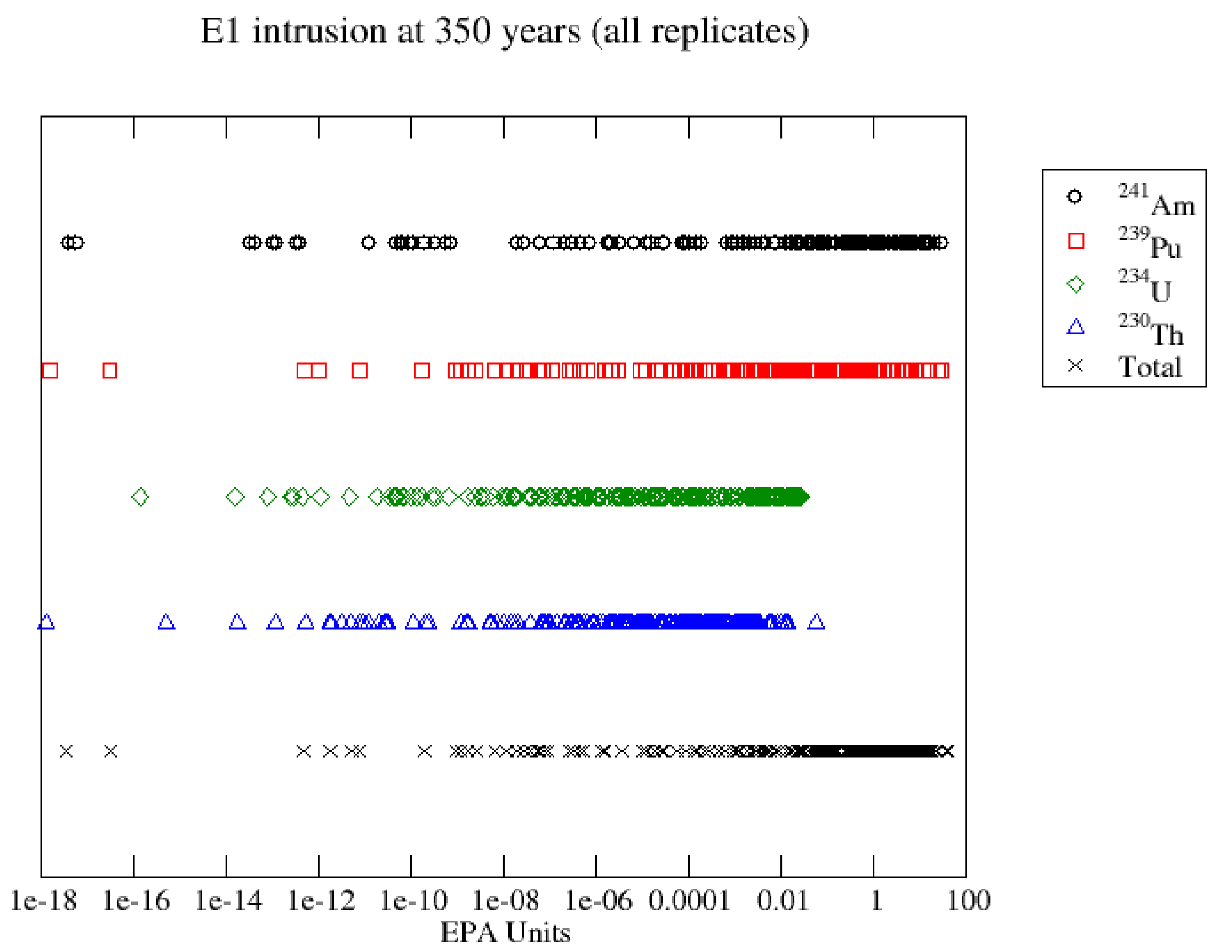
PABC Results for NUTS: Screening

- 167 or 168 vectors screened in per replicate
  - Most screened in for Scenarios 2 and 3
  - Most releases only through borehole
    - Approximately 50 vectors in each replicate show releases through markerbeds
    - 18 vectors across all replicates show possible releases through markerbeds only (no borehole releases)
- Between 75 and 80 vectors also run for Scenario 1 per replicate
  - Provides run conditions for other scenarios
  - No vectors screened in because of releases in undisturbed scenario

PABC Results for NUTS: Isotope Runs



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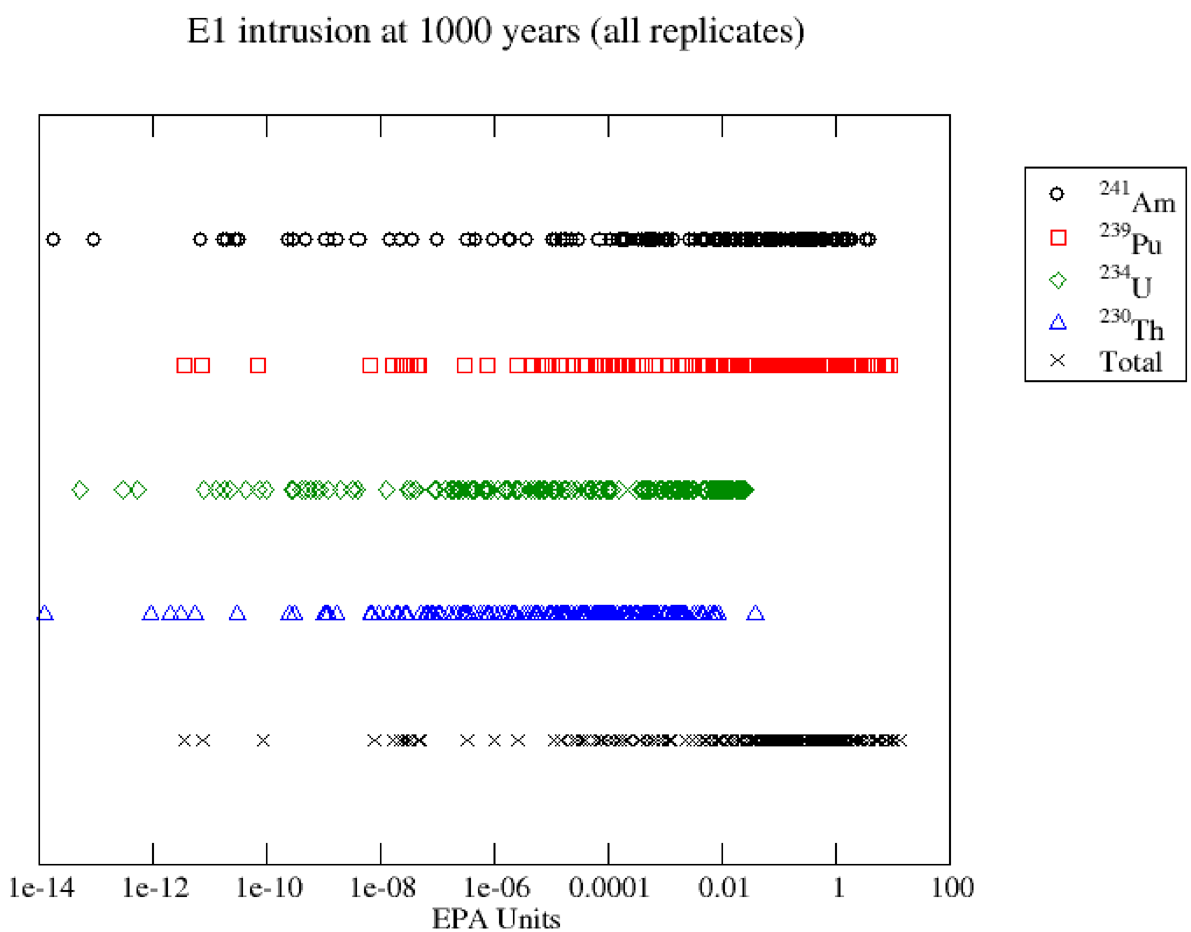
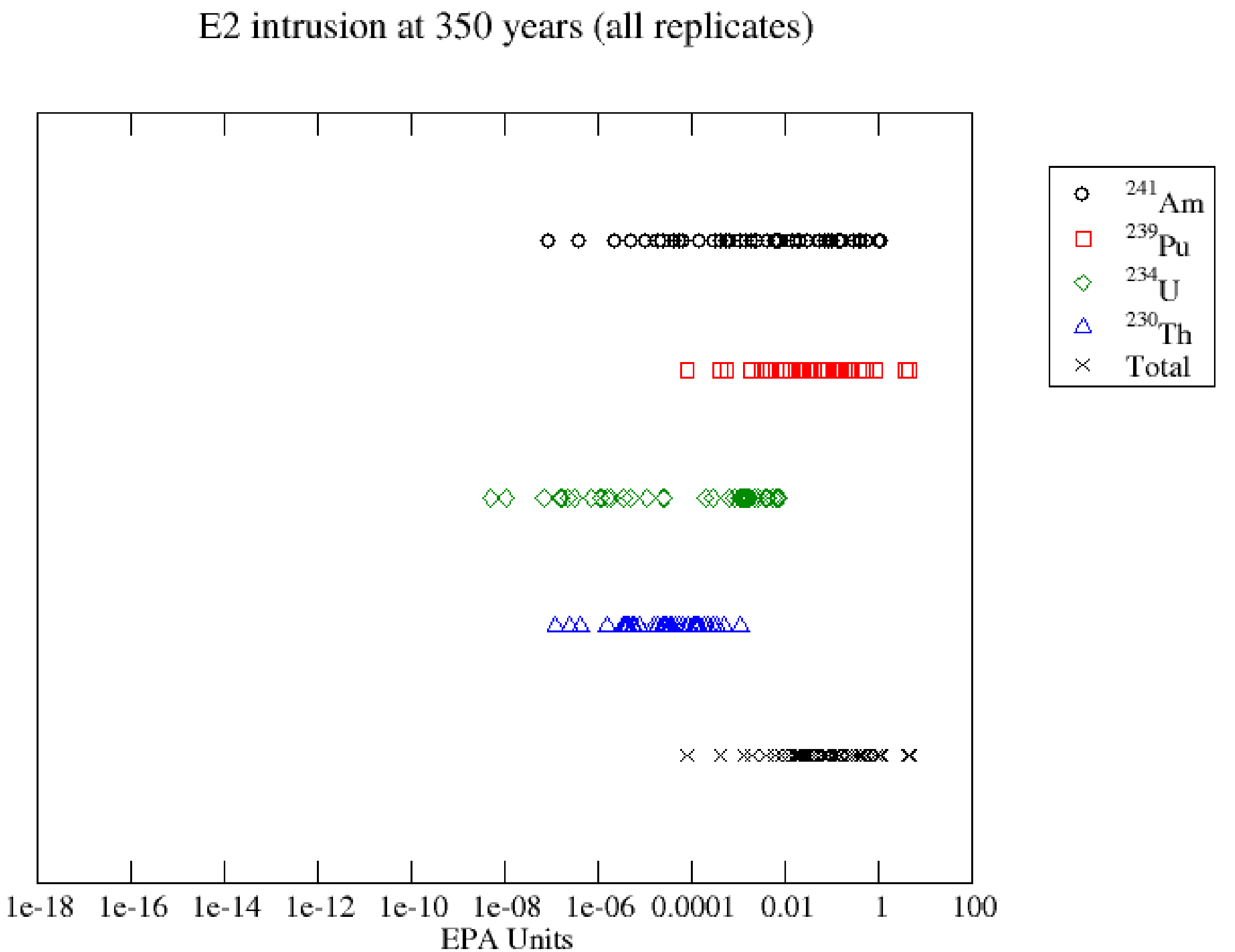
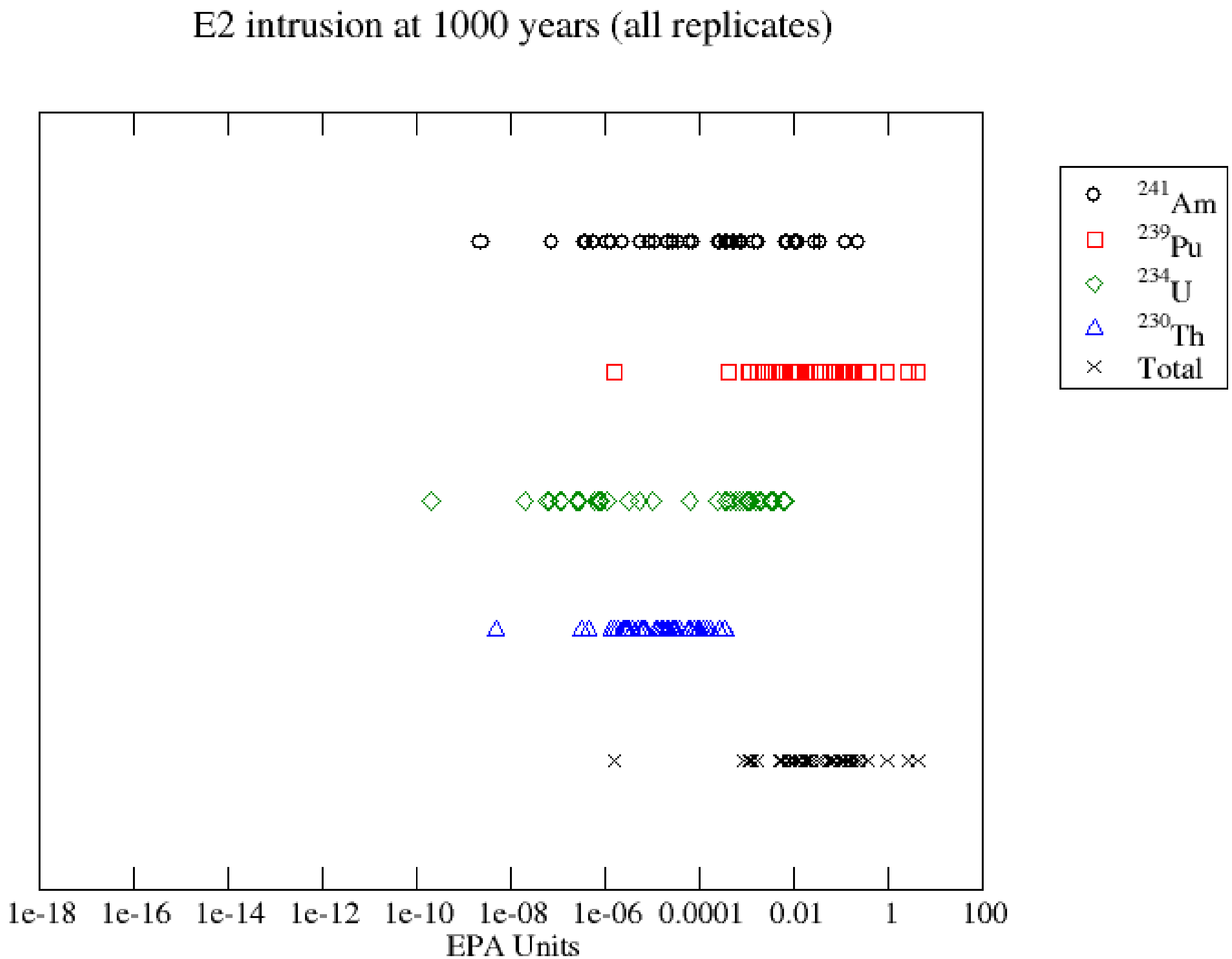
PABC Results for NUTS: Isotope Runs



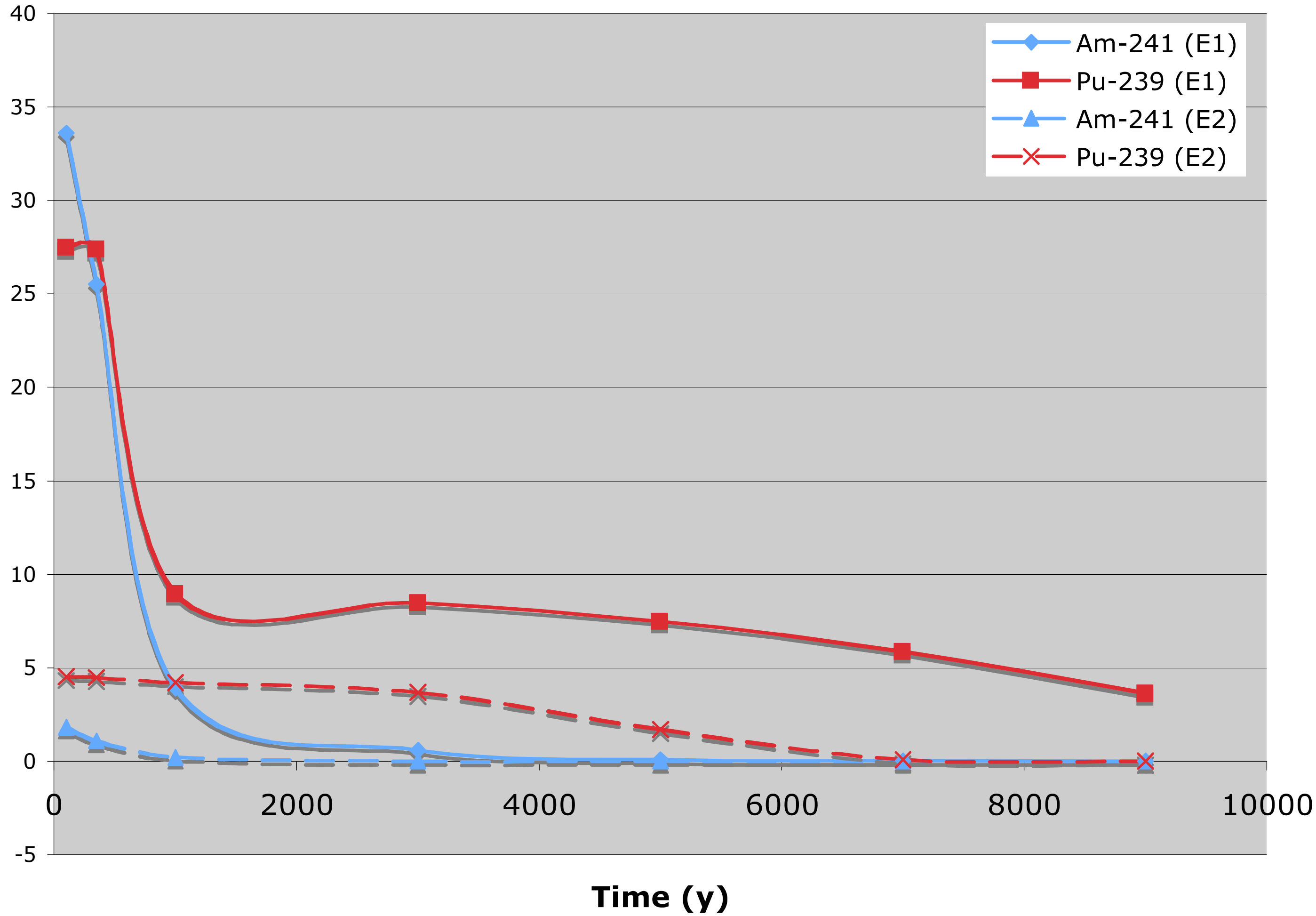
PABC Results for NUTS: Isotope runs



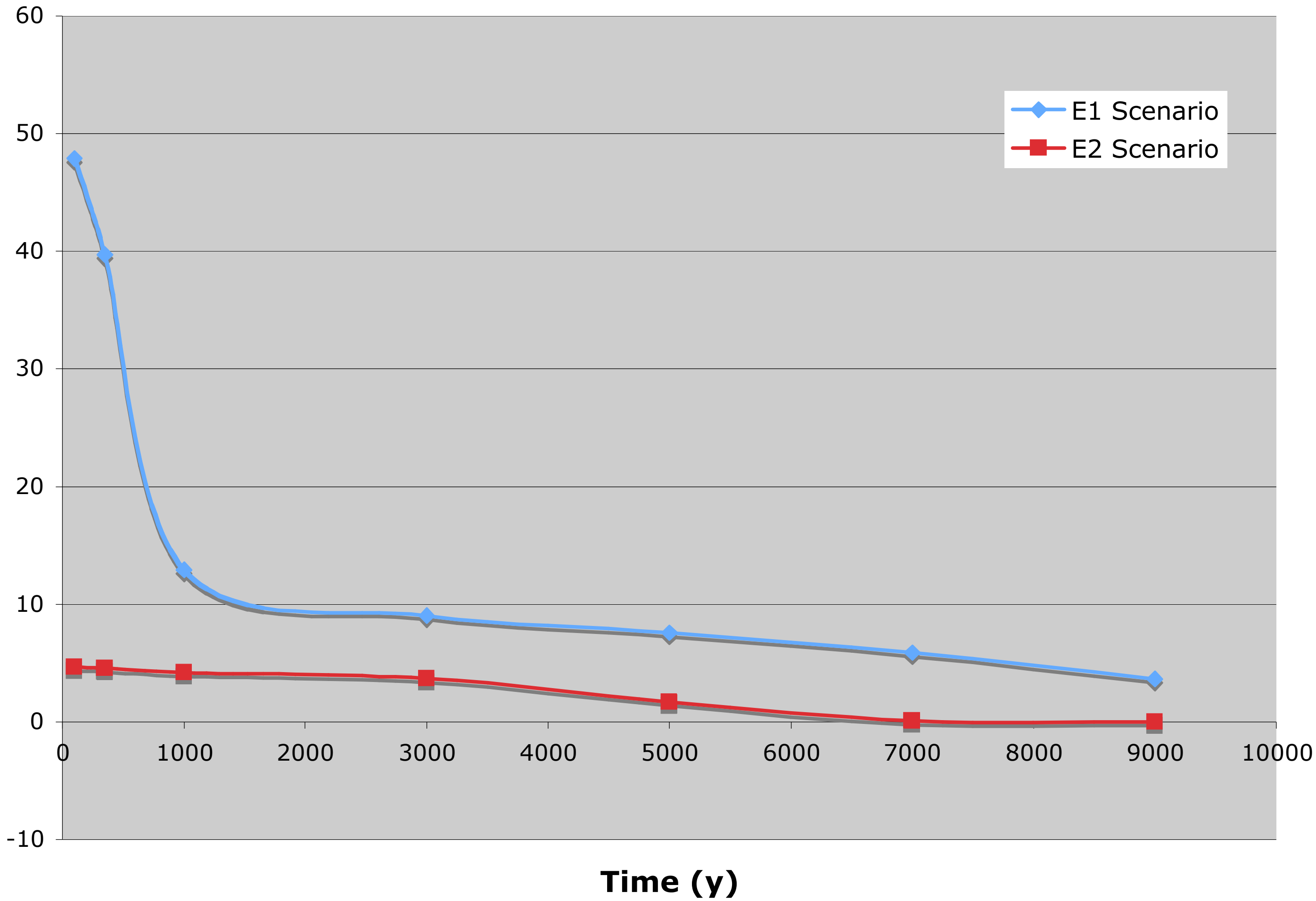
PABC Results for NUTS: Isotope Runs



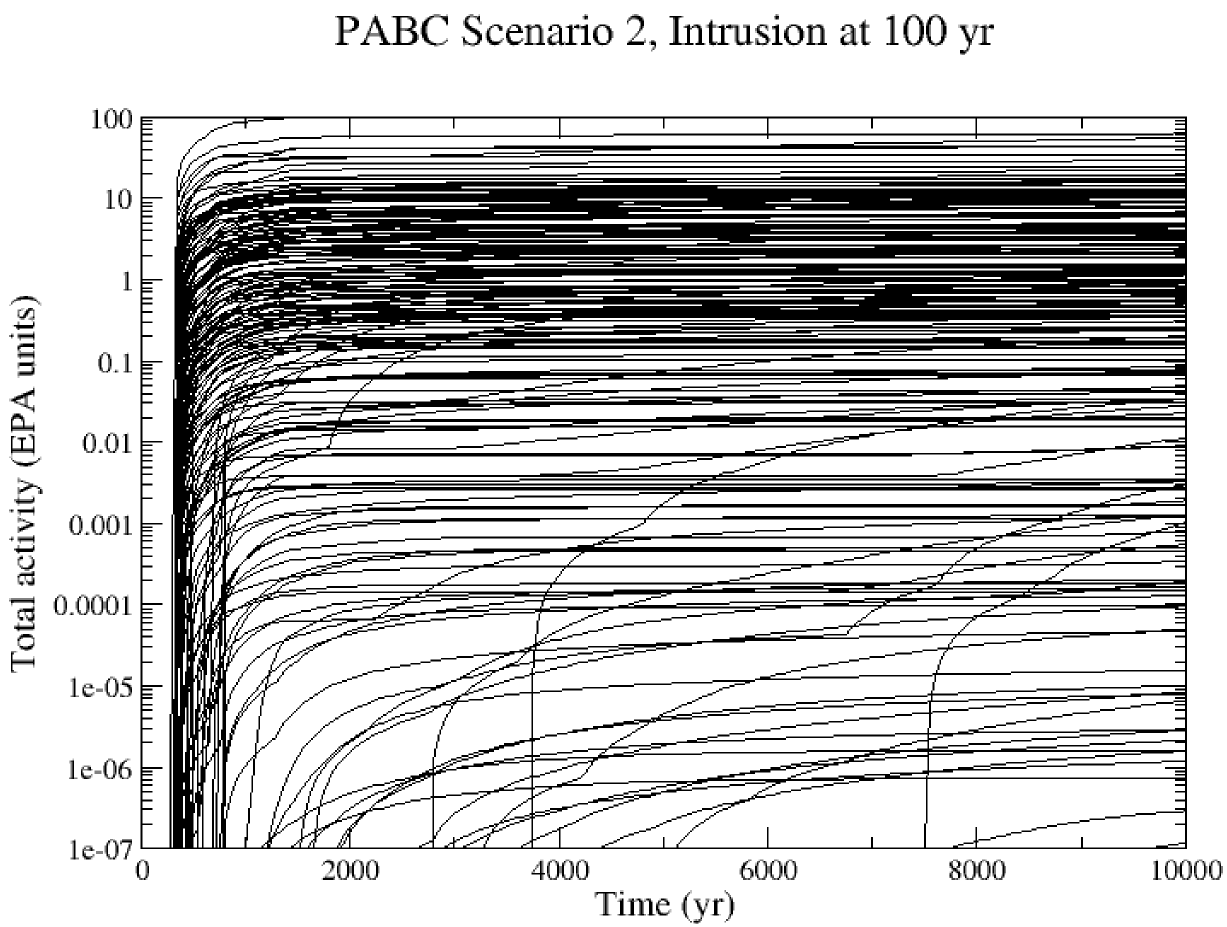
NUTS: Maximum releases for Am, Pu



NUTS: Maximum total releases

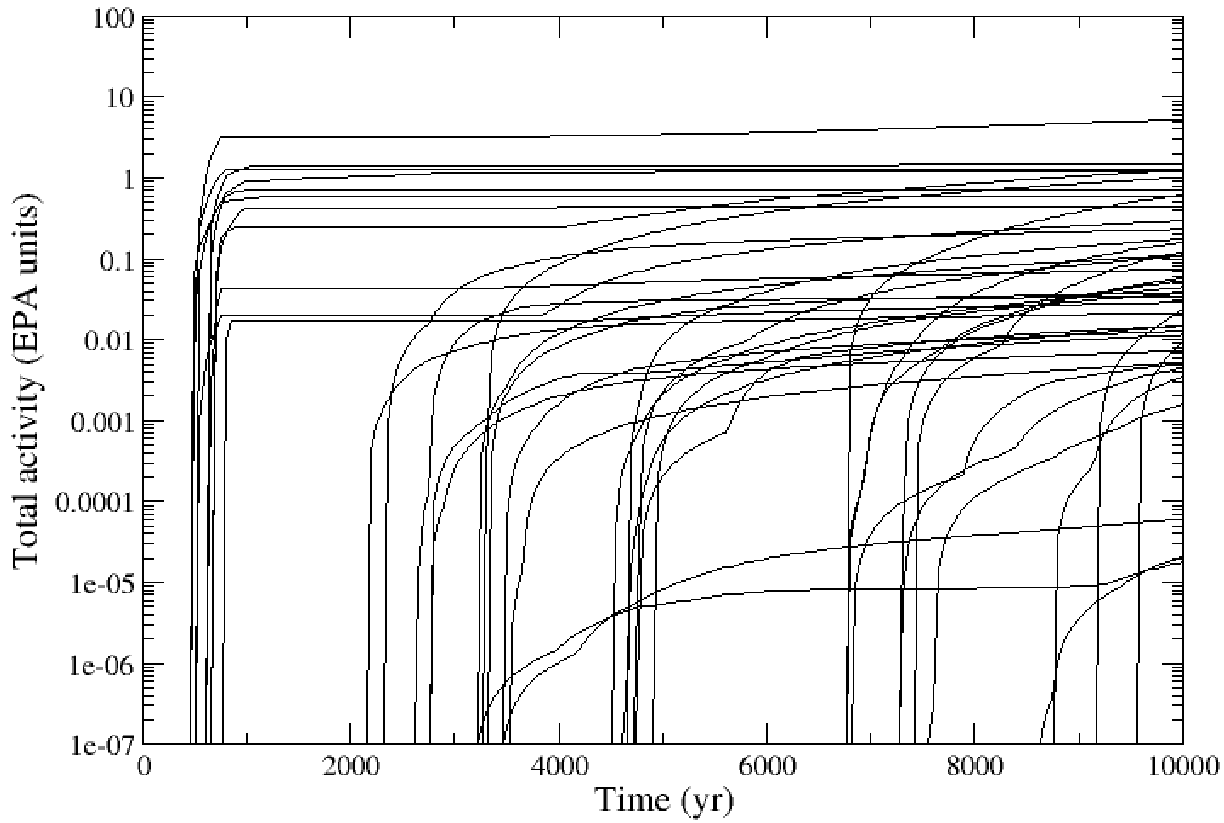


NUTS: Time-intrusion horsetail plots

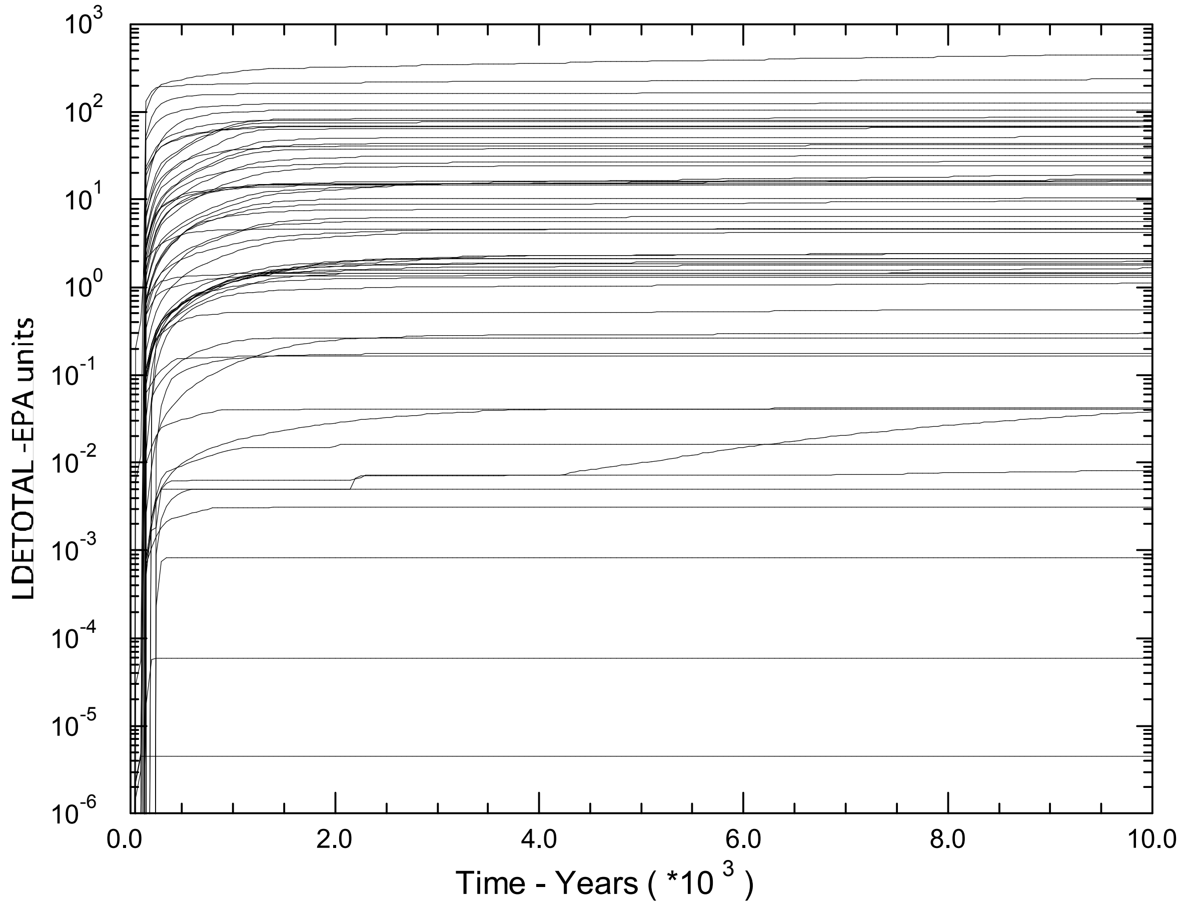


NUTS: Time-intrusion horsetail plots

PABC Scenario 4, Intrusion at 100 yr



PABC Results for PANEL: E2-E1 intrusion



PABC Results for PANEL