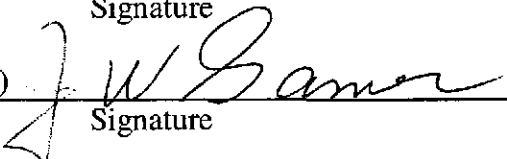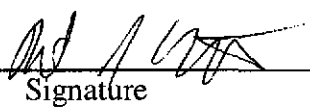548845

Sandia National Laboratories

Waste Isolation Pilot Plant

Analysis Package for Salado Transport Calculations:

Compliance Recertification Application 2009

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1 Introduction

The Waste Isolation Pilot Plant (WIPP) is a deep geologic repository developed by the US Department of Energy (DOE) for the disposal of transuranic (TRU) radioactive waste. Containment of TRU waste at the WIPP is regulated by the U.S. Environmental Protection Agency (EPA) according to the regulations set forth in Title 40 of the Code of Federal Regulations (CFR), Parts 191 (EPA 1985) and 194 (EPA 1996). In December 2007 and January 2008, Sandia National Laboratories (SNL) completed a Performance Assessment (PA) of the WIPP. This PA supports the 2009 Compliance Recertification Application (CRA-2009) to be submitted by the DOE to the EPA to demonstrate continued compliance with the radiation protection regulations of 40 CFR 191 and 40 CFR 194. This analysis has been termed the CRA-2009 PA.

This analysis package documents the CRA-2009 PA calculations performed by the codes NUTS (NUclide Transport System) and PANEL. NUTS (Treadway 1997) is designed to model multidimensional, multi-component, and radioactive-contaminant transport and to analyze the transport of selected radionuclides from the WIPP repository through the Salado Formation and estimates the mobilized radioactive contaminant load in the brine phase of the brine/gas mixture that seeps or flows through the repository's waste panels. PANEL (Garner 2005a) estimates the mobilized radioactive contaminant load in the brine phase of the brine-gas mixture that seeps or flows through the repository's waste panels. The contaminants introduced into the brine are the aged radioisotopes that are assumed to reside in the repository at the time of closure plus any progeny of those radioisotopes that may have been produced through radioactive decay.

Three potential pathways for migration of radioisotopes in dissolved brine are considered in this analysis. The first and most important pathway is a human intrusion through the repository. Under this scenario, brine may be released up the borehole toward the Culebra Dolomite member of the Rustler formation. In the second pathway, brine may migrate through or around the panel seals through the disturbed rock zone (DRZ) surrounding the repository to the shaft and then upward toward the Culebra. In the third pathway, brine may migrate from the repository through the DRZ and then laterally toward the subsurface land withdrawal boundary within the anhydrite inter-beds (marker beds) of the Salado formation.

Initially, brine may flow into the repository from any one of the migration pathways mentioned above. If sufficient brine enters the repository, the radioisotopes become mobilized in both solute and colloidal sorbed forms. Once the radioisotopes are mobilized, transport away from the repository can only occur if the head potential within the repository exceeds that outside the repository and if brine saturation in the waste exceeds residual brine saturation.

1.1 *Purpose*

This analysis package describes the Salado transport calculations that are part of AP-137, Analysis Plan for the Performance Assessment for the 2009 Compliance Recertification Application (Clayton 2008), which are carried out using the codes NUTS and PANEL. In particular, we determine the amount of radionuclides released to the Culebra and at the Land Withdrawal Boundary as a function of time for six different intrusion scenarios. To quantify these releases, the mobilization and subsequent migration of radioisotopes throughout the repository, the shaft system, the Salado formation, and possible human intrusion through boreholes are calculated using information regarding the radionuclide inventory in the repository as well as fluid flow profiles of

brine and gas present in the repository. We also compare the results obtained for NUTS and PANEL in the CRA-2009 PA to those in the CRA-2004 PABC, with consideration also given to the results of changes implemented between the two sets of PA calculations.

1.2 *Outline*

The rest of this document is organized as follows. Section 2 presents the computational methodology of the analysis, including software and hardware environment and the modeling grid, plus information on modeling scenarios and uncertainty. Section 3 presents the major assumptions that are an integral part of the analysis. Section 4 presents and analyzes the results, and Section 5 provides conclusions.

2 Methodology

2.1 *Modeling Scenarios*

The repository is excavated from bedded salt approximately 650 m below the land surface in the Salado Formation. It is connected to the surface by four shafts to be sealed after waste emplacement is complete. The geologic formations directly above and below the Salado are the Rustler and Castile Formations, respectively. The Rustler Formation, located above the repository, has higher transmissivity than the surrounding formations; its most transmissive sub-unit is the Culebra Dolomite Member. The Castile Formation, which lies below the repository, contains areas of pressurized brine; it is unknown if any of these pressurized pockets are located underneath the repository itself.

To represent possible future states of the repository and to predict possible releases through the Salado, six modeling scenarios are defined in Table 1. Scenario S1 assumes that the repository remains undisturbed throughout the 10,000-year compliance period of WIPP PA. Four of the scenarios assume that a single drilling intrusion into the repository occurs. Two scenarios, S2 and S3, assume that a brine pocket in the Castile Formation is encountered during the drilling intrusion, while the other two scenarios, S4 and S5, assume that a Castile brine pocket is not encountered. Intrusions that hit a brine pocket are called E1 intrusions, while intrusions that do not encounter a brine pocket are called E2 intrusions. The remaining scenario, S6, describes a two-intrusion process consisting of an E2 intrusion after 1,000 years and an E1 intrusion after 2,000 years.

Table 1 – Intrusion Scenarios Considered in WIPP PA

Scenario	Number of Drilling Intrusions	Intrusion Time(s) (Years)	Castile Brine Pocket Encountered (Intrusion type)
S1	0	N/A	N/A
S2	1	350	Yes (E1)
S3	1	1000	Yes (E1)
S4	1	350	No (E2)
S5	1	1000	No (E2)
S6	2	1000 and 2000	Only for intrusion at 2000 years (E2-E1)

The first five scenarios are modeled using the code NUTS, while the sixth scenario is modeled using the code PANEL. Scenario S6 cannot be modeled in NUTS because the model for the two-

intrusion scenario assumes that the two boreholes are drilled in different locations; this assumption cannot be explicitly handled in NUTS, which has a fixed grid of coordinates based on a single borehole intruding into the repository.

2.2 *Summary of Potential Pathways*

We present below a brief overview of the physical processes leading to releases from the Salado formation; Nemer and Clayton (2008) give a complete analysis of the Salado transport calculation results.

When brine enters the disposal region, gas is generated by anoxic corrosion of iron and biodegradation of organic materials, resulting in the eventual release of radioisotopes into the brine from the waste. If sufficient quantities of gas are generated, pressures in the disposal region will increase, reducing brine flow into the repository. Brine containing dissolved radioisotopes may be expelled from the repository if pressure in the repository exceeds the brine pressure in the immediately surrounding formation. Brine saturation in the waste must exceed residual brine saturation in order for brine to be expelled from the repository.

Three potential pathways for migration of radioisotopes in dissolved brine are considered in this analysis. The first and most important pathway is a human intrusion through the repository. Under this scenario, brine may be released up the intrusion borehole toward the Culebra Dolomite member of the Rustler formation. Once in the Culebra, contaminated brine may then move toward the subsurface land withdrawal boundary. Direct brine releases to the surface are modeled and analyzed separately. In the second pathway, brine may migrate through or around the panel seals through the disturbed rock zone (DRZ) surrounding the repository to the shaft and then upward toward the Culebra. In the third pathway, brine may migrate from the repository through the DRZ and then laterally toward the subsurface land withdrawal boundary within the anhydrite inter-beds (Marker Beds 138 and 139 in Figure 1).

The dynamics of brine movement are complex and highly dependent on the BRAGLO input parameters. Initially, brine may flow into the repository from any one of the migration pathways mentioned above. If sufficient brine enters the repository the radioisotopes become mobilized in both solute and colloidal sorbed forms. Once the radioisotopes are mobilized, transport away from the repository can only occur if the head potential within the repository exceeds that outside the repository and if brine saturation in the waste exceeds residual brine saturation.

2.3 *Uncertainty*

To address uncertainty in many of the input parameters used in performance assessment calculations, sets of Latin hypercube-sampled parameters are defined; each unique set is called a vector. Latin Hypercube Sampling (LHS) is a structured Monte Carlo sampling method in which samples are drawn from bins of equal probability with correlations between parameters minimized. Each group of 100 vectors is called a replicate. Three replicates (R1, R2, and R3) are run in a full PA calculation. Consequently, a full PA calculation requires five scenarios of 100 vectors for three replicates in NUTS, plus one scenario of 100 vectors for three replicates in PANEL for a total of 1,800 simulations. As will be discussed below, screening runs are used to substantially reduce the number of simulations that must be run in NUTS.

Figure 1 – Computational grid used for Salado Flow and transport calculations.
DRZ represents the Disturbed Rock Zone surrounding the repository area and MB refers to the marker beds. The green area between the upper and lower DRZ's is the repository area and the grayed cells extending from the Castile to the surface shows the intrusion borehole location. CONC_MON represents a concrete monolith, CONC_PCS is the concrete portion of the panel closure system, DRZ_PCS is the disturbed rock zone directly above the concrete portion of the panel closure system, OPS and EXP are the operations and experimental areas of the repository, and RoR is the rest of the repository. The x-axis corresponds to north, the y-axis to depth, and the z-axis to east; all distances are given in meters.

2.4 *Modeling Grid*

The grid used for the NUTS calculations is the same as used for the BRAGFLO calculations, and is stored in the OpenVMS PA system in library LIBCRA09_BF, class CRA09-0, file *gm_bf_CRA09.cdb*. The grid remains unchanged from the CRA-2004 PABC calculations and is illustrated in Figure 1. The extent of the modeling domain is 46,630 m in the horizontal north (x) direction by 940 m in the vertical (y) direction, which is the same as for the CRA-2004 PABC calculations. The domain is discretized into a non-uniform 68×33 grid of (x,y) cells with higher resolution in the repository area and lower resolution towards the edges of the modeling domain. PANEL uses a one-cell grid that encompasses the intruded panel.

2.5 *Other Codes*

The codes that perform the modeling calculations are NUTS (scenarios S1 to S5) and PANEL (scenario S6). BRAGFLO, POSTBRAG, and PREBRAG must be run prior to NUTS and PANEL because the former codes provide input files necessary for the execution of the latter. Uncertainty in the input parameters is included through the use of LHS. The other codes are used for data manipulation and visualization. A listing of the codes is shown in Table 2; more information for each code can be found in the respective design documents and user manuals.

For the NUTS calculations, ALGEBRACDB calculates the integrated fluxes up the borehole, up the shafts, or out through the marker beds. SUMMARIZE is then used to provide a summary of the fluxes. The output from SUMMARIZE is used as input to a plotting/visualization program to view the results. Here, SigmaPlot version 10 and SPLAT are used to plot the breakthrough curves for each replicate/vector/isotope combination.

Since the completion of the CRA-2004 PABC, the OpenVMS operating system used on the WIPP PA Alpha cluster was upgraded from version 7.3-1 to version 8.2. The change in the operating system caused a minor incompatibility with NUTS version 2.05a regarding the handling of dates. To correct the error, some minor changes were made to version 2.05a, which was then re-released as version 2.05c (Gilkey 2006). No changes to the calculation process were made.

Table 2 – List of the major codes used for Salado transport analysis for the CRA-2009 PA

Code	Version	Code Function
ALGEBRACDB	2.35	Data processor
BRAGFLO*	6.00	Brine and gas flow
GENMESH	6.08	Grid generation
ICSET	2.22	Sets initial conditions
LHS	2.42	Latin hypercube sampler
MATSET	9.10	Sets material parameters
NUTS	2.05c	Salado transport
PANEL	4.03	Salado transport, actinide mobilization
POSTBRAG*	4.00a	BRAGFLO postprocessor
POSTLHS	4.07	LHS postprocessor
PREBRAG*	8.00	BRAGFLO preprocessor
PRELHS	2.30	LHS preprocessor
SPLAT	1.02	Plot generation
STEPWISE**	2.21	Correlation analysis
SUMMARIZE	2.20	Data interpolation

*Not directly used as part of the analysis of Salado transport, but must be run to provide input files for NUTS and PANEL.
**Receives output from NUTS and PANEL.

3   An Overview of NUTS and PANEL

3.1   *NUTS*

For scenarios S1 through S5, the overall transport and decay of radionuclides are calculated using the computer code NUTS, version 2.05c. NUTS is a five-point finite-difference code designed to model multi-dimensional, multi-component, and radioactive-contaminant transport in single-porosity, dual-porosity, or dual-permeability porous media, including parent/daughter first-order decay.

The analysis is composed of three types of modeling runs: screening (SCN) runs, isotope (ISO) runs, and time-intrusion (TI) runs, which are discussed in detail in Section 3.1.3 below.

3.1.1 Modeling Assumptions

This section examines the major data inputs, modeling factors, and assumptions for the NUTS PA model. It is not intended to fully document the NUTS code, but rather to provide the reader with sufficient details to interpret and understand the results. For more detail, the reader is referred to the NUTS user's manual (Treadway 1997). NUTS is designed to model mobilization and decay of selected isotopes. For mobilization, the code requires the isotope inventory and element solubility. The isotope inventory is apportioned among the various computational cells according to their volume or areal fractions of the repository; this approach is equivalent to assuming a homogeneous waste inventory.

Radionuclide releases from the repository to the Culebra depend on the rate of brine flow, the solubility limit, and the amount of radionuclide available for transport. Radionuclides are assumed to exist in five states that can be transported from the repository by flowing groundwater (Helton et al. 1998): dissolved, humic colloids, microbial colloids, mineral fragment colloids, and actinide intrinsic colloids. The concentration in each of these states is a function of one or more sampled variables. Element solubility is defined to be the maximum concentration that the brine can hold both suspended on colloids and dissolved in the brine. Stockman et al. (1996) and Garner (2003) provide a full discussion on effective solubility related to the radionuclide transport calculations. Mobilization is assumed to be instantaneous at the solubility limit (up to the inventory limit) such that the radionuclide concentration in the brine and on the colloids is always at equilibrium. However, since the isotope inventory changes with time as a result of decay and ingrowth, steady-state equilibrium is not achieved.

The key processes modeled are advective transport, or transport caused by the velocity field of the fluid; decay of radionuclides; precipitation of radionuclides out of solution; solubility limits controlling the amount of radionuclides permitted in the aqueous phase; and interior sources in a single-porosity, continuous matrix; dispersion, which smears the concentration profile in the direction of fluid flow, is not modeled (Treadway 1997).The initial condition for each run is to assume no radionuclides present within the model domain, with the exception of the source term in the waste panel area.

3.1.2 Data Flow

Any flow of brine up the shafts or boreholes or through the marker beds is calculated using the code BRAGFLO, which must be run prior to running NUTS. NUTS uses multiple input files, including the BRAGFLO ASCII input file containing the grid specifications, initialization parameters, and material maps as well as the BRAGFLO post-processed binary file (CDB) that describes the flow-field. These CDB files are the source for brine fluxes at the cell interfaces, porosity, saturation, pressure, and the geometric information. In addition, NUTS uses a CDB file that contains "effective solubilities," and "lumped inventory" source terms created by PANEL, and atomic weights and half-lives of the modeled isotopes plus an input file specific to NUTS, containing run parameters and isotope decay data information.

The NUTS binary output file is used by ALGEBRACDB, which in turn produces output used by SUMMARIZE. The output from SUMMARIZE is imported into a graphics package such as

SigmaPlot or BLOT and then plotted. Figure 2 shows the relationship between the major codes used in the NUTS analysis.

Figure 2 – Run sequence for NUTS in the CRA-2009 PA

3.1.3 Type of Model Runs

NUTS can perform three different types of model runs: screening (SCN) runs, which identify those vectors which must be analyzed in greater detail; isotope (ISO) runs, which determine the amount of radionuclides transported throughout the repository; and time-intrusion (TI) runs, which repeat the ISO calculations with different starting times. The following sections describe each type of run.

3.1.3.1 Screening (SCN) Runs

Full transport calculations are computationally intensive. NUTS screening runs increase computational efficiency by filtering out scenario-vector combinations that have no potential to release radionuclides either to the Culebra or across the land withdrawal boundary (LWB). SCN runs calculate the transport of a temporally continuous conservative tracer (constant concentration, Dirichlet boundary condition) with an initial concentration of 1 kg/m^3 in all waste disposal areas over 10,000 years. A vector is considered "screened in" if the concentration of cumulative tracer that enters the accessible environment (either by crossing the LWB or by entering the Culebra via the borehole and/or shaft) exceeds 10^{-7} kg/m^3. The magnitude of the initial tracer and screening cutoff concentrations are considered conservative: as discussed in Stockman *et al.* (1996), the tracer concentration was chosen to be greater than the maximum observed concentration of any

radionuclide in the repository, while the cumulative limits underestimate the minimum amount of mass required for a release. Vectors not "screened in" are excluded from ISO and TI calculations, where specific isotopes and more complicated chemistry are modeled.

SCREEN.FOR, a Fortran 90 program, post-processes the output from the SUMMARIZE screening runs and lists which vectors satisfy the screening criteria and where the breach occurs (borehole, markerbeds, shaft). It also totals the number of "screened in" vectors for each scenario. Although no changes have been made to SCREEN.FOR since the CRA-2004 PABC, because SCREEN.FOR is not a qualified PA code, we have verified SCREEN.FOR for the CRA-2009 PA. Details of the verification process are provided in 6Appendix B. [See Long (2008) for information on the run control used for SCREEN.FOR.]

3.1.3.2 Isotope Runs

The ISO runs consist of modeling each isotope for each scenario and calculating the time-integrated flux laterally across the LWB and vertically to the Culebra (via boreholes or shaft) in EPA units. The NUTS ISO runs consist of the undisturbed scenario (S1) as well as the 350- and 1000-year intrusion scenarios (S2 through S5) as calculated by BRAGFLO.

Unlike the screening runs, the isotope and time intrusion runs model specific isotopes and decay chains. To further reduce computational overhead, the complete set of isotopes and decay chains was examined to determine the minimum number of isotopes required to describe the compliance behavior of the WIPP (Stockman et al. 1996). Isotopes having similar decay behaviors and transport characteristics were combined into "lumped isotopes" such that little or no release information is lost. The analysis of Stockman et al. yielded five lumped isotopes (^{241}Am, ^{238}Pu, ^{239}Pu, ^{234}U, and ^{230}Th) in three decay chains:

$$^{241}Am;^{238}Pu \rightarrow {}^{234}U \rightarrow {}^{230}Th; \text{ and } {}^{239}Pu.$$

As these are the same isotopes and chains modeled in both the CRA-2004 PABC and the CRA-2009 PA, no changes to the code or analysis scripts are needed. Note that while ^{241}Am and ^{239}Pu have parent and daughter isotopes, those other isotopes are not considered part of the chain. Moreover, since the half-life of ^{238}Pu is 87.7 years, most of the ^{238}Pu initially present in the repository will have decayed in the time frames of interest. Therefore ^{238}Pu is not considered individually in the remainder of this analysis, although total releases presented below do include contributions from ^{238}Pu.

The total release to the environment, R_n, is reported in normalized "EPA units":

$$R_n = \sum \frac{Q_i}{L_i}\left(\frac{1 \times 10^6 \text{Ci}}{C}\right), \tag{1}$$

where Q_i is the 10,000-year cumulative release of radionuclide i, L_i is the release limit for radionuclide i (as specified by 40 CFR 194), and C is the total transuranic inventory in the WIPP; all measurements are in curies (Ci). All values of EPA units quoted and used in this report are calculated using ALGEBRACDB and are contained in the appropriate ALGEBRACDB output files stored in the Configuration Management System (CMS).

3.1.3.3 Time Intrusion (TI) Runs

By shifting the initial conditions from the BRAGFLO runs to the appropriate time, the NUTS TI runs simulate intrusion times that occur at times other than the 350- and 1000-year intrusions modeled in the ISO runs. For instance, the BRAGFLO results for E1 and E2 intrusions at 350 years are used as input to NUTS at both 100 and at 350 years. For the 100-year intrusion, the flow pattern used in NUTS subsequent to the intrusion is assumed to be the same as the flow pattern predicted by BRAGFLO subsequent to an intrusion at 350 years. Transport calculations are also done with intrusion times of 3000, 5000, 7000, and 9000 years. For times greater than 1000 years, "shifted intrusion-time" calculations are performed, assuming an undisturbed scenario until the time of intrusion and then the 1000-year intrusion flow-field after the intrusion.

This approach is justified since previous BRAGFLO simulations for intrusion times greater then 1000 years have shown that undisturbed conditions reach steady state prior to intrusion. In addition, repository performance is most sensitive to gas-pressure relief and brine inflow (from the high-pressure brine pocket or marker beds) that occurs at or soon after intrusion. However, it is insensitive to changes, such as fracturing, that occur prior to intrusion (Stockman *et al.* 1996; Nemer and Clayton 2008). Thus, the flow-field after intrusion is much more dependent on an intrusion event occurring than on the conditions before intrusion.

3.1.4 Computational Procedure

This section documents the input and output files used for NUTS, ALGEBRACDB, and SUMMARIZE for the Salado transport calculations as well as the library locations within the CMS where the final versions are archived. A detailed description of the run control procedures used for the CRA-2009 PA, including the NUTS calculations, and the input, log, script, and output files for each step are described in Long (2008).

3.1.4.1 Step 1: NUTS "Screening Mode"

Step 1 invokes NUTS in "screening mode" to compute the transport of a conservative tracer for BRAGFLO scenarios S1 through S5. Step 1 is run for each replicate for each of these scenarios. The script loops over all 100 vectors for each replicate/scenario combination.

3.1.4.2 Step 2: SUMMARIZE and SCREEN

Step 2 uses SUMMARIZE and SCREEN to determine the vectors to be included in the full transport simulations. Step 2 is run for each replicate for scenarios S1 through S5. For each replicate/scenario combination, the script writes an input control file, and then runs SUMMARIZE to tabulate transport of the conservative tracer at key locations. The script then runs the SCREEN utility on the SUMMARIZE table. The SCREEN utility output file lists vectors "screened in" for use in the full transport simulations. Because the undisturbed simulation results are needed as initial conditions to compute the consequences of intrusions, a vector is automatically "screened in" for scenario S1 if it was "screened in" for any of scenarios S2 through S5, regardless of the tracer transport results.

SCREEN output files have two sections, UNION and NONUNION. Vectors listed in the NONUNION section have concentrations of the conservative tracer greater than the tolerance. The UNION section is only used in S1 to list vectors screened in for scenarios S2 through S5.

Any S1 vectors that had tracer concentrations greater than the tolerance are listed in the NONUNION section of the S1 output file.

3.1.4.3 Step 3: Isotope Mode (ISO)

Step 3 invokes NUTS in "isotope" mode to compute radionuclide transport for BRAGFLO scenarios S1 through S5. Step 3 is run for each replicate for each of these scenarios. The script loops over only the screened-in vectors specified in the SCREEN output file from Step 2 for each replicate/scenario combination.

3.1.4.4 Step 4: Time Intrusion Mode (TI)

Step 4 invokes NUTS in "time intrusion" mode to compute radionuclide transport for single intrusions (BRAGFLO scenarios S2 through S5, but at times different from the intrusion times in the BRAGFLO scenarios). Step 4 is run for each replicate for scenarios S2 through S5. The script loops over the screened-in vectors specified in the SCREEN output file for each replicate/scenario combination.

3.2 *PANEL*

PANEL is unique in the WIPP PA framework in that it produces information for several of the downstream WIPP PA codes: NUTS (for Salado transport), CCDFGF (for DBR releases), and CCDFGF (for Culebra releases). The calculated outputs in each case are different. NUTS needs information for the "lumped" radionuclides ^{241}Am, ^{238}Pu, ^{239}Pu, ^{234}U, and ^{230}Th. CCDFGF (for DBR releases) needs the mobilized radionuclide concentrations in brine (Salado and/or Castile brine), while CCDFGF (for Culebra releases in the S6 scenario) needs the EPA units of the "lumped" radionuclides ^{241}Am, ^{238}Pu, ^{239}Pu, ^{234}U, and ^{230}Th up the borehole to the Culebra. In addition to providing inputs used by other PA codes, PANEL is frequently used in a stand-alone mode to calculate radionuclide decay.

Since the inventory and the minimum significant brine volume were unchanged from the CRA-2004 PABC, PANEL was not rerun in either the DECAY mode, which calculates the decay pathways for the inventory as a function of time, or the CONCENTRATION mode, which calculates the amount of radionuclides mobilized for a given volume of brine; for these results, see Garner and Leigh (2005). For Scenario S6, PANEL was run in STANDARD mode, which computes the amount of radionuclides transported up the borehole to the Culebra. The run control pathway for STANDARD mode is shown in Figure 3, where the output from MATSET and POSTLHS (see Table 2) on the left-hand-side of the figure and the output from BRAGFLO on the right-hand side are processed by ALGEBRACDB before being used as inputs by PANEL. Because the DECAY and CONCENTRATION runs were not performed for the CRA-2009 PA, the ALGEBRACDB output files from the CRA-2004 PABC were used unaltered (Long 2008). Reference information on the files generated by GENMESH, MATSET, POSTLHS and ALGEBRACDB for the DECAY and CONCENTRATION runs are given in Garner and Leigh (2005). (See Table 2 for descriptions of the codes listed above.)

A detailed description of the run control procedures used for the PANEL calculations, as well as the input, log, script, and output files for each step, are described in Long (2008).

Figure 3 – Run sequence for PANEL in the CRA-2009 PA

3.2.1 BRAGFLO Output to PANEL

As mentioned above, PANEL requires BRAGFLO results (right-hand-side of Figure 1). The re-quired PANEL input for the S6 scenario is generated by the BRAGFLO run and written to the files ALG2_BF_CRA09_Rr_S6_Vvvv.CDB (r = 1, 2, or 3; vvv = 001, 002, ... 100) which are stored in CMS libraries LIBCRA09_BFRrS6 (r = 1, 2, or 3).

3.2.2 SUMMARIZE and SPLAT

The SUMMARIZE code (Baker 2003b) extracts data from the PANEL binary output files (.CDB) to produce ASCII tables organized according to analytical needs. One common use of SUMMARIZE is to create a table of output variables with values for 100 vectors reported at specified time intervals. Tables from SUMMARIZE are used to make cumulative release plots that show the values of output variables for each of the 100 vectors in a scenario over time (usu-ally the full 10,000 year regulatory period). These plots are generated using the SPLAT code (Baker 2003a).

Information Only

4 Results

This section presents the results from NUTS and PANEL simulations for transport of the major lumped radioisotopes within the Salado formation for scenarios S1 through S6 as discussed above. As mentioned, although NUTS models five isotopes, ^{238}Pu is a small fraction of the inventory within the repository and has a relatively short half-life (87.7 years), and is therefore excluded from further consideration in our analysis, although total releases presented below do include contributions from ^{238}Pu.

4.1 *NUTS*

4.1.1 Screening Runs

Screening runs reduce the total number of simulations necessary by eliminating vectors that cannot transport sufficient quantities of radionuclides beyond the LWB. Screening runs model a conservative tracer with a concentration of 1 kg/m^3. The cumulative mass of tracer is monitored at the intersection of the borehole and the Culebra intersection, at the intersection of the shaft and the Culebra, and at the LWB in the marker beds. Vectors with a cumulative tracer release of 10^{-7} kg/m^3 or more at any of these key points are "screened in" and passed through to the full radionuclide transport simulations. The results of the screening runs are presented in Table 3.

For this analysis, replicates R1, R2, and R3 screened in 155, 161, and 165 vectors out of a possible 500 each. These vectors are listed in Table 3, sorted by replicate and scenario. The total of 481 screened-in vectors represents an increase of roughly 2 percent over the CRA-2004 PABC, which had 471 screened-in vectors. In addition to these vectors, it was also necessary to screen in 70 vectors from replicate R1, 76 vectors from replicate R2, and 77 vectors from replicate R3 for Scenario 1 to provide the flow conditions needed for the time-intrusion calculations. As in the CRA-2004 PABC calculations, we find that only one vector showed potential releases to the markerbeds—vector 53 in replicate R1, which was also the only vector to be screened-in for the undisturbed scenario in all three replicates. No vector in this analysis showed releases at the shaft/Culebra interface. The remaining vectors from scenario S1, listed in Table 4, are analyzed only to provide the fluid flow profiles needed for the intrusion scenarios.

Table 3 – Screened-in vectors for each scenario/replicate combination

Rep.	Scen.	Vectors[a]	Count
R1	S1	(53M)	1
	S2	2, 3, 6, 7, 8, 9, 10, 12, 13, 14, 16, 17, 19, 20, 22, 23, 24, 25, 26, 27, 28, 29, 30, 34, 35, 36, 38, 41, 43, 45, 46, 47, 48, 49, 50, 51, 52, (53M), 54, 55, 58, 59, 60, 61, 62, 63, 64, 66, 67, 69, 70, 71, 72, 73, 74, 76, 78, 79, 80, 82, 83, 84, 86, 88, 89, 90, 92, 93, 94, 98	70
	S3	2, 3, 7, 8, 9, 10, 12, 13, 14, 16, 17, 20, 22, 23, 24, 25, 27, 28, 29, 30, 34, 35, 36, 41, 43, 45, 46, 47, 49, 50, 54, 55, 58, 59, 60, 61, 62, 63, 66, 67, 70, 71, 76, 78, 79, 80, 82, 83, 84, 86, 89, 90, 93, 94, 98	55
	S4	2, 7, 9, 12, 16, 17, 27, 36, 45, 50, (53M), 55, 76, 78, 82	15
	S5	7, 9, 12, 16, 17, 27, 36, 45, 50, (53M), 55, 76, 78, 82	14
R2	S1	None	0

Rep.	Scen.	Vectors[a]	Count
	S2	2, 3, 4, 6, 8, 9, 10, 11, 12, 14, 16, 17, 18, 19, 20, 21, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 43, 44, 45, 48, 49, 50, 51, 52, 53, 54, 55, 56, 59, 61, 62, 63, 64, 65, 66, 67, 68, 69, 71, 72, 74, 75, 77, 79, 80, 81, 83, 84, 87, 89, 90, 91, 92, 95, 96, 98, 99, 100	76
	S3	3, 4, 6, 8, 9, 12, 14, 16, 17, 18, 20, 21, 24, 25, 26, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 39, 40, 41, 44, 48, 50, 51, 52, 53, 54, 55, 59, 63, 65, 66, 67, 68, 71, 72, 74, 75, 77, 79, 80, 84, 87, 89, 90, 92, 95, 96, 98, 99	58
	S4	4, 17, 24, 28, 34, 36, 40, 53, 55, 63, 68, 79, 92, 95	14
	S5	4, 17, 24, 28, 34, 40, 53, 55, 63, 68, 79, 92, 95	13
R3	S1	None	0
	S2	2, 3, 4, 7, 10, 11, 13, 14, 15, 17, 18, 19, 21, 22, 24, 25, 26, 27, 28, 29, 30, 32, 33, 34, 35, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 49, 50, 52, 53, 56, 57, 58, 59, 60, 61, 62, 63, 64, 65, 66, 67, 68, 69, 70, 71, 73, 74, 76, 77, 78, 79, 84, 85, 86, 88, 89, 90, 91, 93, 94, 95, 96, 97, 98, 99, 100	77
	S3	2, 10, 11, 14, 15, 18, 21, 24, 25, 26, 27, 28, 29, 30, 32, 33, 34, 35, 37, 38, 39, 40, 42, 43, 44, 45, 46, 47, 49, 50, 53, 56, 58, 59, 60, 61, 63, 64, 65, 66, 67, 68, 69, 73, 74, 77, 78, 79, 84, 85, 86, 88, 89, 91, 93, 94, 95, 96, 97, 98	60
	S4	30, 35, 37, 42, 44, 47, 49, 53, 59, 66, 77, 79, 86, 93, 96	15
	S5	30, 35, 42, 47, 49, 53, 59, 66, 77, 79, 86, 93, 96	13

[a]Borehole releases except where indicated by an M (for markerbed releases).

Table 4 – Undisturbed vectors run to provide conditions for intrusion scenarios

Rep.	Vectors	Count
R1	2, 3, 6, 7, 8, 9, 10, 12, 13, 14, 16, 17, 19, 20, 22, 23, 24, 25, 26, 27, 28, 29, 30, 34, 35, 36, 38, 41, 43, 45, 46, 47, 48, 49, 50, 51, 52, **53**, 54, 55, 58, 59, 60, 61, 62, 63, 64, 66, 67, 69, 70, 71, 72, 73, 74, 76, 78, 79, 80, 82, 83, 84, 86, 88, 89, 90, 92, 93, 94, 98	70
R2	2, 3, 4, 6, 8, 9, 10, 11, 12, 14, 16, 17, 18, 19, 20, 21, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 43, 44, 45, 48, 49, 50, 51, 52, 53, 54, 55, 56, 59, 61, 62, 63, 64, 65, 66, 67, 68, 69, 71, 72, 74, 75, 77, 79, 80, 81, 83, 84, 87, 89, 90, 91, 92, 95, 96, 98, 99, 100	76
R3	2, 3, 4, 7, 10, 11, 13, 14, 15, 17, 18, 19, 21, 22, 24, 25, 26, 27, 28, 29, 30, 32, 33, 34, 35, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 49, 50, 52, 53, 56, 57, 58, 59, 60, 61, 62, 63, 64, 65, 66, 67, 68, 69, 70, 71, 73, 74, 76, 77, 78, 79, 84, 85, 86, 88, 89, 90, 91, 93, 94, 95, 96, 97, 98, 99, 100	77

Vector 53 of replicate R1 was also screened in as a result of the potential for releases through the markerbed.

4.1.2 ISO Runs

ISO runs represent the undisturbed case (scenario S1), as well as 350- and 1000-year E1 intrusions (scenarios S2 and S3) and of type E2 (scenarios S4 and S5). The maximum releases for each species in the various ISO cases analyzed are summarized in Table 5.

These values represent the integrated releases for each vector over the 10,000-year compliance period of WIPP PA. Note that the total maximum releases for each scenario do not equal the sum of the individual maximum releases for each of the lumped isotopes because the values for the individual isotopes may be taken from different vectors. Because the solubility of the nuclides is a variable parameter in WIPP PA, and because ^{239}Pu has markedly different solubilities when speciated as Pu(III) versus Pu(IV), it is unlikely that the same vector will have the maximum concentration of every radionuclide in a given scenario.

Table 5 – Maximum radionuclide and total releases at the Borehole/Culebra interface in NUTS ISO calculations

Intrusion	Scenario	Time	Maximum Releases (EPA units)				
			^{241}Am	^{239}Pu	^{234}U	^{230}Th	Total
None	S1	N/A	0.0	0.0	0.0	0.0	0.0
E1	S2	350 yr	29.4	36.1	0.0619	0.135	49.3
	S3	1000 yr	14.2	28.3	0.0543	0.124	28.8
E2	S4	350 yr	2.72	5.11	0.00822	0.00157	7.83
	S5	1000 yr	0.336	2.65	0.00716	0.00141	2.69

In addition to the maximum releases for each radionuclide and the maximum overall releases shown in Table 5, the average release for each scenario plus the percentage contribution of each of the lumped isotopes to the scenario average has been calculated in Table 6. The average release, reported in EPA units, is determined by taking the average of all of the cumulative releases across the three replicates. The percentage assigned to each isotope is the average release for the given isotope divided by the average cumulative release.

Table 6 – Percentage of lumped isotopes relative to average release at the Borehole/Culebra interface for ISO scenarios

Intrusion	Scenario	Time	Percentage of Isotope in Average Release (%)				Average Release (EPA units)
			^{241}Am	^{239}Pu	^{234}U	^{230}Th	
None	S1	N/A	0.0	0.0	0.0	0.0	0.0
E1	S2	350 yr	69.2	30.6	0.1	0.0	2.17
	S3	1000 yr	34.5	65.0	0.3	0.1	0.765
E2	S4	350 yr	45.0	54.7	0.3	0.0	0.0520
	S5	1000 yr	10.1	89.2	0.6	0.1	0.0198

Examining Table 6, we notice prominent changes in the distribution of isotopes between the E1 and E2 intrusion types, and between the 350-yr and 1000-yr intrusion times. Because of the shorter half-life of ^{241}Am (approximately 430 yr) relative to ^{239}Pu (approximately 24,000 yr), a much larger fraction of the ^{241}Am will decay between 350 and 1000 years than for the ^{239}Pu. Comparing the intrusion types, we can see by comparing the average total release to the maximum total release that a handful of vectors dominate the releases in each scenario. Differences in

the brine volumes between the two scenarios, combined with speciation-dependent variations in the solubility, are largely responsible for the difference in compositions between the E1 and E2 releases. The relative magnitude of the E1 and E2 releases is a result of the smaller brine volumes available in the E2 scenarios.

4.1.2.1 Scenario S1: Undisturbed Scenario

Scenario S1 represents the undisturbed state of the repository. In replicates R1, R2, and R3, there are 70, 76, and 77 screened-in vectors, respectively; these vectors are listed in Table 4. These vectors were included because their flow and transport profiles were needed for the time intrusion runs. Only one vector, vector 53 in replicate R1, was screened in because of the potential for significant releases in the undisturbed scenario. However, the actual cumulative release for vector 53 is 2.64×10^{-10} EPA units, which is orders of magnitude lower than the average releases for the disturbed scenarios shown in Table 6. In addition, the instantaneous concentration of radionuclides detected at the LWB was computed for vector 53 as a function of time. The maximum concentration of radionuclides observed was 3.84×10^{-13} Ci/L (Ismail 2008); this concentration is below 4.93×10^{-12} Ci/L, the maximum concentration observed in the CCA (U.S. DOE 2004).

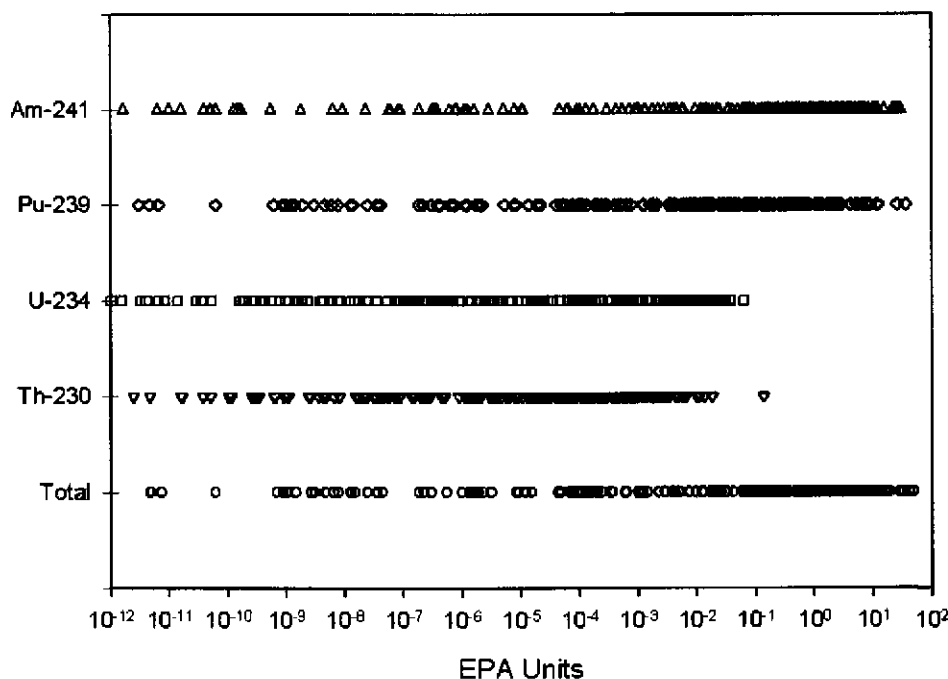**Figure 4** – Instantaneous total concentration of transuranic isotopes at the Land Withdrawal Boundary for replicate R1, vector 53 for the undisturbed scenario (S1)

4.1.2.2 Scenario S2: E1 Intrusion at 350 Years

Scenario S2 models an E1 intrusion, which penetrates the repository and a brine pocket in the lower Castile formation 350 years after closure. The S2 scenario is highly influenced by condi-

tions within the brine pocket. The timing of the 350-year intrusion allows for brine inflow into the repository, but is not long enough to have secondary processes, such as gas production, displace the brine. Consequently, the S2 scenario has both the greatest number of screened-in vectors and the largest outward fluxes of brine and radioisotopes. All but one of the vectors screened-in for scenario S2 showed movement of the tracer up the borehole, vector 53 in replicate R1 was screened in exclusively because of contaminant movement through the marker beds. In the ISO runs, however, that vector did not show any significant integrated activity at the LWB. In fact, only two vectors, vectors 53 and 59 in replicate R1, showed any activity at the LWB, with total integrated activities of 3.62×10^{-10} EPA units and 3.14×10^{-24} EPA units, respectively, which are both orders of magnitude lower than the average releases for this scenario. (Although nonzero, the activity of vector 59 in replicate R1 is so small that it is most likely the result of numerical dispersion effects rather than advective transport across the LWB.) For this reason, the remainder of this discussion focuses on the balance of the replicate/vector combinations, and in particular on the total activity in EPA units at the point where the borehole intersects the Culebra.
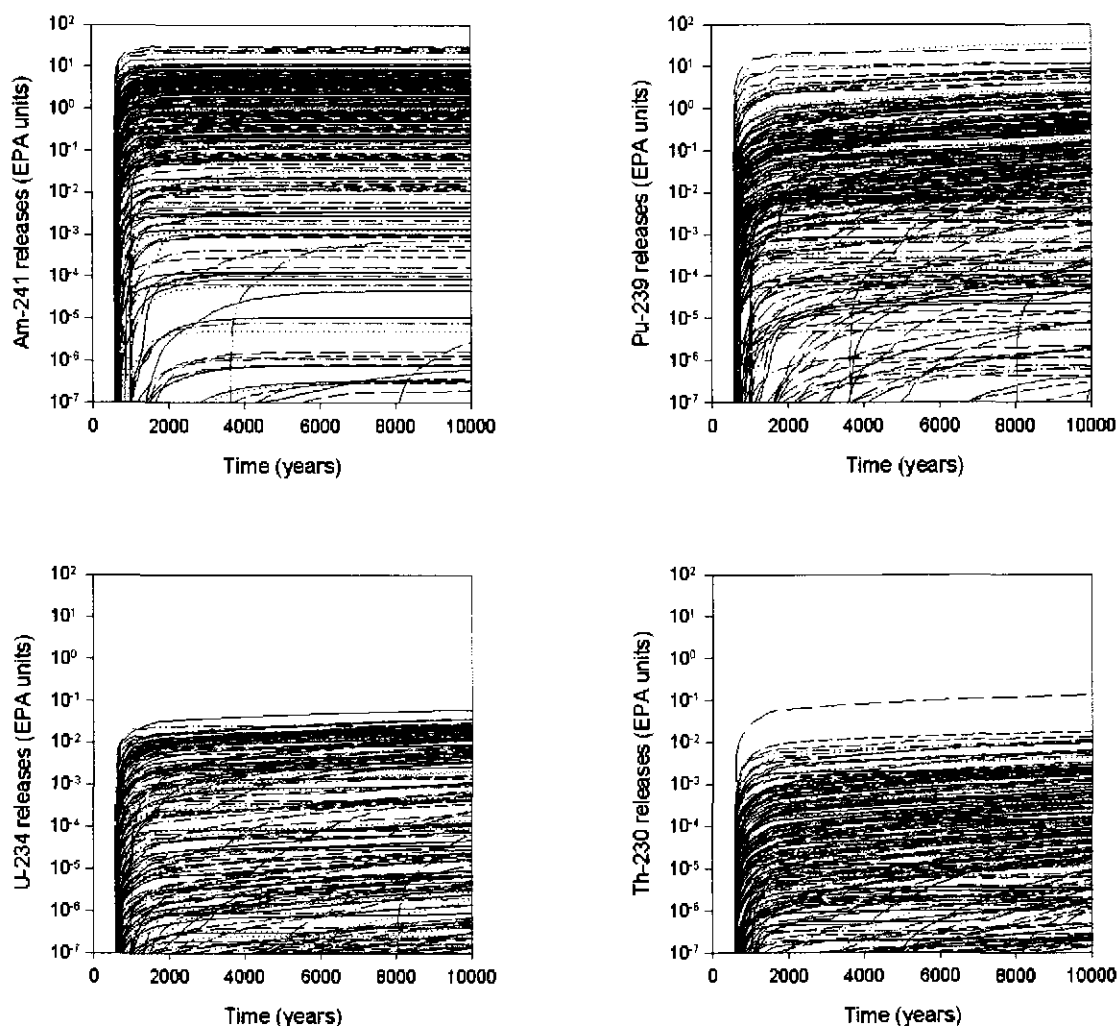

Figure 5 – Normalized cumulative release (EPA units) to the Culebra from the borehole for each isotope and the total for an E1 intrusion at 350 years (scenario S2)

The distribution of releases in EPA units for each isotope and the total release are shown in Figure 5, while the time series plots for each isotope are shown in Figure 6. Most vectors result in little or no release due to limited brine flow. Most of the release occurs over a relatively short period of time shortly after the borehole intrusion, and then continues at a reduced rate or stops entirely. The maximum activity for any individual isotope occurred in replicate R2, vector 31, which had an integrated activity of 36.1 EPA units for ^{239}Pu. For ^{241}Am, R1, replicate R1, vector 17 had the maximum integrated activity, 29.4 EPA units. These values are somewhat lower than

the values of 43.1 and 36.6 EPA units obtained in the CRA-2004 PABC (Lowry 2005), but are very close to the values of 36.3 and 29.9 EPA units obtained after correcting errors discovered in the CRA-2004 PABC calculations (Ismail 2007a). The total activities of ^{234}U and ^{230}Th are negligible in comparison: the maxima for those isotopes were 0.0619 and 0.135 EPA units in replicate R3, vector 42 and replicate R1, vector 17, respectively.

Given the relative magnitude of the differences between the original CRA-2004 PABC results and the CRA-2009 PA results compared to the differences between the corrected CRA-2004 PABC results and the CRA-2009 PA results, it is reasonable to conclude that most of the discrepancies are the result of the error correction; the other changes introduced between the revision and the CRA-2009 have an extremely limited effect on the activities, which changed by only about 2 percent between the corrected CRA-2004 PABC and the CRA-2009 PA.
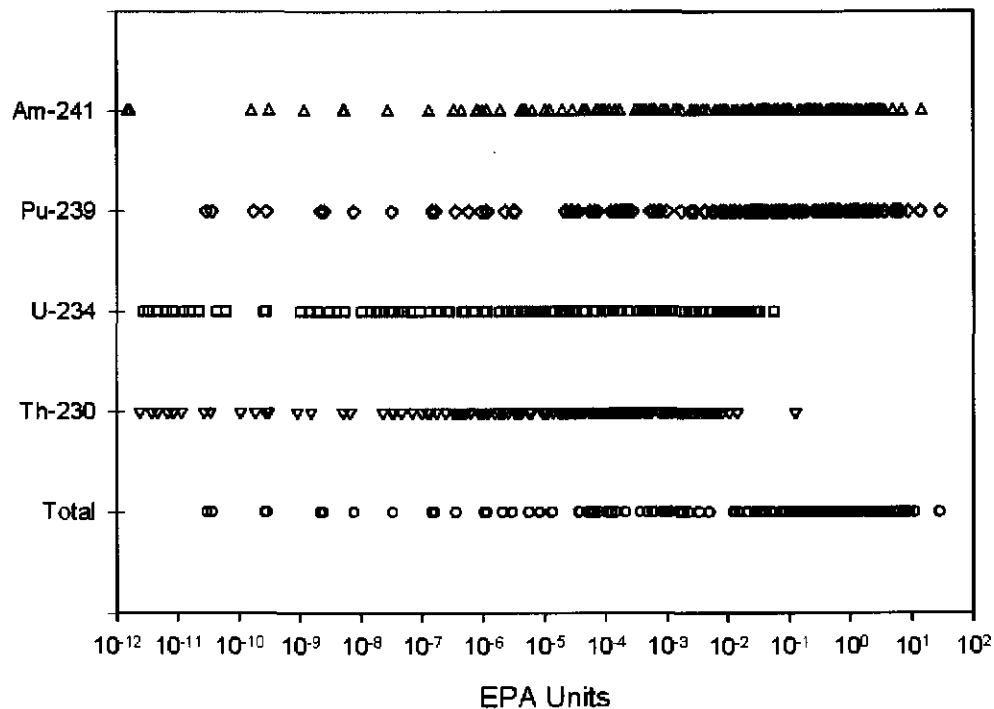

Figure 6 – Cumulative releases in the borehole at the Culebra versus time by species for an E1 intrusion at 350 years (scenario S2)

4.1.2.3 Scenario S3: E1 Intrusion at 1000 Years

The time difference between the intrusion in the S2 and S3 scenarios allows more time for chemical and biological activity to either consume brine or produce gas, both of which reduce the amount of brine in the repository at the time of intrusion. This in turn reduces the capacity for nuclide transport. However, like scenario S2, the results of scenario S3 are highly influenced by the conditions in the pressurized Castile brine pocket and thus we see that scenario S3 has similar characteristics to the S2 scenario, although the number of screened-in vectors is slightly smaller and the maximum activities are lower.
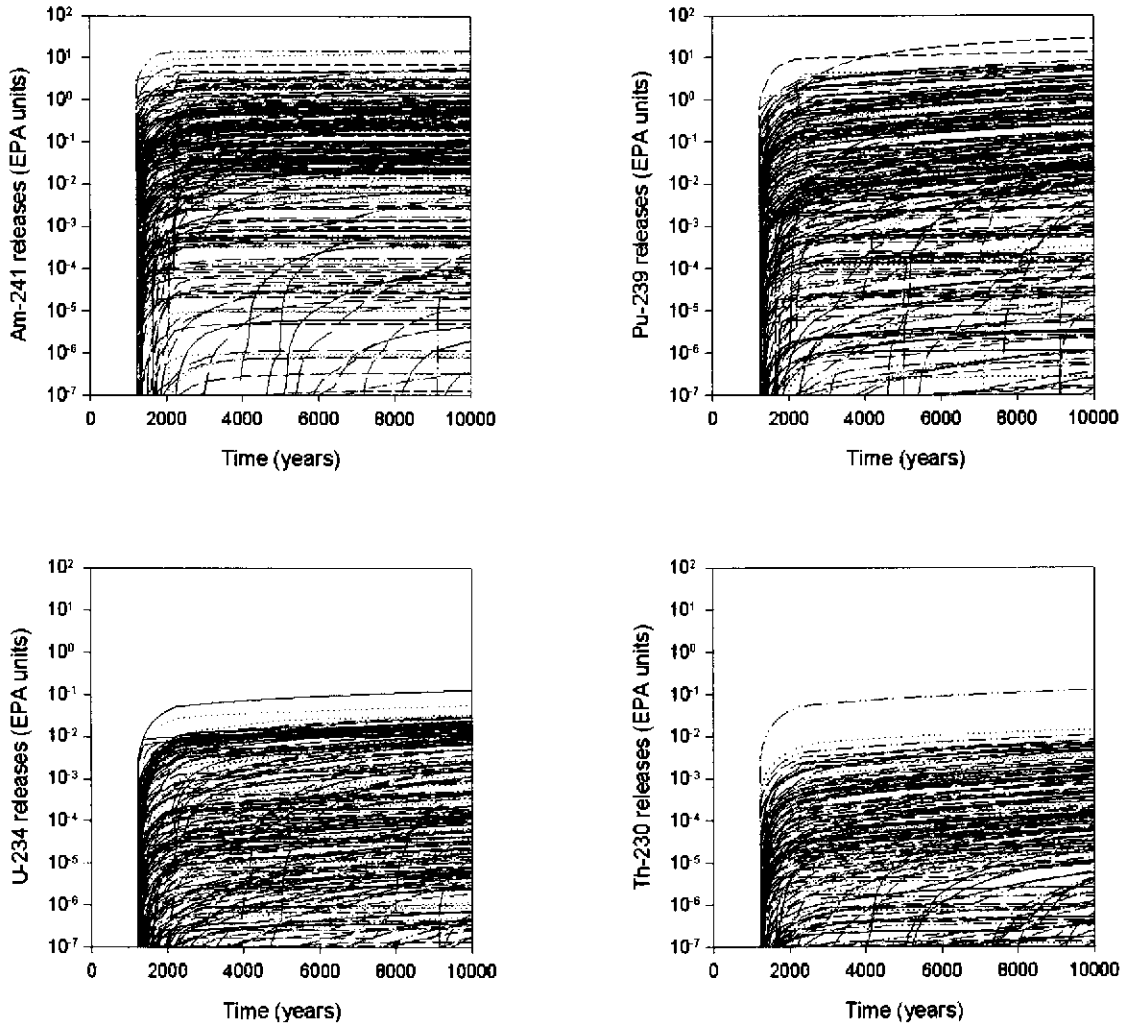
The only pathway with any cumulative releases in scenario S3 is through the borehole. No releases occur through the marker beds or the shaft for any of the vectors. The releases in EPA units for each isotope and the total release are shown in Figure 7, while the time series plots for each isotope, vector, and replicate are shown in Figure 8. As can be seen in the figures, and like the S2 scenario, the releases for the S3 scenario primarily take place over a short period of time. The maximum activity for any isotope occurred in replicate R2, vector 31, which had an integrated activity of 28.3 EPA units for ^{239}Pu. Replicate R1, vector 17 had the maximum activity of ^{241}Am, 14.2 EPA units. The releases of ^{234}U and ^{230}Th were significantly smaller, with maxima of 0.0543 and 0.124 found in replicate R3, vector 42 and replicate R1, vector 17, respectively.

Figure 7 – Normalized cumulative release (EPA units) to the Culebra from the borehole for each isotope and the total for an E1 intrusion at 1000 years (scenario S3)

The difference in the distribution of releases between scenarios S2 and S3 can be attributed to the time lag between the intrusions in the S2 and S3 scenarios. At early times, releases will be dominated by ^{241}Am, with an additional contribution from ^{238}Pu at very early times (not shown). With

increasing time, ^{241}Am is lost due to decay, and the release is dominated by ^{239}Pu due to its long half-life.
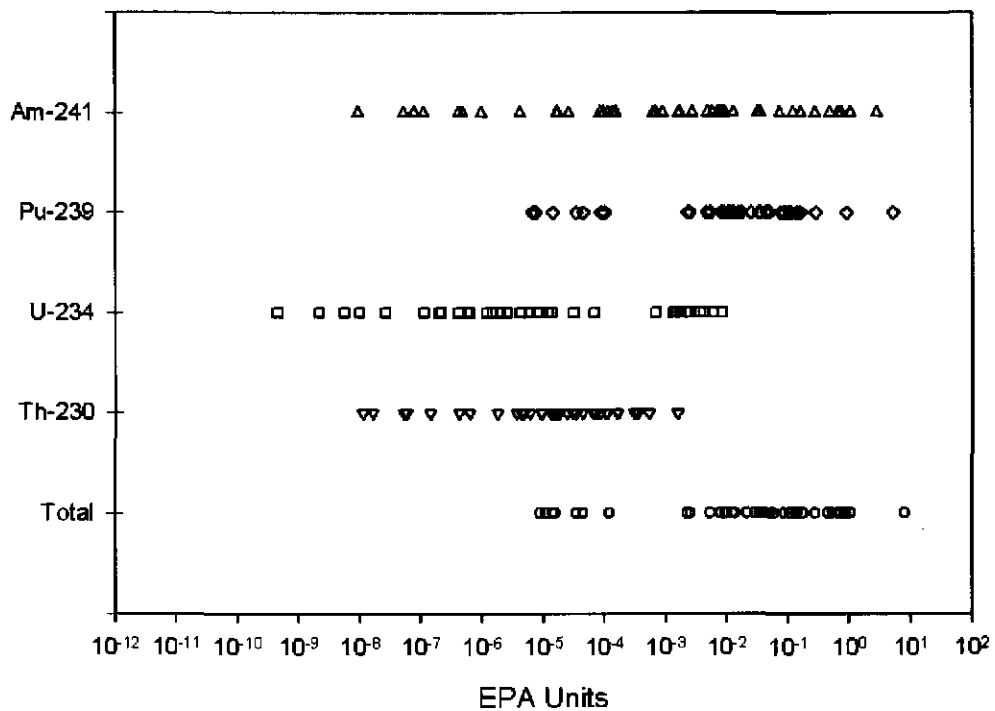

Figure 8 – Cumulative releases in the borehole at the Culebra versus time by species for an E1 intrusion at 1000 years (scenario S3)

4.1.2.4 Scenario S4: E2 Intrusion at 350 Years

For most vectors associated with an E2 intrusion, BRAGFLO predicts no or very little brine flow from the repository to the Culebra, as can be seen from Figure 9 and Figure 10; less than a fifth of all vectors demonstrate the possibility of a significant release. The releases in EPA units for each isotope and the total release are shown in Figure 9, while Figure 10 shows the time-series plots for each vector across all replicates. Unlike the brine pocket pressure release associated with an E1 intrusion, physical processes do not dominate E2 releases; greater variation therefore exists in the distribution of times at which releases first occur. This also creates a difference in the distribution of total activities, with the activities nearly an order of magnitude smaller than

the comparable releases in scenario S2. The maximum activities for ^{241}Am, ^{239}Pu, ^{234}U, and ^{230}Th are 2.72, 5.11, 0.00822, and 0.00157 EPA units, respectively.

Figure 9 – Normalized Cumulative Release (EPA Units) to the Culebra from the borehole for each isotope and the total for an E2 intrusion at 350 years (scenario S4)

Figure 10 – Cumulative releases in the borehole at the Culebra versus time by species for an E2 intrusion at 350 years (scenario S4)

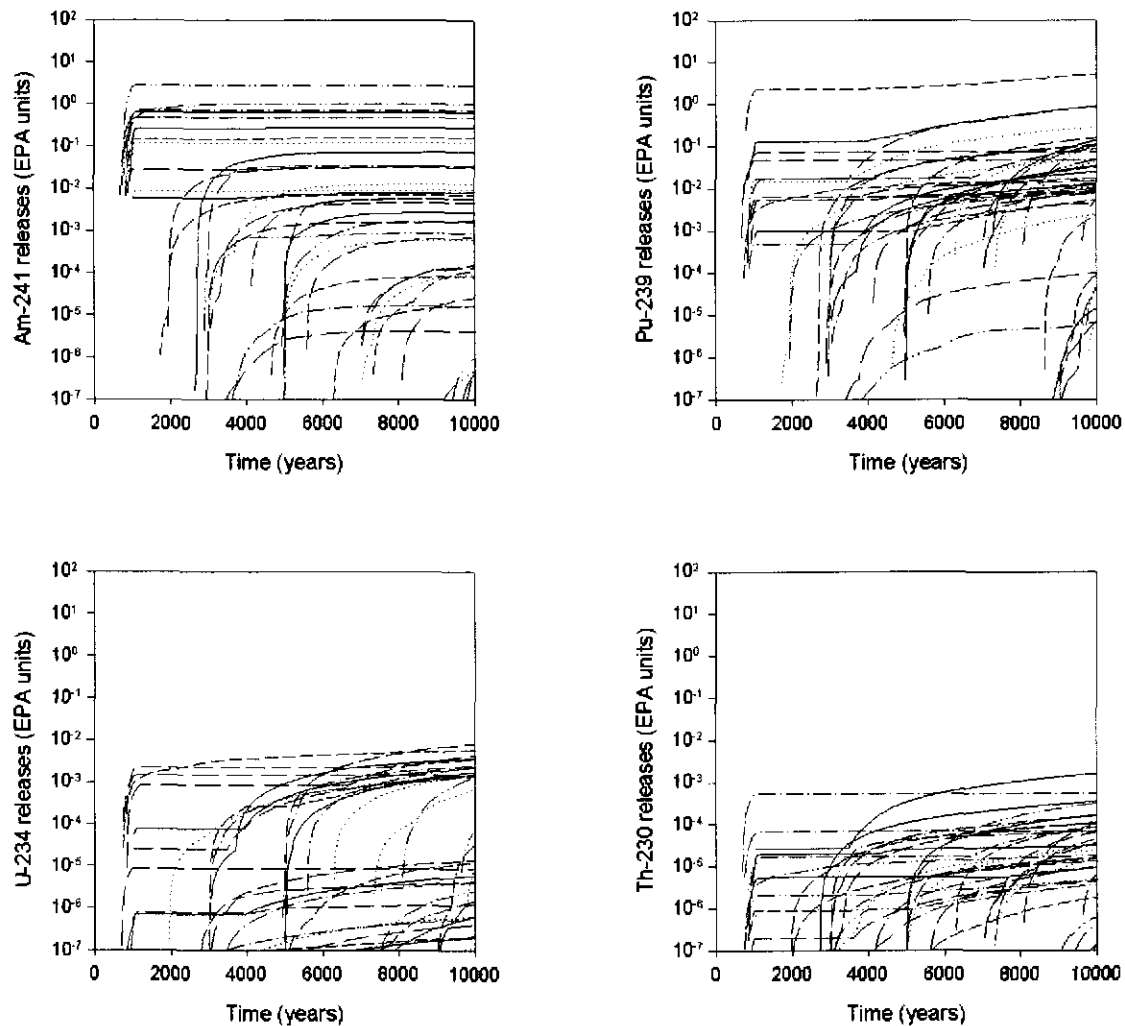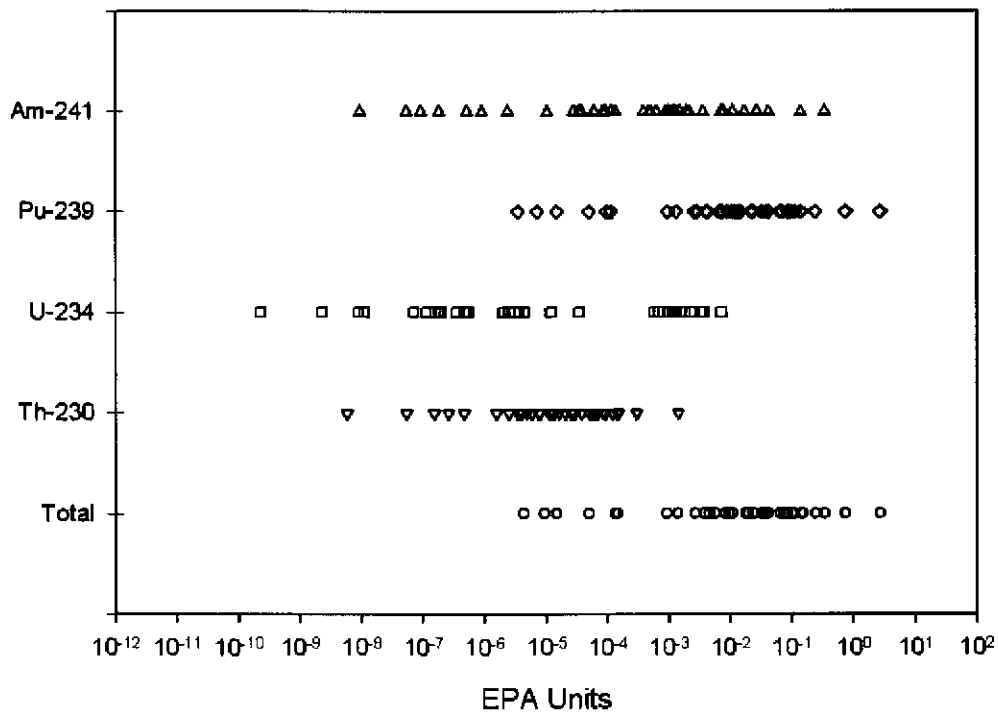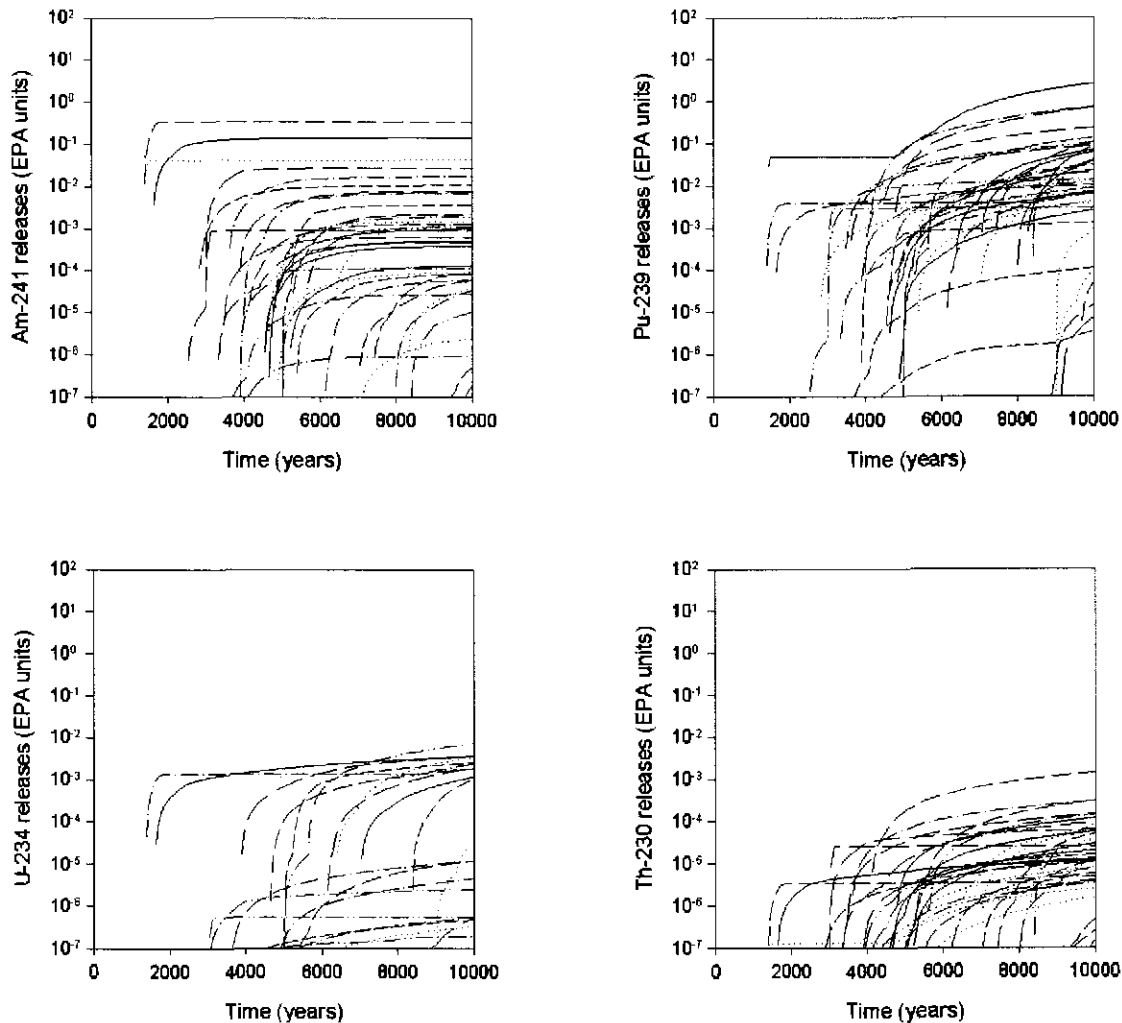### 4.1.2.5 Scenario S5: E2 Intrusion at 1000 Years

Like the 350-year E2 intrusion scenario (S4), the 1000-year E2 intrusion scenario (S5) shows very few vectors with significant amounts of radionuclide releases. Over the 1000 years before the intrusion, gas pressure builds up and brine is consumed through chemical and biological processes. This in turn reduces the brine movement through the repository in comparison to the earlier intrusion times.

The releases in EPA units for each isotope and the total release are shown in Figure 11. Figure 12 show the time-series plots for each vector across all replicates. Again, the time plots show greater variation in the occurrences of releases than the corresponding E1 intrusion plots. The 1000-year intrusion time allows for greater decay of the ^{241}Am than is found in the 350-year intrusion time of scenario S4, and a greater relative amount of ^{239}Pu than in scenario S4. The maximum activities for ^{241}Am, ^{239}Pu, ^{234}U, and ^{230}Th are 0.336, 2.65, 0.00716, and 0.00141 EPA units, respectively.

Figure 11 – Normalized Cumulative Release (EPA Units) to the Culebra from the borehole for each isotope and the total for an E2 intrusion at 1000 years (scenario S5)

Figure 12 – Cumulative releases in the borehole at the Culebra versus time by species for an E2 intrusion at 1000 years (scenario S5)

4.1.3 Time Intrusion (TI) Runs

The TI runs show the same pattern in terms of nuclide transport as do the ISO runs in that the E1 intrusions associated with early time intrusions show the highest activities, while the E2 intrusions associated with late time intrusions show the lowest. The reasons behind this are the same as discussed above. Table 7 shows the maximum normalized release in EPA units for each scenario/intrusion time combination. The time series plots for each isotope at each time/replicate/vector combination are presented in Appendix A.

^{241}Am for a 100-year intrusion of type E1 shows the highest maximum activity (35.1 EPA units) of all the isotopes across all TI runs. Under all other time intrusion scenarios, the maximum activity is from ^{239}Pu. ^{234}U and ^{230}Th never dominate the releases; however, because of ^{241}Am's relatively short half-life (approximately 432 yr), ^{234}U and ^{230}Th can occur at greater concentrations than ^{241}Am, particularly for intrusions close to the end of the 10,000-year horizon. This

trend is shown in Table 7; cumulative release plots for the various time intrusion scenarios are provided in Appendix A.

Table 7 – Maximum normalized release of each isotope at the Borehole/Culebra interface for TI scenarios

Intrusion	Time	Maximum Releases (EPA Units)				
		[241]Am	[239]Pu	[234]U	[230]Th	Total[a]
E1	100 yr	35.1	31.3	0.0632	0.136	60.6
	3000 yr	1.54	23.5	0.0475	0.108	23.5
	5000 yr	0.172	17.6	0.0407	0.0898	17.6
	7000 yr	0.0552	9.73	0.0338	0.0710	9.73
	9000 yr	0.0433	3.93	0.0211	0.0402	4.01
E2	100 yr	3.99	5.28	0.00864	0.00164	9.27
	3000 yr	0.00840	1.31	0.00376	0.000893	1.32
	5000 yr	0.000840	0.233	0.00217	0.000396	0.234
	7000 yr	0.0000973	0.0493	0.00143	0.0000314	0.0493
	9000 yr	0.00000625	0.0492	0.00133	0.00000332	0.0492

[a]The total maximum release is the maximum for a single vector whereas the maximum for each isotope for each scenario may be from different vectors. For this reason, the sum of the maximum for each isotope may not sum to the total maximum.

As done for the ISO runs shown in Section 4.1.2, we can calculate the average percentage of each isotope as a fraction of the average total release. Table 8 shows that for either an E1 or an E2 intrusion at 100 years, [241]Am is the primary component of releases; at later times, [239]Pu comprises at least 94 percent of the total observed activity. [234]U and [230]Th never dominate releases, and only in E2 scenarios at 5000 years or later does [234]U exceed 1 percent of the average total release. Table 8 also demonstrates the large differences in the magnitude of releases between E1 and E2 intrusions; the average release for an E1 intrusion is nearly two orders of magnitude larger than the comparable average release for an E2 intrusion occurring at the same time.

Table 8 – Percentage of lumped isotopes relative to average release at the Borehole/Culebra interface for TI scenarios

Intrusion	Time	Percentage of Isotope in Average Release (%)				Average Release (EPA units)
		^{241}Am	^{239}Pu	^{234}U	^{230}Th	
E1	100 yr	74.9	25.0	0.1	0.0	2.62
	3000 yr	5.0	94.3	0.5	0.2	0.436
	5000 yr	0.8	98.5	0.5	0.2	0.329
	7000 yr	0.2	99.0	0.6	0.2	0.224
	9000 yr	0.3	98.6	0.8	0.3	0.0875
E2	100 yr	50.5	49.2	0.3	0.0	0.0603
	3000 yr	0.8	98.4	0.7	0.1	0.00885
	5000 yr	0.3	98.4	1.1	0.1	0.00227
	7000 yr	0.3	96.2	3.5	0.1	0.0002730
	9000 yr	0.0	97.1	2.9	0.0	0.000185

4.1.4 Comparison to CRA-2004 PABC Results

There are two sets of results for radionuclide releases in the CRA-2004 PABC to which the present results can be compared. The earlier set of results (Lowry 2005) represents the official results considered as part of the CRA-2004 PABC. However, during the preparations for the CRA-2009 PA, several errors were found in the input files for NUTS used in the CRA-2004 PABC calculations (Ismail 2007a). The errors occurred in the NUTS input file, which misidentified several of the cells that were part of the waste area, and the ALGEBRACDB file used to process the NUTS output, which misidentified which cells to use in the calculation of radionuclide fluxes out of the repository. Consequently, the CRA-2004 PABC calculations were re-run with the correct files, and the results between the two analyses compared (Ismail 2007a). The primary change between the CRA-2004 PABC calculations and the CRA-2009 PA calculations affecting the results obtained from NUTS are changes and updates that affected the fluid flow profiles calculated by BRAGFLO (Clayton 2008). Among these changes is the correction of the porosity distribution for the DRZ (Ismail 2007b), which greatly increases the amount of brine available for dissolution of radionuclides in many vectors, particularly for E2 vectors.

Comparing the maximum releases in Table 7 to those obtained from the original CRA-2004 PABC calculations (Lowry 2005), we find that the maximum total releases in the CRA-2009 PA are lower for all E1 intrusion cases, and for E2 intrusions at 3000 and 5000 years. For the E2 intrusion at 100 years, for which the largest total release in the CRA-2009 PA is nearly twice as big as the corresponding maximum release in the CRA-2004 PABC. Similarly, for the E2 intrusion at 7000 years and 9000 years, the maximum release is significantly larger, although essentially the entire contribution to total releases comes from ^{239}Pu. For the individual isotopes, no general trend emerges; however, for ^{239}Pu and ^{230}Th, the maximum releases in the CRA-2009 PA are consistently lower than the corresponding CRA-2004 PABC maximum releases for E1 intrusions.

Results from the three analyses are compared in Figure 13, Figure 14, and Table 9. Figure 13 shows the average releases for E1 and E2 intrusions as a function of time for each of the analyses. The number of nonzero vectors in each intrusion scenario is shown in Table 9.

There is general agreement between the three analyses with respect to average releases. For the E1 scenarios, the revision to the CRA-2004 PABC had lower smaller average releases than the original CRA-2004 PABC calculations and the CRA-2009 PA calculations, which were roughly equal to one another.

In E2 intrusions, the primary trend is that the largest average releases are found in the CRA-2009 PA. However, even in this case, the average release never exceeds 0.1 EPA units, even for intrusions occurring only 100 years after closure of the repository. The increase in average releases for the E2 intrusion scenarios at 9000 years is largely the result of the small sample sizes: only three of the 300 vectors in each of the scenarios considered showed non-zero releases. Moreover, the relatively small magnitude of the average release (less than 0.001 EPA units) indicates that the consequences of the differences among the three analyses on total releases will be negligible.
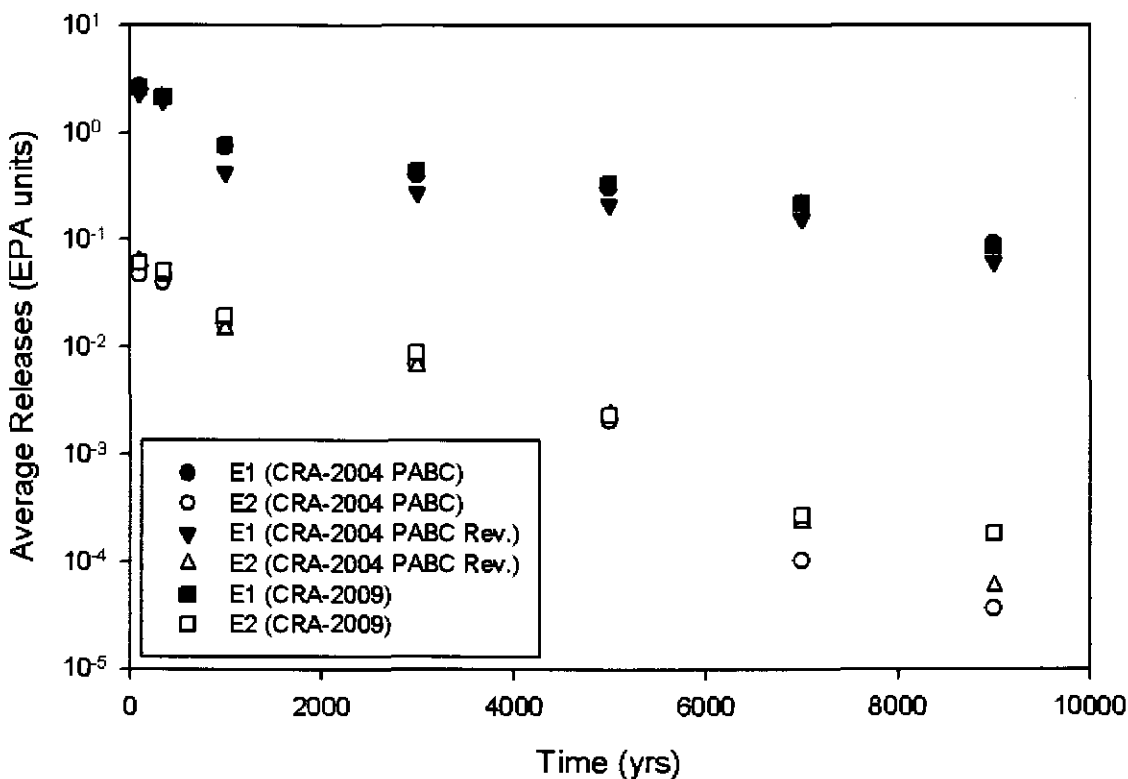

Figure 13 – Average releases (in EPA units) as a function of time and intrusion type for the CRA-2004 PABC, the revision to the CRA-2004 PABC, and the CRA-2009 PA

The maximum releases, shown in Figure 14, demonstrate no clear trends. The maximum releases for the E1 intrusions show only small differences among the three analyses. For the E2 intrusions, the maximum releases for the CRA-2009 PA are larger than the corresponding releases from the revised CRA-2004 PABC.
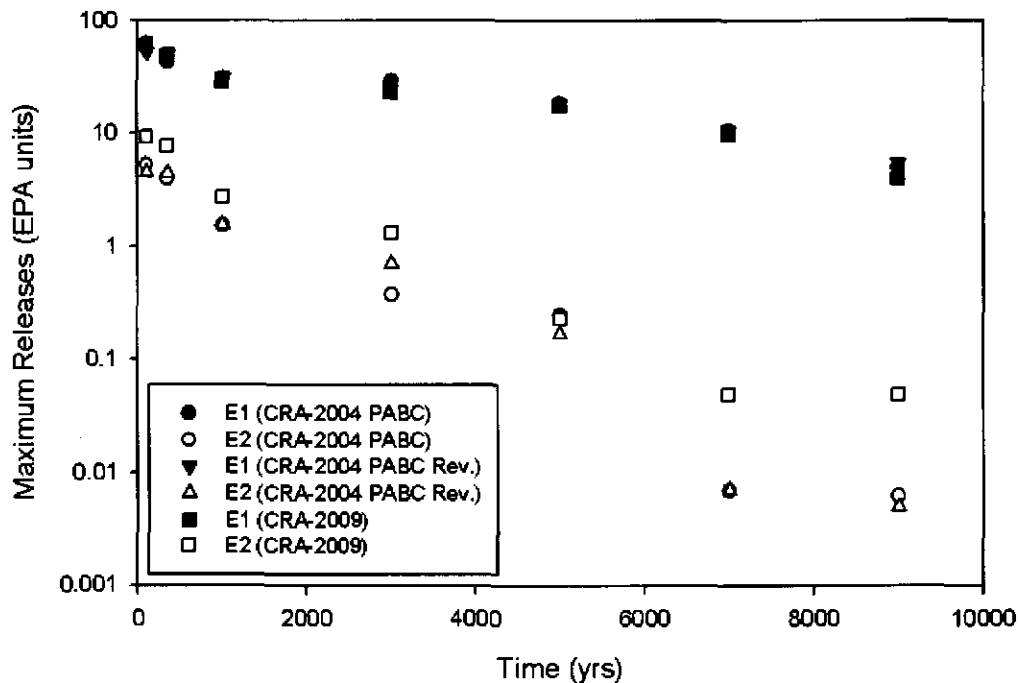

Figure 14 – Maximum releases (in EPA units) as a function of time and intrusion type for the CRA-2004 PABC, the revision to the CRA-2004 PABC, and the CRA-2009 PA

Table 9 – Number of vectors with releases for intrusion scenarios for the CRA-2004 PABC, the CRA-2004 PABC Revision, and the CRA-2009 PA

| Intru-sion | Time | Number of Vectors With Releases | | |
		CRA-2004 PABC	CRA-2004 PABC Revision	CRA-2009
E1	100 yr	218	203	223
	350 yr	218	202	223
	1000 yr	173	154	173
	3000 yr	172	154	173
	5000 yr	170	149	171
	7000 yr	167	147	169
	9000 yr	160	144	166

Intru-sion	Time	Number of Vectors With Releases		
		CRA-2004 PABC	CRA-2004 PABC Revision	CRA-2009
E2	100 yr	41	40	43
	350 yr	41	40	43
	1000 yr	39	39	39
	3000 yr	34	37	33
	5000 yr	27	32	27
	7000 yr	13	17	14
	9000 yr	3	6	3

Finally, Table 9 lists the number of vectors with non-zero releases for each of the intrusion scenarios examined. The revision to the CRA-2004 PABC shows fewer vectors with releases than either the original CRA-2004 PABC or the CRA-2009 PA calculations. The corrections to the input files in the CRA-2004 PABC appears to have increased the number of pathways for radionuclides to leave the repository, thereby lowering the amount of radionuclides available for transport up the borehole and thus the number of vectors showing releases as well. However, the increase in the upper end of the porosity distribution increases the amount of brine available in the repository and the amount of radionuclides that can be dissolved and transported up the borehole. In addition, as discussed in Nemer and Clayton (2008), the increase in porosity leads to an increase in the pressure in the repository, which can lead to greater brine flow.

4.2 PANEL

4.2.1 Scenario 6: E1-E2 Intrusion

PANEL is run in STANDARD mode for scenario S6 to determine the amount of releases, measured in EPA units, up the borehole to the Culebra. PANEL calculates the mobilized radionuclide concentrations using panel brine volumes and brine flow volumes from BRAGFLO. The volume of brine in the panel and the flow of brine past the disturbed rock zone (DRZ) of the Salado are obtained from postprocessed BRAGFLO results. It is assumed that any brine that gets past the DRZ reaches the Culebra instantly.

The PANEL results from replicate R1 for the releases up the borehole to the Culebra are shown in Figure 15 through Figure 19, which display cumulative release plots of the releases for individual vectors as a function of time for the entire 10,000-year regulatory compliance period. The abscissa in these figures is time in years, while the ordinate is EPA units released up the borehole to the Culebra.

Figure 15 shows the cumulative total releases up the borehole to the Culebra for scenario S6 given an E2 intrusion at 1000 years and an E1 intrusion at 2000 years. Prior to 2000 years, only two vectors have radionuclides that move up the borehole to the Culebra. At 2000 years, the time of the E1 intrusion, radionuclides are washed up the borehole to the Culebra. The shape of the

curves, with an immediate rise in the ordinate value at 2000 years followed by almost no increase in the ordinate value as time progresses, indicates that movement up the borehole to the Culebra is rapid and essentially complete at the time of the E1 intrusion. The same behavior is apparent for ^{241}Am, ^{239}Pu, ^{234}U, and ^{230}Th (Figure 16 through Figure 19, respectively).

The cumulative total EPA Units up the borehole to the Culebra for replicate R1 of scenario S6 given an E1 intrusion at 100, 350, 1000, 4000, 6000, and 9000 years respectively are shown in Appendix A. In general, the amount of material moved up the borehole to the Culebra remains essentially unchanged between the CRA-2004 PABC and the CRA-2009 PA.

The maximum contribution in the CRA-2009 PA up the borehole to the Culebra from radionuclides that are not typically transported in the Culebra—primarily ^{237}Np and ^{243}Am—in PA is 0.1 EPA units; this is the same value as found in CRA-2004 PABC. For comparison, the maximum value for EPA units up the borehole for the radionuclides that are tracked (the "lumped" radionuclides) in PA is on the order of 1000 EPA units for CRA-2009 PA. Thus, the contribution made by the radionuclides that are not tracked is several orders of magnitude lower than the ones that are tracked.
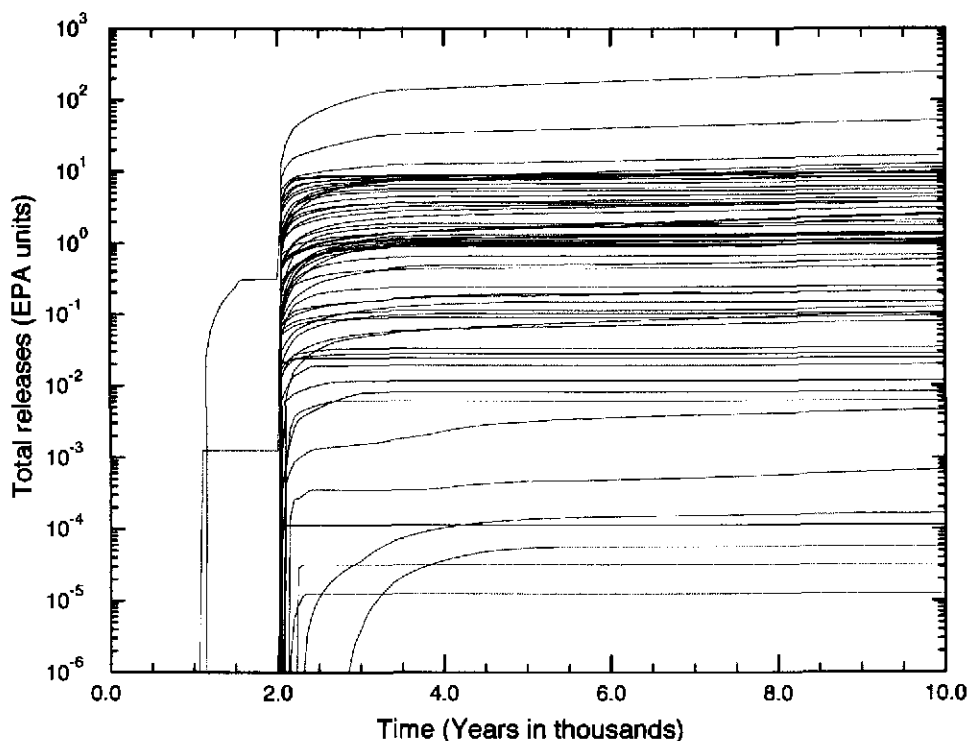

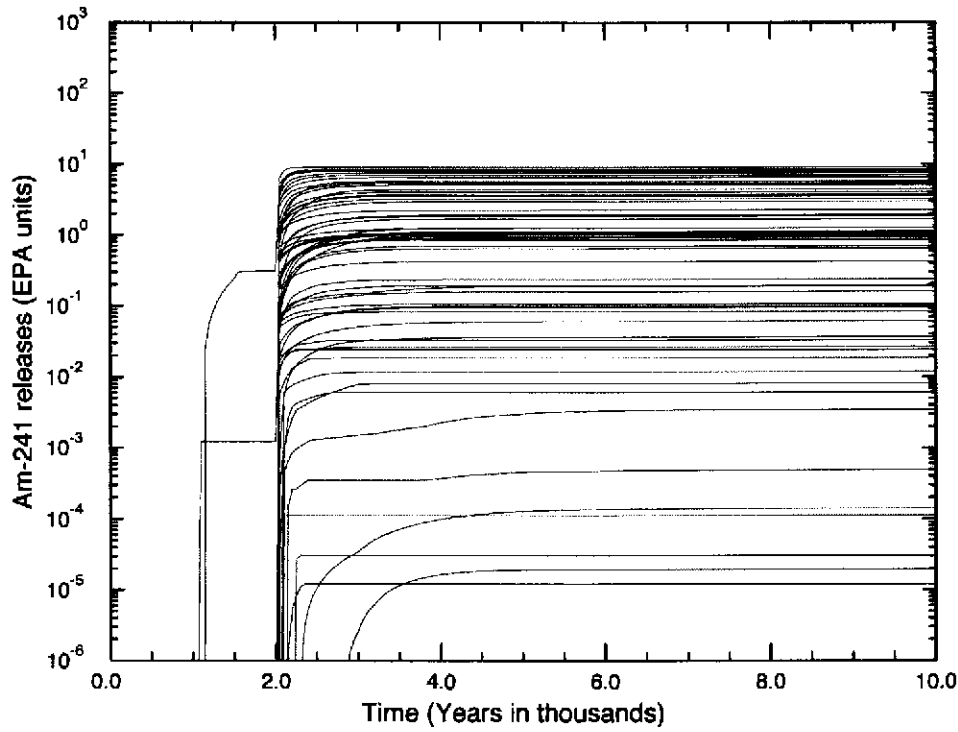**Figure 15** – Total releases to the Culebra for replicate R1, scenario S6

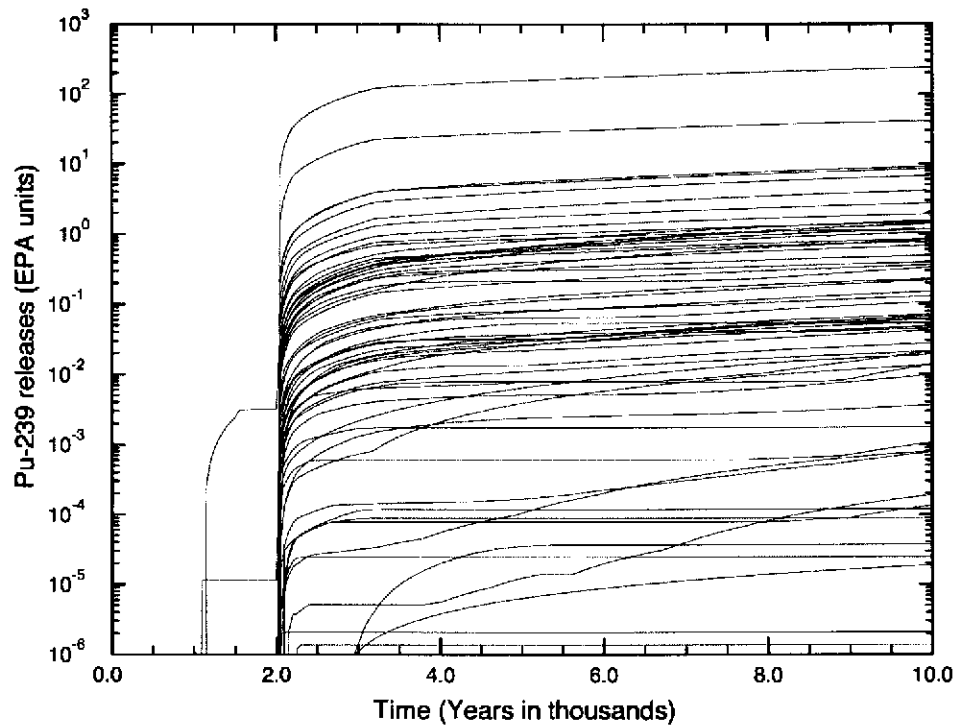**Figure 16** – Releases of [241]Am to the Culebra for replicate R1, scenario S6

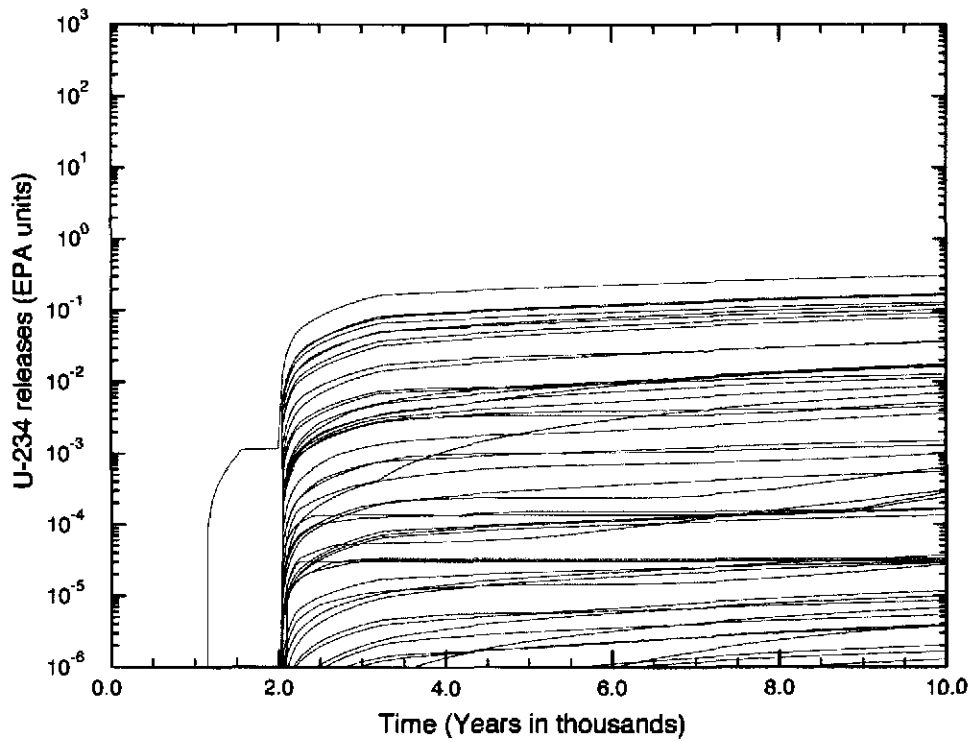**Figure 17** – Releases of [239]Pu to the Culebra for replicate R1, scenario S6

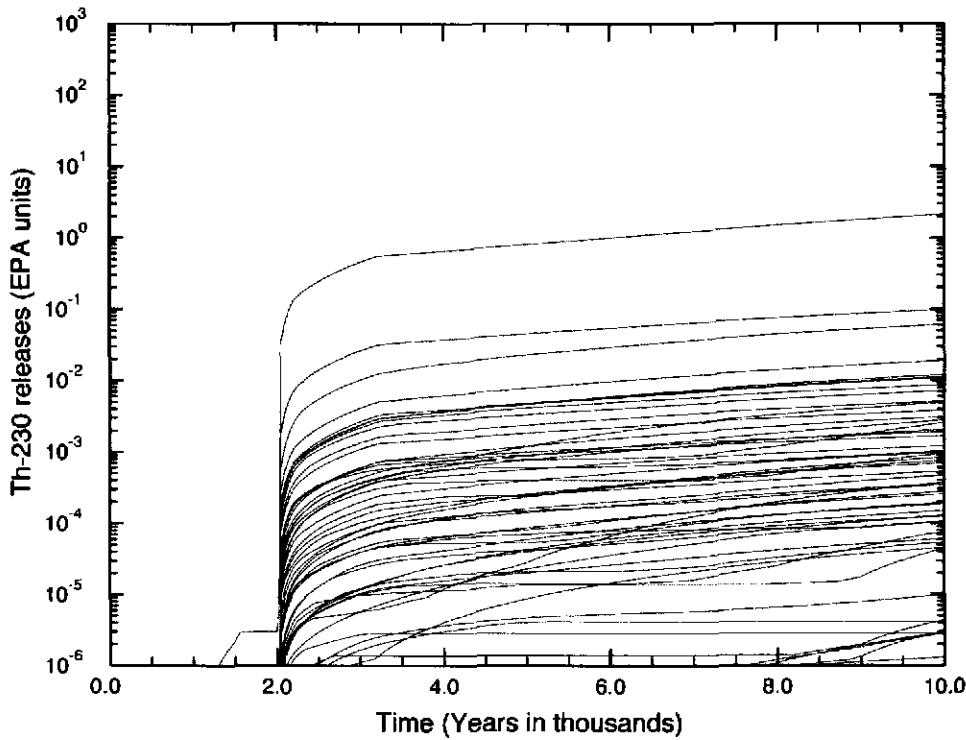**Figure 18** – Releases of ^{234}U to the Culebra for replicate R1, scenario S6

Figure 19 – Releases of ^{230}Th to the Culebra for replicate R1, scenario S6

4.2.2 Comparison to CRA-2004 PABC

Because source-term sampled parameters in the CRA-2009 PA were the same as in the CRA-2004 PABC, it is possible to directly compare vectors between the two sets of data. In Figure 20, the horizontal axis shows the flow up the borehole past the DRZ for replicate R1 of the CRA-2004 PABC calculations, while the vertical axis gives the flow up the borehole past the DRZ for replicate R1 of the CRA-2009 PA calculations. The data from this plot are taken by processing the files ALG2_BF_CRA1BC_R1_S6_Vvvv.CDB and ALG2_BF_CRA09_R1_S6_Vvvv.CDB (vvv = 001, 002, ... 100) using SUMMARIZE to extract the flow up the borehole past the DRZ. This plot shows that all flows of 10^2 cubic meters or more are essentially equal; flows of 10^1 to 10^2 cubic meters are almost the same as well. Since the source term for the two calculations are the same, this shows that the released to the Culebra are essentially identical.
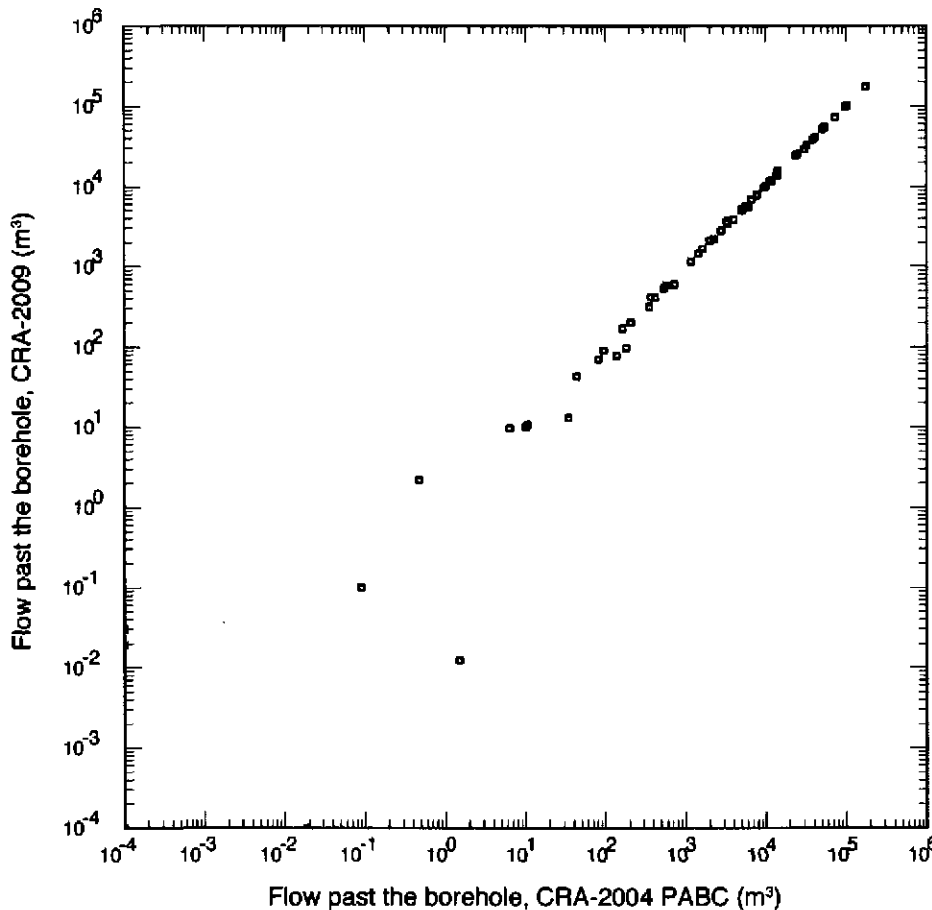

Figure 20 – CRA-2004 PABC versus CRA-2009 PA release volumes for replicate R1, scenario S6

5 Summary

This analysis package describes the Salado transport calculations that are part of the CRA-2009 PA as outlined in Clayton (2008). Specifically, it covers the calculations to determine the mobilization and subsequent migration of radioisotopes throughout the repository, the shaft system, the Salado formation, and possible human intrusion boreholes.

The calculations presented in this report are based on the same PA process as the CRA-2004 PABC (Lowry 2005, Garner and Leigh 2005). The only changes are the revisions and error corrections cited in Clayton (2008) and discussed above. The most important changes with respect to NUTS are the corrections to the NUTS input files and the probability distribution for the halite porosity. In NUTS, the screening runs produced 480 "screened-in" vector-scenario combinations out of 1200 involving an intrusion (three replicates of 100 vectors across four scenarios). In addition, 223 vector-scenario combinations out of the 300 not involving an intrusion were screened-in to provide flow fields for the intrusion scenarios; one of those vectors was also screened-in for possible releases to the markerbeds, although further analysis revealed that releases of actual radionuclides were insignificant. Results of the isotope (ISO) and time-intrusion (TI) runs yield only two vectors that show releases through the Land Withdrawal Boundary (LWB). However, since the releases through the LWB never exceed 10^{-9} EPA units, there is effectively no release out of either the marker beds or the Culebra.

The E1 intrusion scenarios (S2 and S3) produced the highest releases, with a maximum total activity at the borehole/Culebra intersection of 60.6 EPA units occurring for an E1 intrusion 100 years after closure, compared to an average release of 2.62 EPA units for an E1 intrusion at 100 years. As the intrusion time increases, the maximum total release tends to decrease. For example, at an intrusion time of 5000 years, the maximum total release for an E1 intrusion is predicted to be 17.6 EPA units, and the average release is 0.329 EPA units.

The E2 intrusions produced somewhat lower maximum total activities at all intrusion times than the E1 intrusion. The maximum total activity at the borehole/Culebra intersection for all intrusion times is predicted to be 9.27 EPA units (100-year E2 intrusion time). This also declines with increasing intrusion times, with 0.0493 EPA units predicted at a 7000- or 9000-year intrusion time. Like the other scenarios, little or no activity is predicted in the marker beds or at the shaft/Culebra intersection.

Calculations from PANEL show only small differences in the results between the CRA-2004 PABC and the CRA-2009 PA. Release volumes were essentially unchanged between the two sets of calculations, and any changes were for release volumes less than about 10 m^3, which are not large enough to have a significant effect on overall releases.

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Appendix A   Time Intrusion (TI) Cumulative Release Plots

Figure 21 – Cumulative total releases in the borehole at the Culebra for an E1 intrusion at 100 years
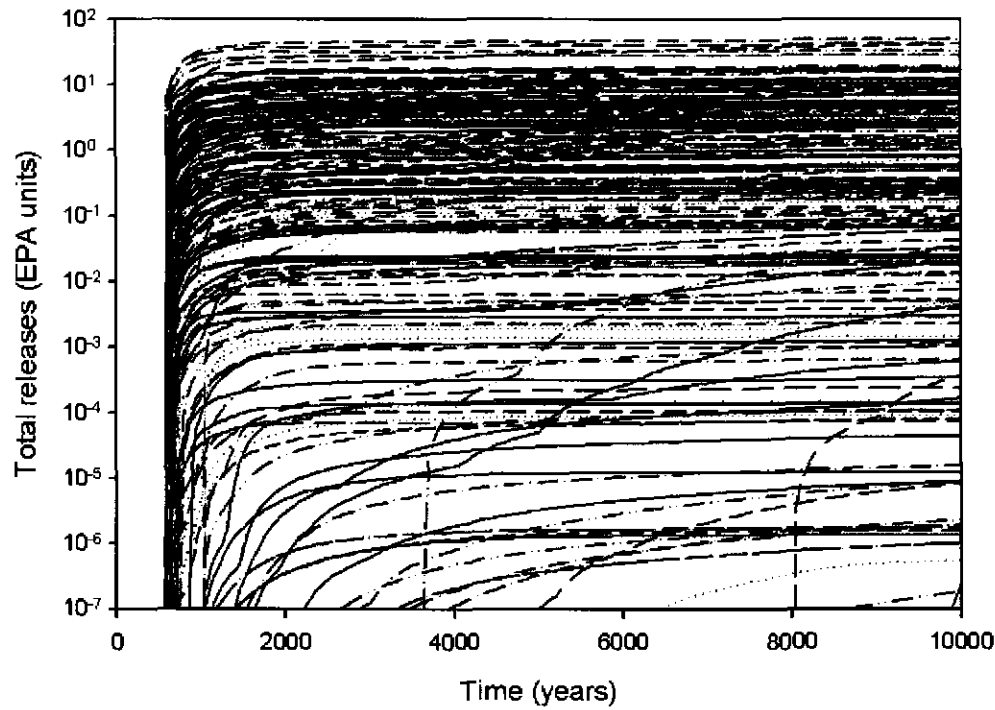

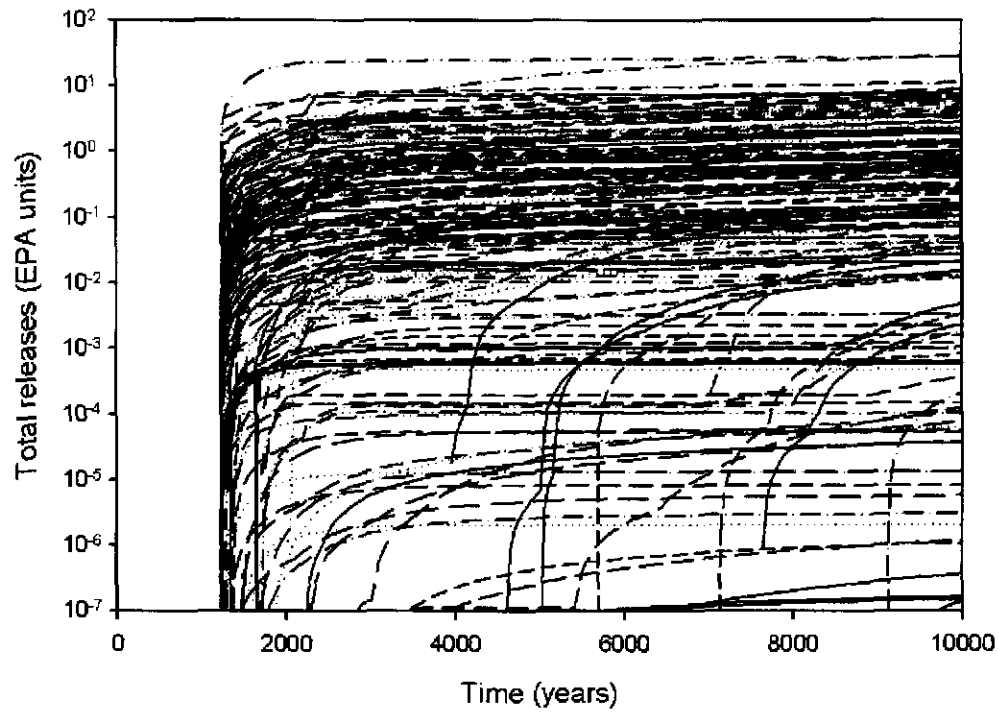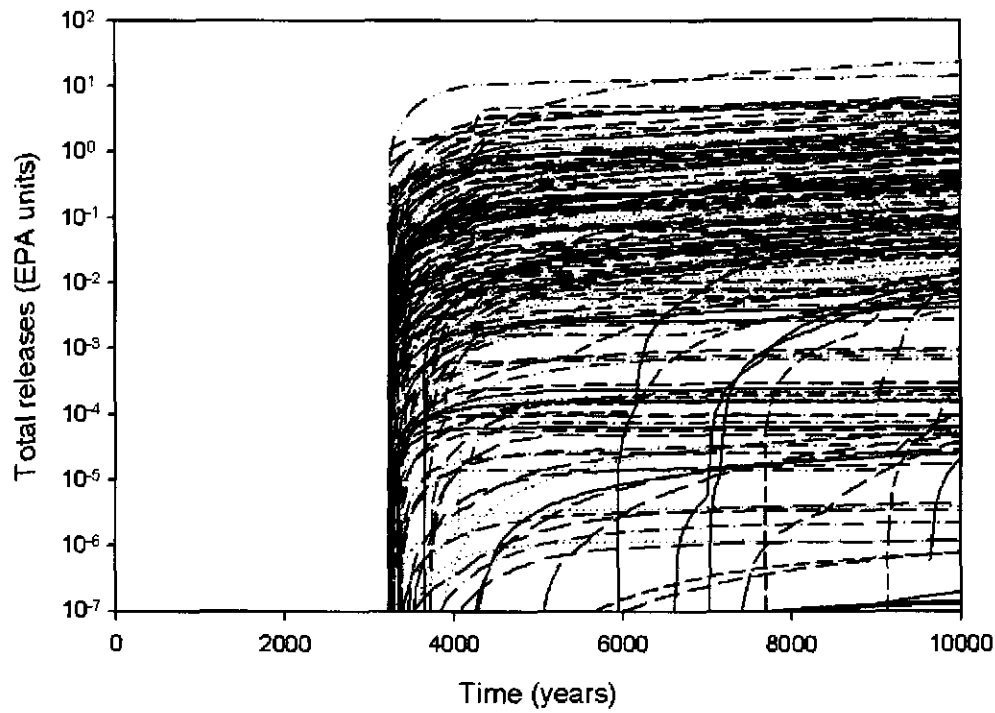**Figure 22** – Cumulative total releases in the borehole at the Culebra for an E1 intrusion at 350 years

Information Only

Figure 23 – Cumulative total releases in the borehole at the Culebra for an E1 intrusion at 1000 years

Figure 24 – Cumulative total releases in the borehole at the Culebra for an E1 intrusion at 3000 years
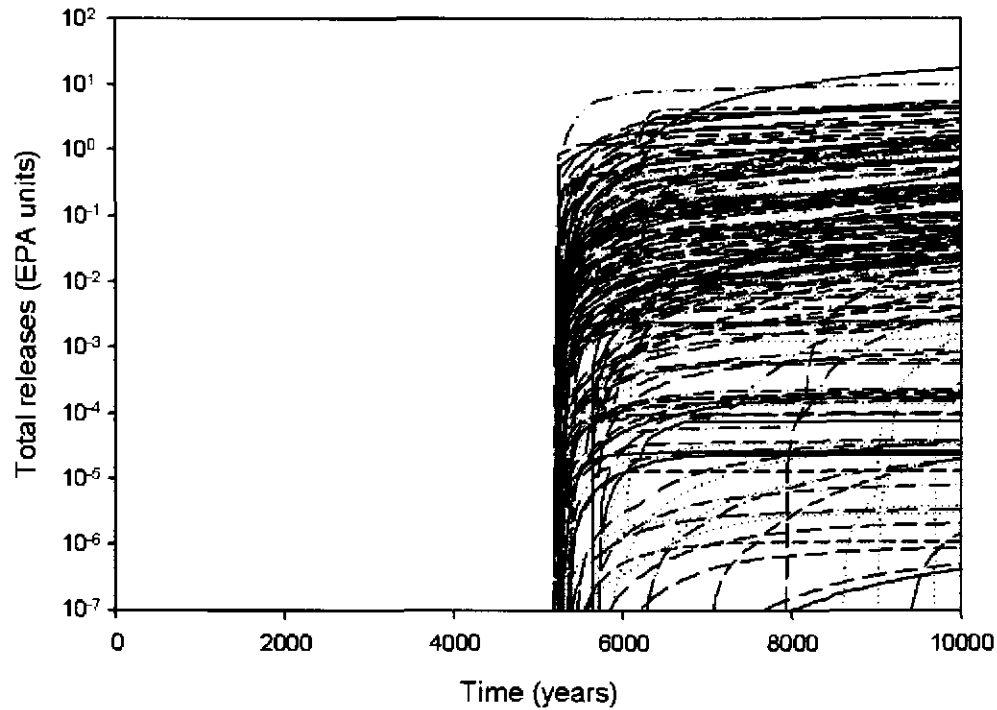
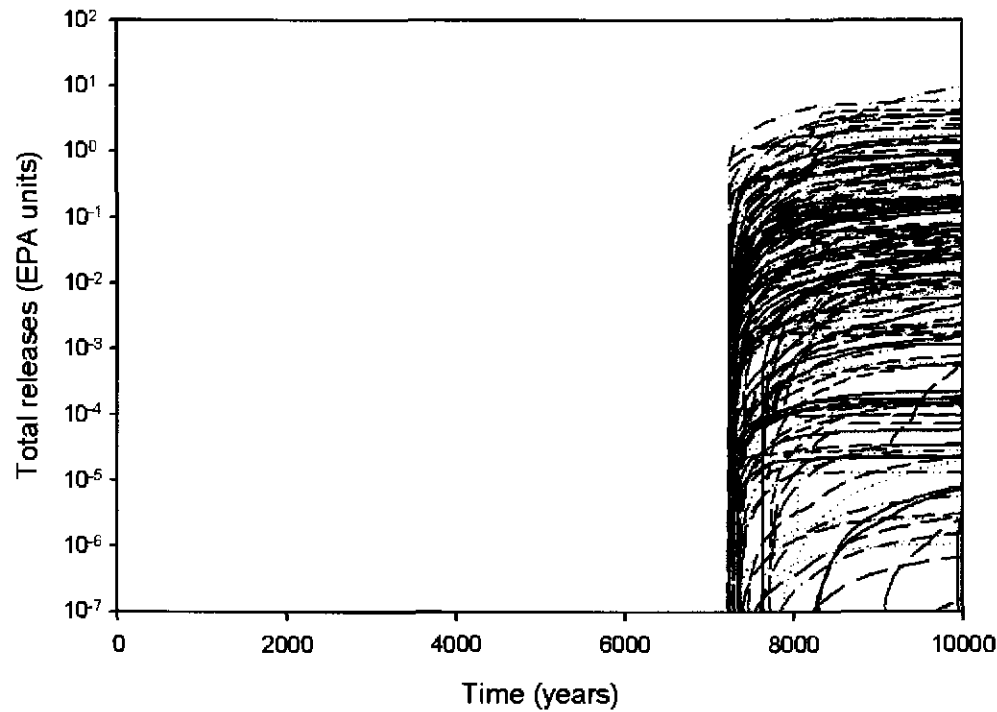**Figure 25** – Cumulative total releases in the borehole at the Culebra for an E1 intrusion at 5000 years

Figure 26 – Cumulative total releases in the borehole at the Culebra for an E1 intrusion at 7000 years
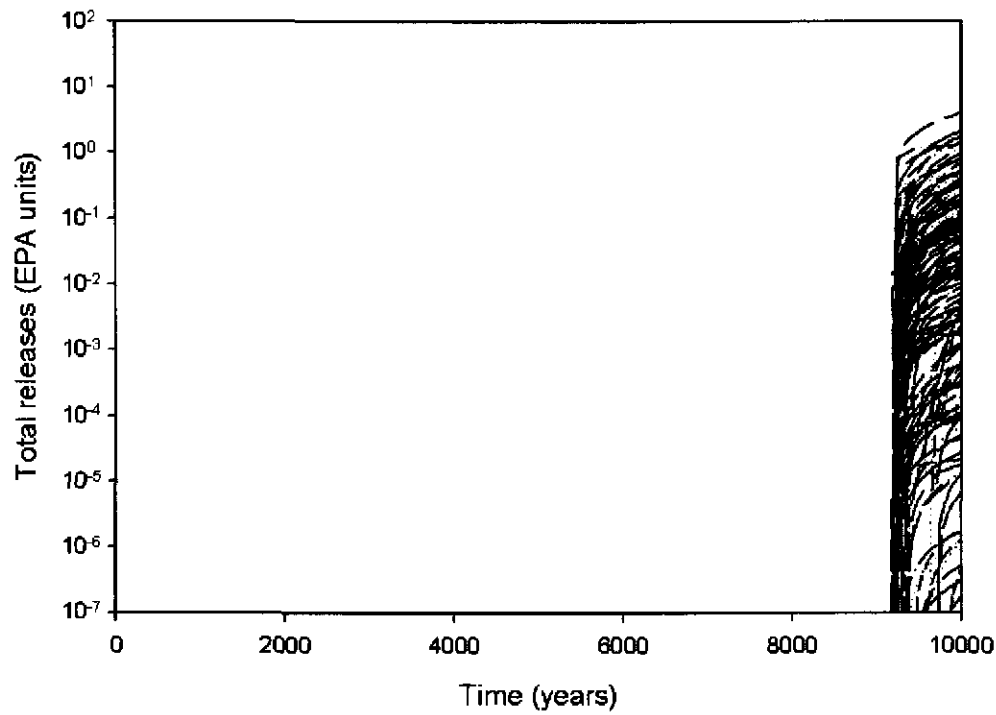
Figure 27 – Cumulative total releases in the borehole at the Culebra for an E1 intrusion at 9000 years
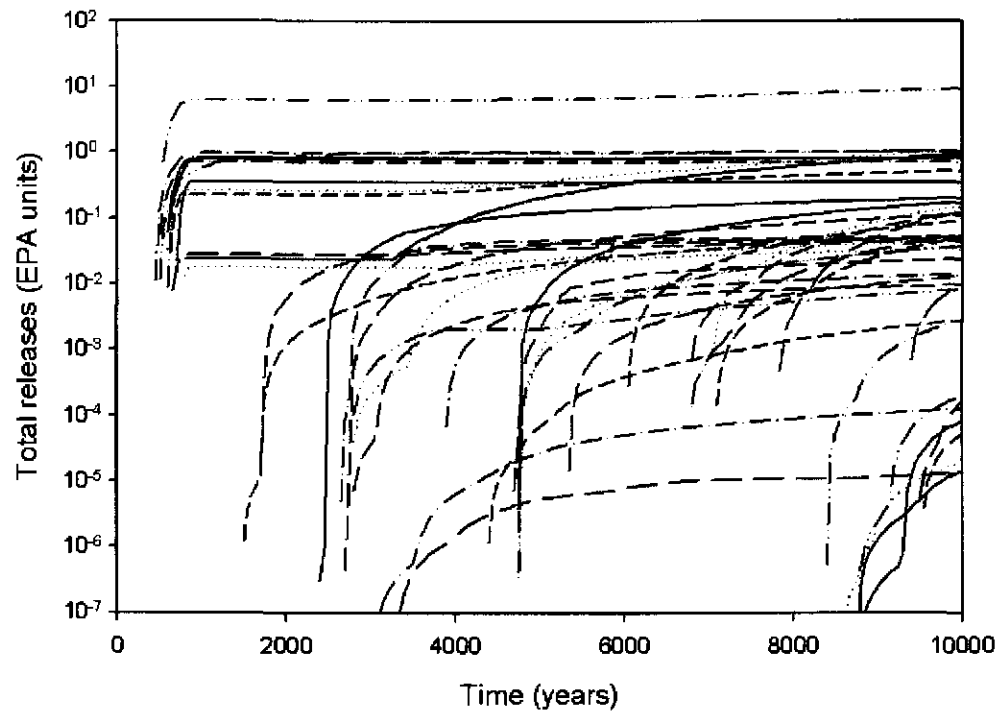

Figure 28 – Cumulative total releases in the borehole at the Culebra for an E2 intrusion at 100 years

Figure 29 – Cumulative total releases in the borehole at the Culebra for an E2 intrusion at 350 years

Figure 30 – Cumulative total releases in the borehole at the Culebra for an E2 intrusion at 1000 years

Figure 31 – Cumulative total releases in the borehole at the Culebra for an E2 intrusion at 3000 years

Figure 32 – Cumulative total releases in the borehole at the Culebra for an E2 intrusion at 5000 years
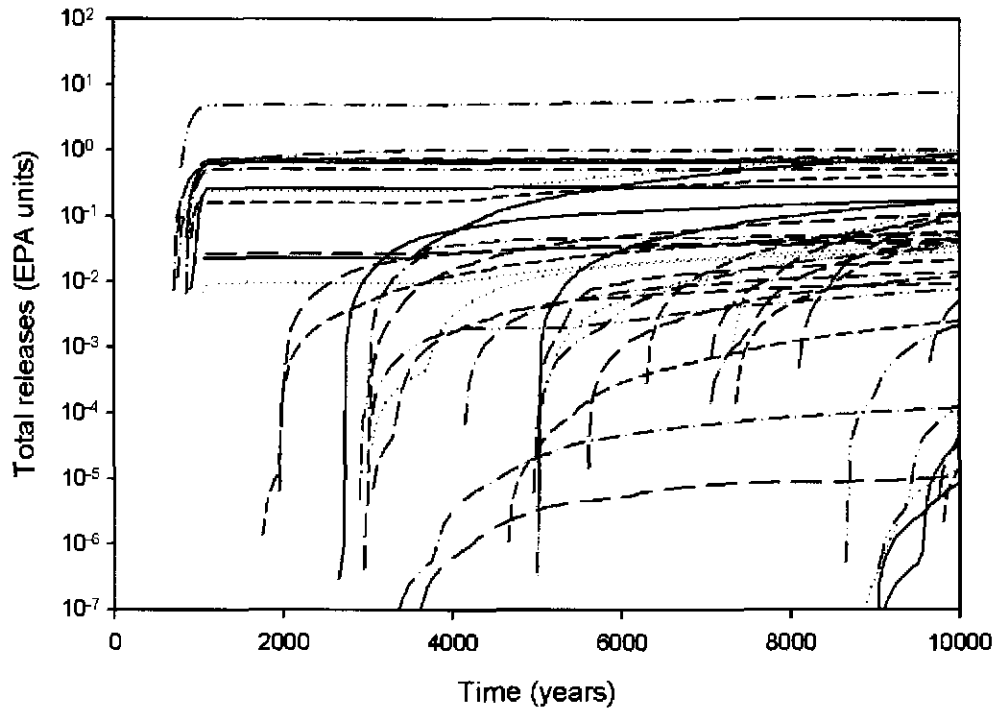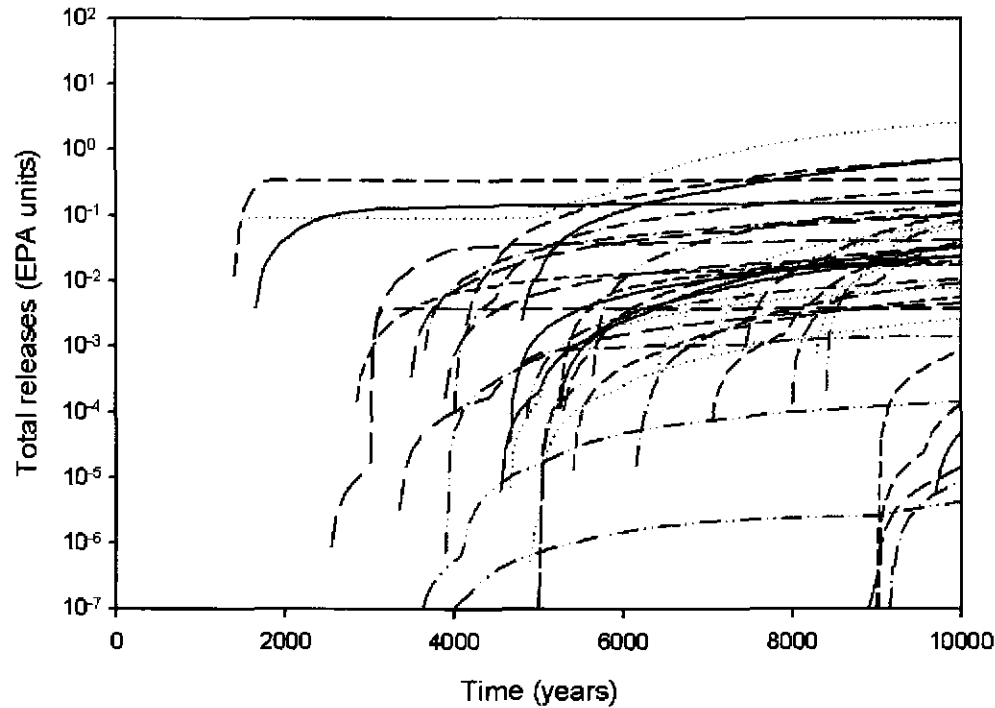
Information Only

Figure 33 – Cumulative total releases in the borehole at the Culebra for an E2 intrusion at 7000 years

Figure 34 – Cumulative total releases in the borehole at the Culebra for an E2 intrusion at 9000 years
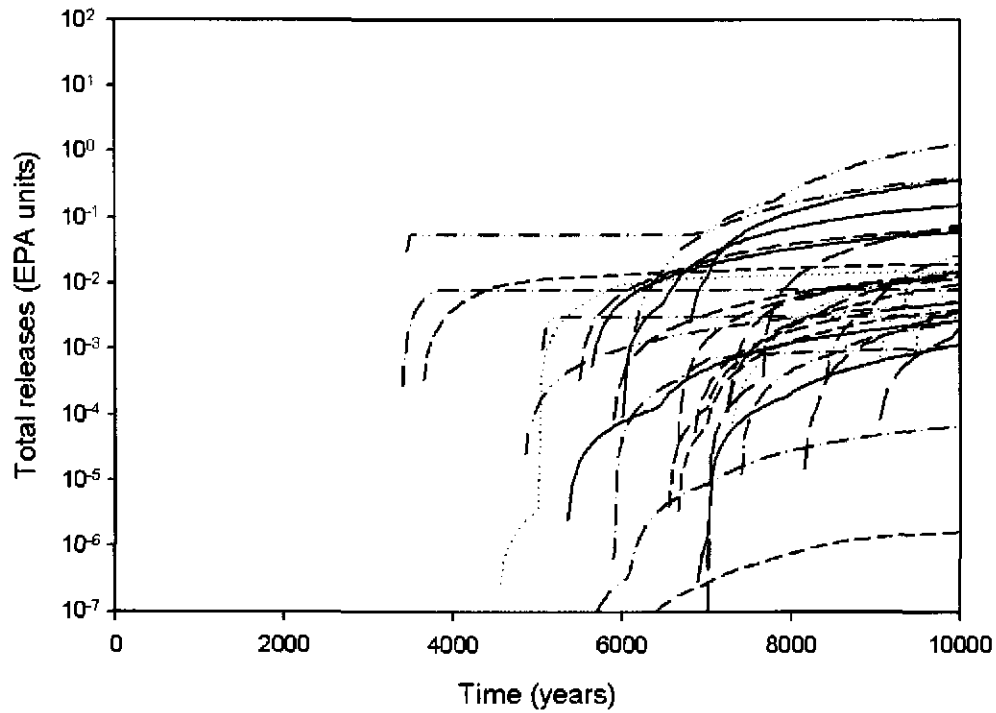
Information Only

Figure 35 – Cumulative total releases in the borehole at the Culebra for an E2-E1 intrusion at 100 years

Figure 36 – Cumulative total releases in the borehole at the Culebra for an E2-E1 intrusion at 350 years
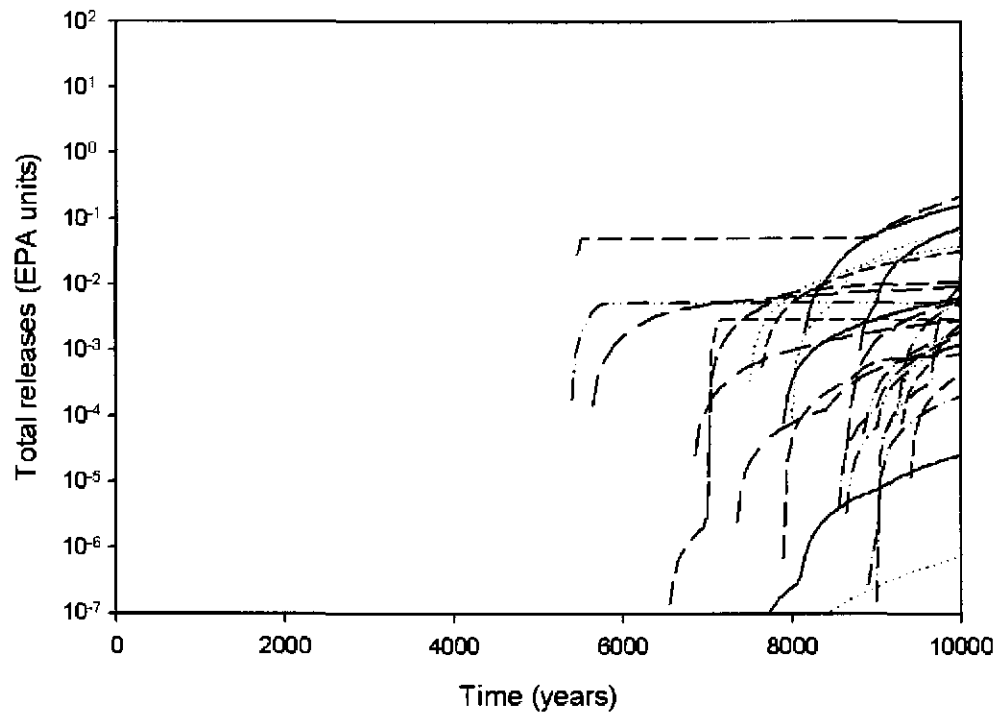
Information Only

Figure 37 – Cumulative total releases in the borehole at the Culebra for an E2-E1 intrusion at 1000 years
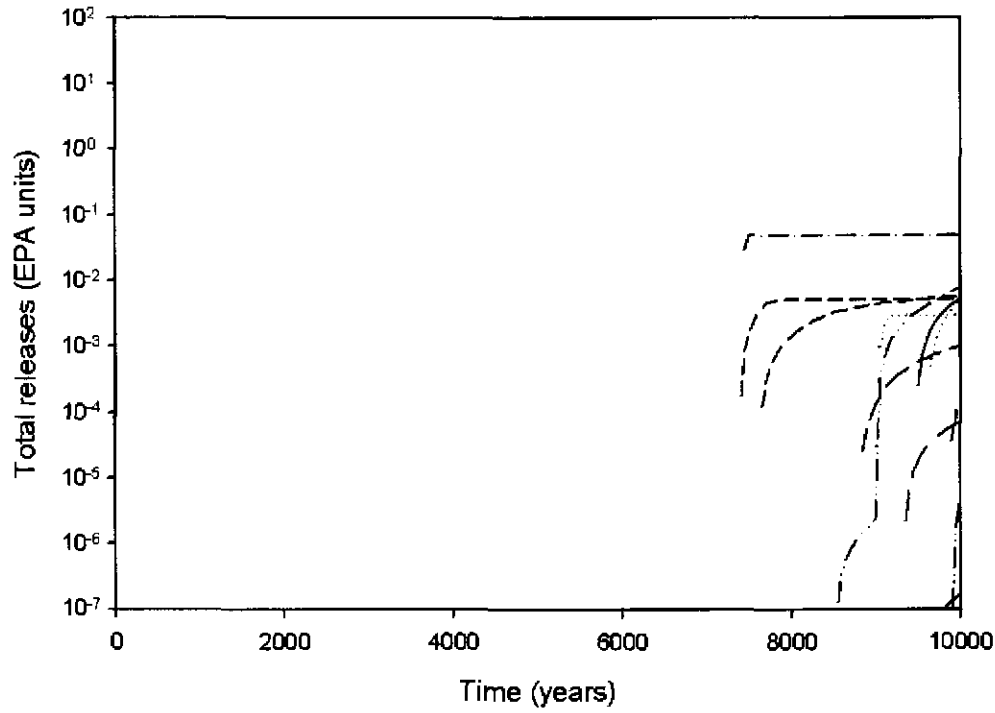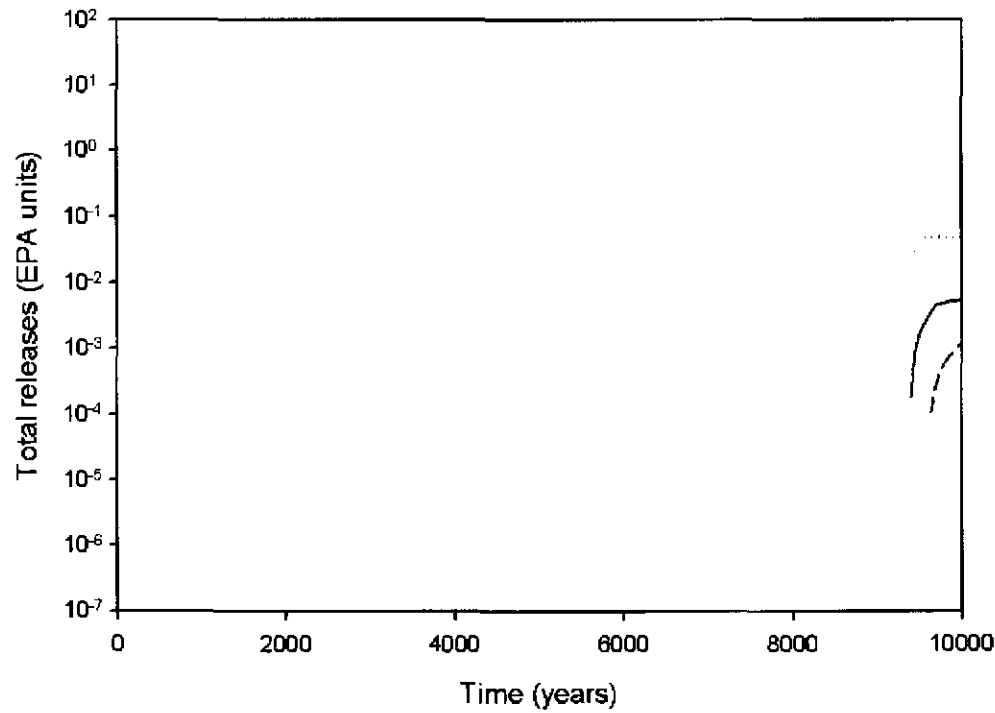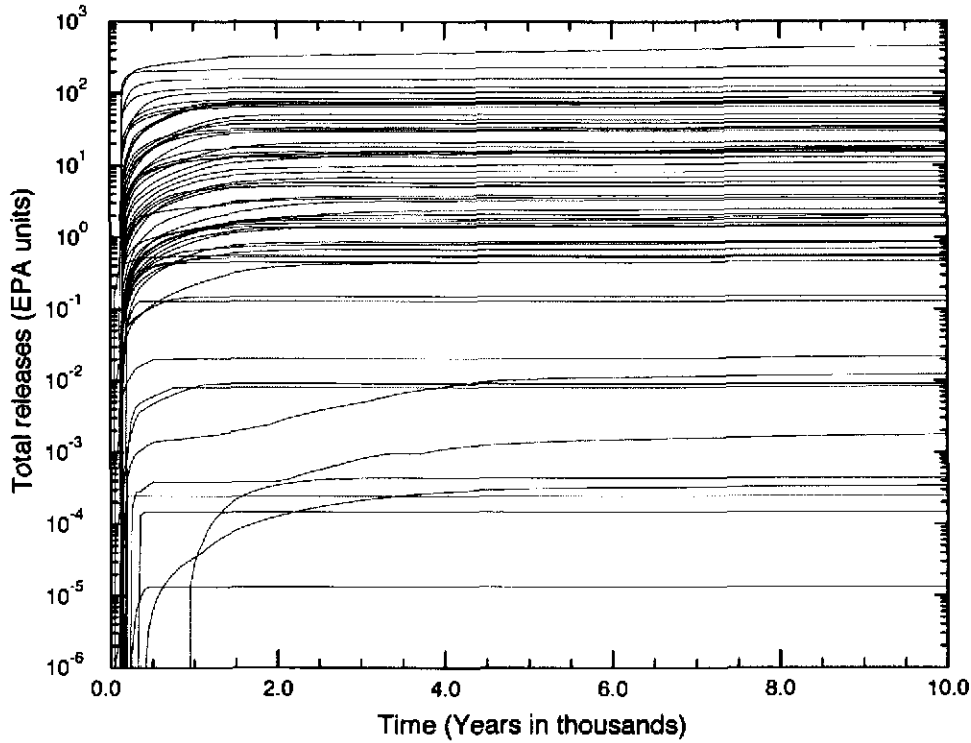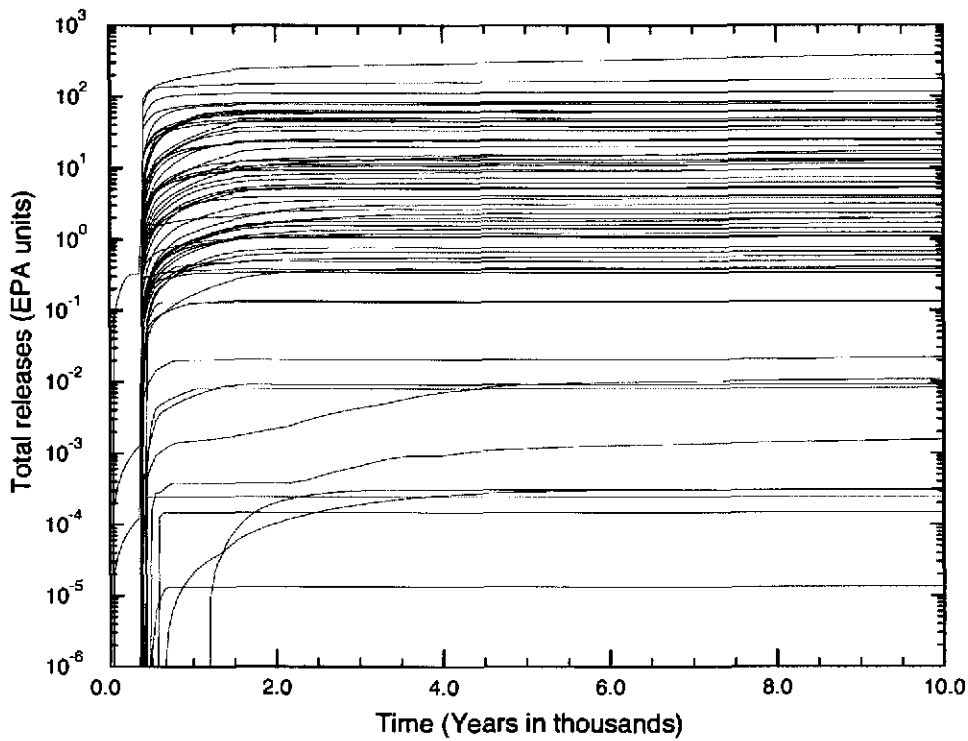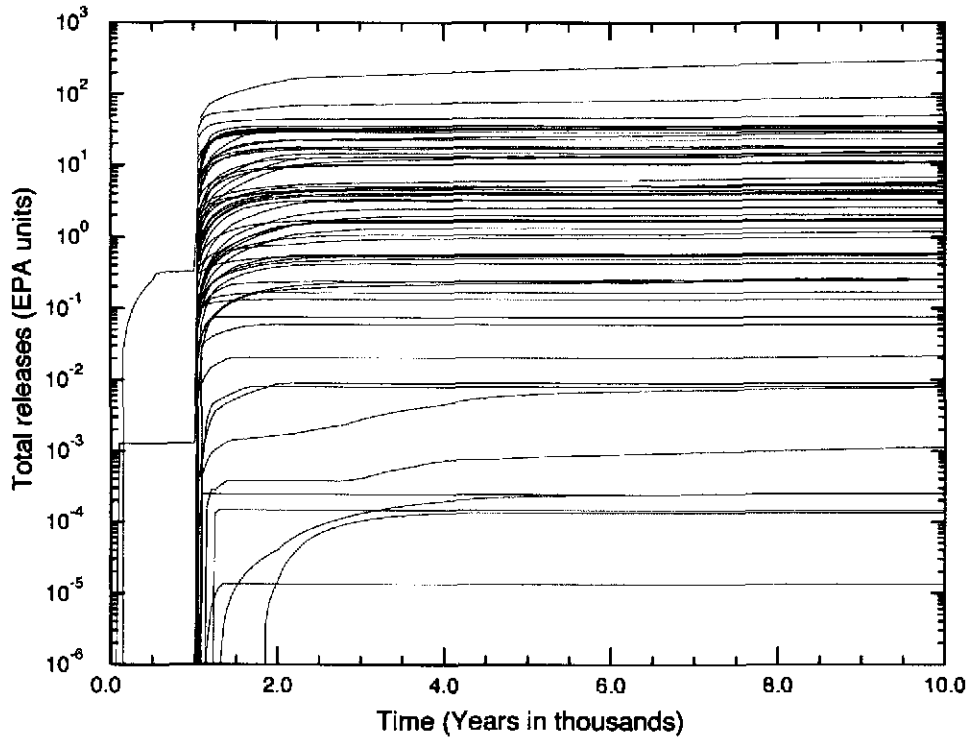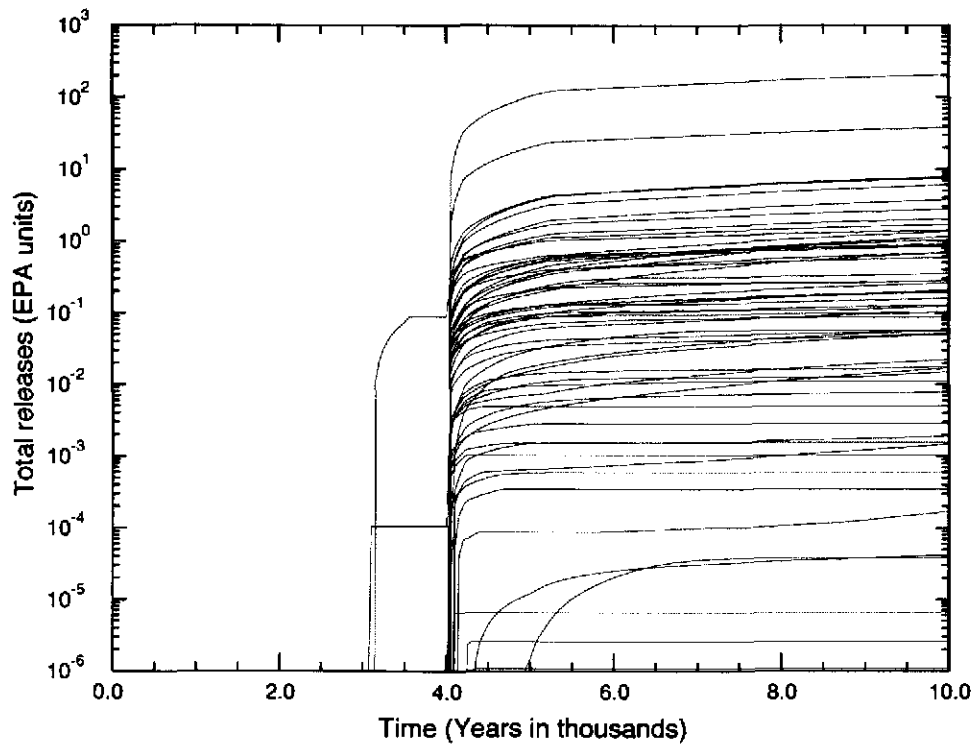

Figure 38 – Cumulative total releases in the borehole at the Culebra for an E2-E1 intrusion at 4000 years
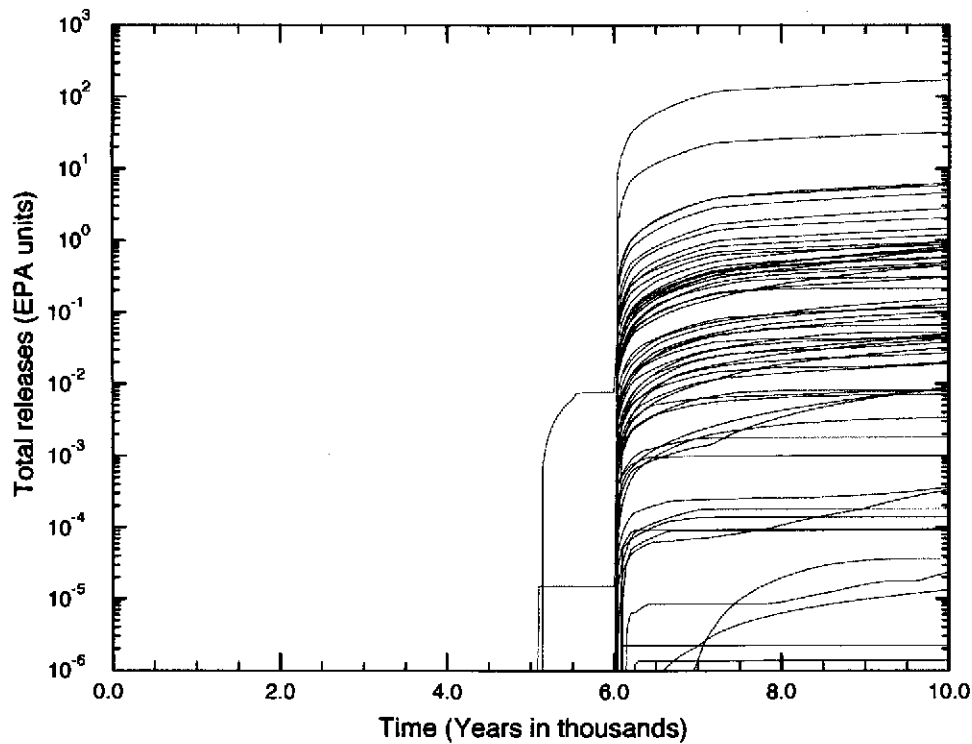
Figure 39 – Cumulative total releases in the borehole at the Culebra for an E2-E1 intrusion at 6000 years
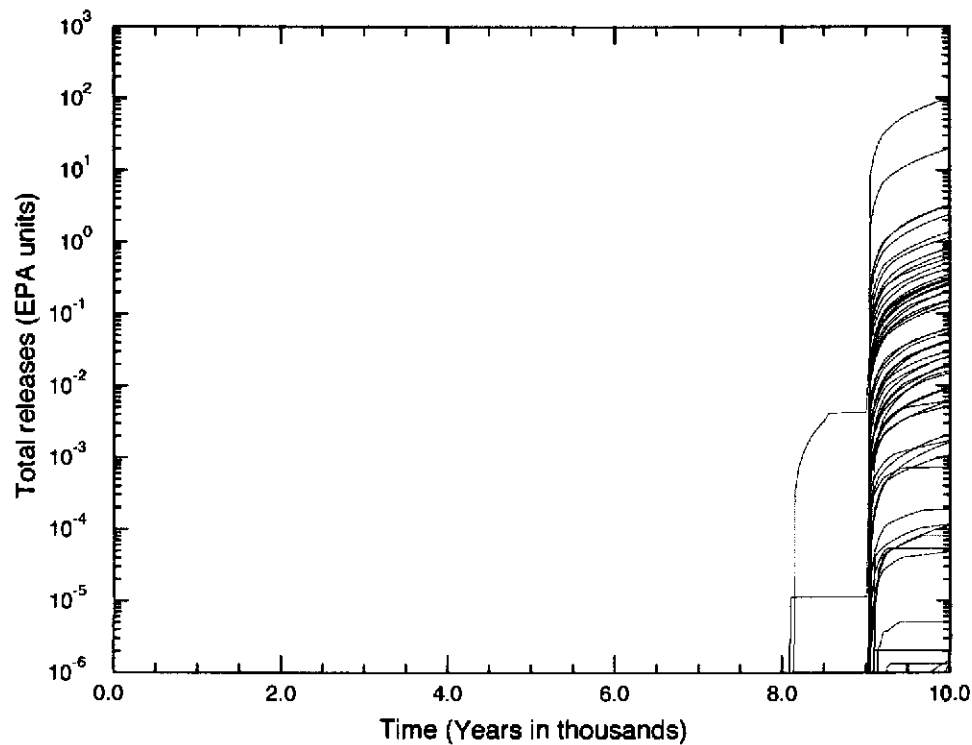

Figure 40 – Cumulative total releases in the borehole at the Culebra for an E2-E1 intrusion at 9000 years

Appendix B   Scripts Used to Analyze NUTS Results

The scripts included below have been used in the processing of the NUTS output files to prepare some of the tables and figures included in this Analysis Report. The source codes for these scripts are stored in CMS library LIBCRA09_NUT in class ANALYSIS. The results of the code were confirmed by visual inspection and hand calculations where appropriate.

Appendix B.1   read_screened.pl

The script *read_screened.pl* reads files SCREEN_NUT_SCN_*ANALYSIS*_R*r*_S*s*.OUT, where *ANALYSIS* is the designation given to the analysis plan in the CMS system (*ANALYSIS* = CRA09, CRA1BC, or AP132), R*r* is the replicate number, and S*s* is the scenario number; these files are stored in CMS library LIB*ANALYSIS*_R*r*S*s*. The result is a single output file, called *screened.results*, which lists the nonzero vectors for each scenario, as well as the number of vectors. This script was used to prepare Table 3.

```perl
#!/usr/bin/perl

# A. E. Ismail
# 5/13/07

# read_screened.pl: Uses output from SCREEN to determine which
# vectors have been "screened-in" for further study.
#
# It also returns a count of the number of vectors in each scenario
# that have been screened in.

use strict;

for my $item (@ARGV) {
  my $new_item = substr ($item, 0, -2);
  `mv $item $new_item`;
  &read_file($item);
}

sub read_file {
  my $file = $_;
  my $repl = substr ($file, -8, 1);
  my $scen = substr ($file, -5, 1);
  my %list;

  print "Replicate $repl, Scenario $scen: ";


  open IN, "<$file" or die "Could not open $file.\n";

  <IN> until (/NONUNION_BEGIN/);

  while (<IN>) {
    last if (/NONUNION_END/);
    my @line = split;
    $list{$line[0]} = 1;
  }
```

```
<IN> until (/UNION_BEGIN/);
while (<IN>) {
  last if (/UNION_END/);
  my @line = split;
  $list{$line[0]} = 2;
}

for my $v (sort keys %list) {
  print "$v, "
}

printf "Count %d", scalar(keys %list);
}
```

Appendix B.2　　find_max.pl

The script *find_max.pl* reads SUMMARIZE files SUM_NUT_*ANALYSIS*_R*r*_S*s*_T*ttttt*.TBL, where *ANALYSIS* is the designator given to the analysis plan(*ANALYSIS* = CRA09, CRA1BC, or AP132), R*r* is the replicate number, and S*s* is the scenario number; these files are stored in CMS library LIB*ANALYSIS*_R*r*S*s*. Two output files are created: sum_nut_*analysis*_*rr*_*ss*_*ttttt*.dat lists the releases for each vector individually, while sum_nut_*analysis*_*rr*_*ss*_*ttttt*.sum outputs the maximum releases for each species and the maximum total release for a given replicate-scenario-time combination. These results were used in Table 5 and Table 7, and Figure 5, Figure 7, Figure 9, and Figure 11.

```
#!/usr/bin/perl

# A. E. Ismail
# 5/13/07

# find_max.pl: Determines maximum for each species and for all species
# for a given replicate.

use strict;

# Run algorithm for each routine individually.
&find_max($_) for (@ARGV);

sub find_max {
  my $file = $_[0];
  my $handle = substr(lc($file), 0, -6);
  my $output = $handle . ".sum";
  my $summary = $handle . ".dat";

  # Open data and output files
  print "Processing $file...\n";
  open IN, "<$file" or die "Could not open input $file.\n";
  open OUT, ">$output" or die "Could not open output $output.\n";
  open SUM, ">$summary" or die "Could not open summary $summary.\n";

  # Vectors to store maximum activities and PA vector numbers.
  my @max = {0., 0., 0., 0., 0., 0., 0.};
  my @loc = {0, 0, 0, 0, 0, 0, 0};

  # Discard header from input file
```

```
<IN> for (1 .. 4);

while (<IN>) {
  # Parse each line. Determine if current activity is greater than the
  # maximum currently stored; if so, replace existing value with the new
  # maximum. Also update loc vector, which stores the ID of the PA vector.
  my @array = split;
  next if (!@array);
  my $row = 0;
  # Determine total activity. Am, Pu, U are normalized by 232; Th by 23.2
  # to convert Ci to EPA units.
  for my $q (2 .. 5) {
    my $term = $array[$q] / (($q != 5) ? 232 : 23.2);
    $row += $term;
    $max[$q - 1] = $term, $loc[$q - 1] = $array[0]
      if ($term > $max[$q - 1]);
  }
  $max[5] = $row, $loc[5] = $array[0] if ($row > $max[5]);
  $max[6] = $array[6], $loc[6] = $array[0] if ($array[6] > $max[6]);
  # Print results for each PA vector to output for creation of figures.
  printf SUM "%3d  %10.5g  %10.5g  %10.5g  %10.5g  %10.5g \n",
    $array[0], $array[2] / 232, $array[3] / 232, $array[4] / 232,
    $array[5] / 23.2, $row
      if ($array[1] > 9999);
}

# Print overall replicate maxima to output file.
for (1 .. 6) {
  printf OUT " %12.6g   %3d\n", $max[$_], $loc[$_];
}

close IN;
close OUT;
close SUM;
}
```

Appendix B.3   spec_act.pl

The script *spec_act.pl* reads SUMMARIZE files SUM_NUT_*ANALYSIS*_R*r*_S*s*_T*tttt*.TBL, where *ANALYSIS* is the designator given to the analysis plan (*ANALYSIS* = CRA09, CRA1BC, or AP132), R*r* is the replicate number, S*s* is the scenario number, and T*tttt* is the intrusion time; these files are stored in CMS library LIB*ANALYSIS*_R*r*S*s*. Four output files are created: *rr_ss_ttttt.sp*.dat, where *sp* is the species ("am," "pu," "u," or "th"). These files print out the time-dependent releases for vectors in which the releases are non-zero for the given species. These results were used in Figure 6, Figure 8, Figure 10, and Figure 12, plus Figure 21 through Figure 34, and then exported to SigmaPlot to produce the plots.

```
#!/usr/bin/perl

# A. E. Ismail
# 5/13/07

# spec_act.pl

# Returns the individual releases for each species, and outputs the list of
```

```perl
# nonzero releases to a separate file for each radionuclide.

use strict;

&sum_act($_) for (@ARGV);

sub sum_act {

  my $input = $_[0];
  my @species = ("am", "pu", "u", "th");

  for my $col (2 .. 5) {
    my $output = lc(substr($input, 14, -6)) . ".$species[$col - 2]" . ".dat";

    open IN, "<$input" or die "Could not open input file $input.\n";
    open OUT, ">$output" or die "Could not open output file $output.\n";

    <IN> for (1 .. 4);

    my ($i, $id, @t, @act);

    $id = 1;
    $i = 0;

    while (<IN>) {
      my @line = split;
      next if (!@line);
      $i = ($line[0] == $id) ? $i + 1 : 1;
      $t[$i] = $line[1];
      $act[$id][$i] = $line[$col] / (($col != 5) ? 232 : 23.2);
      $id = $line[0];
    }

    my @valid;

  OUTER: for my $i (1 .. 100) {
      for my $j (1 .. $#t) {
      push(@valid, $i), next OUTER if ($act[$i][$j] > 0);
      }
    }

    for my $k (1 .. $#t) {
      print OUT " $t[$k] ";
      for my $l (@valid) {
      printf OUT "  %8.4g  ", $act[$l][$k];
      }
      print OUT "\n";
    }

    close IN;
    close OUT;
  }
}
```

Appendix B.4   avg_act.pl

The script *avg_act.pl* reads SUMMARIZE files SUM_NUT_CRA09_*Rr*_S*s*_T*tttt*.TBL, where *Rr* is the replicate number, S*s* is the scenario number, and T*tttt* is the intrusion time; these files are stored in CMS library LIBCRA09_*Rr*S*s*. A single output file "average.dat" is created, listing for each table analyzed the average activity found for each species in the vectors with nonzero releases. The file was then imported into Excel, where the total number of vectors per scenario/time combination and the average release (including vectors with zero releases) were calculated. The resulting spreadsheet, called CRA09_averages.xls, is stored in class ANALYSIS of library LIBCRA09_NUT. The results in CRA09_averages.xls were used to generate Table 6, Table 8, and Table 9.

```perl
#!/usr/bin/perl

# A. E. Ismail
# 1/13/08

# avg_act.pl

# Finds normalized activities and totals them for each vector, then
# returns the average activity found for each species and for the
# total of all species.

use strict;

# Process each file individually

open OUT, ">average.dat" or die "Could not open output file average.dat.\n";

&sum_act($_) for (@ARGV);

close OUT;

sub sum_act {

  my $input = $_[0];
  my $output = lc(substr($input, 14, -4));
  my $count;

  # Open data file
  open IN, "<$input" or die "Could not open input file $input.\n";

  # Discard header
  <IN> for (1 .. 4);
  $count = 0;

  my ($i, $id, @t, @sp_act, $act);

  $id = 1;
  $i = 0;

  while (<IN>) {
    # Grab each line, and parse. For each time step, determine if the
    # activity for each species and for the total is greater than the current
    # stored values. If so, replace them.
```

```perl
    my @line = split;
    next if (!@line);
    next unless ($line[1] >= 9999);
    $count++ if ($line[2] > 0 || $line[3] > 0 || $line[4] > 0 || $line[5] >
0);
    for my $q (2 .. 5) {
      $sp_act[$q - 2] += $line[$q];
    }
  }

  $sp_act[$_] /= 232 for (0 .. 3);
  $sp_act[3] *= 10.0;

  $act += $sp_act[$_] for (0 .. 3);

  if ($count) {
      $sp_act[$_] /= $count for (0 .. 3);
      printf(OUT "$output: %3d %12.7f %12.7f %12.7f %12.7f %12.7g\n", $count,
            $sp_act[0], $sp_act[1], $sp_act[2], $sp_act[3], $act);
  }

  close IN;
}
```

Appendix B.5   pct_act.pl

The script *pct_act.pl* reads SUMMARIZE files SUM_NUT_CRA09_R*r*_S*s*_T*ttttt*.TBL, where R*r* is the replicate number, S*s* is the scenario number, and T*ttttt* is the intrusion time; these files are stored in CMS library LIBCRA09_R*r*S*s*. A single output file "percent.dat" is created, storing the total activities for each species across all vectors of a given replicate, as well as the total activity for all species across all vectors. The file is then imported into Excel, where the percentage of each species as a function of the total activity across all three replicates was calculated. The resulting Excel file, CRA09_percentages.xls, is stored in class ANALYSIS of LIBCRA09_NUT. These results were used to generate Table 6 and Table 8.

```perl
#!/usr/bin/perl

# A. E. Ismail
# 1/13/08

# pct_act.pl

# Finds normalized activities and totals them for each vector, then
# returns the percentage of activity found for each species and the
# total activity of all species.

use strict;

# Process each file individually

open OUT, ">percent.dat" or die "Could not open output file percent.dat.\n";

&sum_act($_) for (@ARGV);
```

```
close OUT;

sub sum_act {

  my $input = $_[0];
  my $output = lc(substr($input, 14, -4));

  # Open data file
  open IN, "<$input" or die "Could not open input file $input.\n";

  # Discard header
  <IN> for (1 .. 4);

  my ($i, $id, @t, @sp_act, $act, $count);

  $id = 1;
  $i = 0;
  $count = 0;

  while (<IN>) {
    # Grab each line, and parse. For each time step, determine if the
    # activity for each species and for the total is greater than the current
    # stored values. If so, replace them.
    my @line = split;
    next if (!@line);
    next unless ($line[1] >= 9999);
    $count++ if ($line[2] > 0 || $line[3] > 0 || $line[4] > 0 ||
            $line[5] > 0);

    for my $q (2 .. 5) {
      $sp_act[$q - 2] += $line[$q];
    }
  }

  $sp_act[$_] /= 232 for (0 .. 3);
  $sp_act[3] *= 10.0;

  $act += $sp_act[$_] for (0 .. 3);

  if ($count) {
      printf(OUT "$output: %12.7f %12.7f %12.7f %12.7f %12.7g\n", $sp_act[0],
            $sp_act[1], $sp_act[2], $sp_act[3], $act);
  }

  close IN;
}
```

Appendix B.6   Verification of SCREEN.FOR

The utility SCREEN.FOR has been used to determine which vectors will be considered for further processing in the isotope and time-intrusion scenarios in NUTS. There have been no changes to the code since the CRA-2004 PABC, so the listing provided in Lowry (2005) is still valid. The verification procedure then consists of running the test cases and comparing the results to show that there are no differences other than those related to file processing (such as designation of the analysis title).

The results of using the `diff` command on the results of SCREEN.FOR for SCREEN_TEST1_S1.OUT from the CRA-2004 PABC and the CRA-2009 PA are shown below. The only difference between the two files is the analysis indicator, which has "CRA09" for the CRA-2009 PA and "CRA1BC" for the CRA-2004 PABC.

```
* * * * * * * * * * * *
File PAWORK: [SHARED.AISMAIL.AP137.NUTS.SCREEN.QUAL]SCREEN_TEST1_S1.OUT;1
     1     analysis: CRA09
     2     replicate:           1
* * * * * *
File
PAWORK: [SHARED.AISMAIL.AP137.NUTS.SCREEN.QUAL.CRA1BC]SCREEN_TEST1_S1.OUT;1
     1     analysis: CRA1BC
     2     replicate:           1
* * * * * * * * * * * *

Number of difference sections found: 1
Number of difference records found: 1

DIFFERENCES /IGNORE=()/MERGED=1-
     PAWORK: [SHARED.AISMAIL.AP137.NUTS.SCREEN.QUAL]SCREEN_TEST1_S1.OUT;1-
PAWORK: [SHARED.AISMAIL.AP137.NUTS.SCREEN.QUAL.CRA1BC]SCREEN_TEST1_S1.OUT;1
[End of file]
```

Similarly, the only difference between SCREEN_TEST1_S2.OUT for the CRA-2004 PABC and the CRA-2009 PA is the analysis indicator, which is the same as for SCREEN_TEST1_S2.OUT above.

```
* * * * * * * * * * * *
File PAWORK: [SHARED.AISMAIL.AP137.NUTS.SCREEN.QUAL]SCREEN_TEST1_S2.OUT;1
     1     analysis: CRA09
     2     replicate:           1
* * * * * *
File
PAWORK: [SHARED.AISMAIL.AP137.NUTS.SCREEN.QUAL.CRA1BC]SCREEN_TEST1_S2.OUT;1
     1     analysis: CRA1BC
     2     replicate:           1
* * * * * * * * * * * *

Number of difference sections found: 1
Number of difference records found: 1

DIFFERENCES
/IGNORE=()/MERGED=1/OUTPUT=PAWORK: [SHARED.AISMAIL.AP137.NUTS.SCREEN*
     PAWORK: [SHARED.AISMAIL.AP137.NUTS.SCREEN.QUAL]SCREEN_TEST1_S2.OUT;1-
PAWORK: [SHARED.AISMAIL.AP137.NUTS.SCREEN.QUAL.CRA1BC]SCREEN_TEST1_S2.OUT;1
[End of file]
```

Since there are no changes to the code and the only differences between the two files are in the name of the analysis, we conclude that the code is performing as expected and as verified in Lowry (2005).