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Sandia National Laboratories
Carlsbad Programs Group
Waste Isolation Pilot Plant

Analysis Package for Salado Transport Calculations:
Compliance Recertification Application

Revision 0

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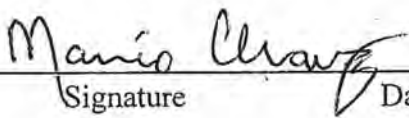
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Introduction

1.1. Background

The Waste Isolation Pilot Plant (WIPP) is located in southeastern New Mexico and has been developed by the U.S. Department of Energy (DOE) for the geologic (deep underground) disposal of transuranic (TRU) 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 and 194. The DOE demonstrates compliance with the containment requirements in the regulations by means of a performance assessment (PA), which estimates releases from the repository for the regulatory period of 10,000 years after closure.

In October 1996, DOE submitted the Compliance Certification Application (CCA) to the EPA, which included the results of extensive PA analyses and modeling. After an extensive review, in May 1998 the EPA certified that the WIPP met the criteria in the regulations and was approved for disposal of transuranic waste. The first shipment of waste arrived at the site in March 1999.

The results of the PA conducted for the CCA were subsequently summarized in a Sandia National Laboratories (SNL) report (Helton, et al, 1998) and in refereed journal articles (Helton and Marietta, 2000).

The DOE is required to submit an application for re-certification every five years after the initial receipt of waste. The re-certification applications take into account any information or conditions that have changed since the original certification decision. Accordingly, the DOE is conducting a new PA in support of the Compliance Recertification Application (CRA).

1.2. Purpose

This analysis package describes the transport calculations that are part of the "Salado Flow and Transport Calculations for the Compliance Recertification Application of the Waste Isolation Pilot Plant" as described in Analysis Plan AP-99 (Stein, 2003a). Specifically, it covers the calculations to determine the mobilization and subsequent migration of radioisotopes throughout the repository, shaft system, Salado formation, and possible human intrusion boreholes. Much of the background information for the CRA is based on the original Compliance Certification Application (CCA). An excellent description of the CCA PA models can be found in Helton et al. (1998) and the CCA version of the tasks described here for the CRA are found in Stockman et al. (1996). This document presents only the changes and updates in the CRA that differ from the CCA and thus the reader is advised to review Helton et al. (1998) and Stockman et al. (1996) prior to reading this document.

1.3. Outline

The rest of this document is organized as follows: Section 2 presents the methodology of the analysis covering the computational aspects such as software, modeling grid, and computational environment, as well as conceptual aspects such as modeling scenarios and

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uncertainty. Section 3 presents the major assumptions and data inclusions that are separate from the methodology but are in integral part of the analysis. Section 4 presents the quantitative aspects of the results. Section 5 covers sensitivity analysis and provides a discussion of the results that are more qualitative in nature. A complete summary is presented in Section 6. The reader is reminded that this report covers only those items that are different from those used in the CCA calculations. However, where it is appropriate, some detail of the CCA calculations, as well as pertinent background information, is presented to provide a better context to the current analyses.

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, which will 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 is of higher transmissivity than the surrounding formations with the Rustler sub-unit, the Culebra Dolomite Member, being the most transmissive. The Castile formation lies directly below the repository and contains areas of pressurized brine. It is not known 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. Five of these scenarios are modeled using the code NUTS (described below) and the sixth scenario is modeled using the code PANEL (Garner, 2003). PANEL is not discussed in this document. The reasoning and methodology surrounding the choice of these scenarios is contained in the above referenced documents and will not be described here. The six scenarios are:

- **S1:** Undisturbed performance (no human intervention or intrusion into the repository during 10,000 years)
- **S2:** An intrusion borehole at 350 years that penetrates both the repository and an underlying pressurized brine reservoir in the Castile formation (E1-type intrusion)
- **S3:** An intrusion borehole at 1000 years that penetrates both the repository and an underlying pressurized brine reservoir in the Castile formation (E1-type intrusion)
- **S4:** An intrusion borehole at 350 years that penetrates the repository but does not encounter a pressurized brine reservoir (E2-type intrusion)
- **S5:** An intrusion borehole at 1000 years that penetrates the repository but does not encounter a pressurized brine reservoir (E2-type intrusion)
- **S6:** A multiple intrusion scenario, which includes an E2 intrusion followed by and E1 intrusion at a later date

2.2. Uncertainty

To address the uncertainty in many of the input parameters used in performance assessment calculations, 100 sets of Latin Hypercube sampled parameters (each unique set is called a vector) are defined. LHS is a method of Monte Carlo sampling that selects parameters values based on individual probability density functions for each parameter. Each group of 100 vectors is called a replicate. Three replicates (R1, R2, and R3) are run in a full PA calculation. This totals to 1500 NUTS simulations; five scenarios of 100 vectors for three replicates. As will be discussed below, screening runs are used to substantially reduce this number.

In order to provide an accurate method for assessing the uncertainty in the results, the code CCDFGF is used to create complimentary cumulative distribution functions (CCDFs) that define the probability of exceeding normalized cumulative radionuclide releases. CCDFs are one of the measures used by the EPA to determine compliance. A complete discussion on the uncertainty involved with the CRA PA modeling can be found in (Hansen, 2003).

2.3. Software

2.3.1. Nuts

The overall transport and decay of radionuclides for scenarios S1 to S5 are calculated using the computer code NUTS (NUclide Transport System), version 2.05a. NUTS is a five-point finite difference code designed to model multi-dimensional, multi-component, and radioactive-contaminant transport in single-porosity (SP), dual-porosity (DP), and/or dual-permeability (DPM) porous media, including parent/daughter first-order decay. Any flow of brine up the shafts, borehole(s), and out the marker beds (see below) is calculated using the code BRAGFLO (Stein and Zelinski, 2003) and these results are required prior to running NUTS. NUTS requires the BRAGFLO ASCII input file containing the grid specifications, initialization parameters, and material maps as well as the BRAGFLO post-processed binary files (CDB) that describes the flow-field. The 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 the 'effective solubilities', 'lumped inventory' (see below) source terms created by PANEL, and atomic weights and half-lives of the modeled isotopes. NUTS also uses its own input file that contains the run parameters and the isotope decay data.

2.3.2. Other Codes

The codes that perform the modeling calculations are BRAGFLO (calculation of brine and gas flow), NUTS (radionuclide transport, scenarios S1 to S5), and PANEL (radionuclide transport, scenario S6). Uncertainty in the input parameters is included through the use of the Latin hypercube sampler code, LHS. The rest of the codes are used as data manipulation and/or visualization. More information for each code in can be found in the respective design document and/or user manual. A listing of the codes is shown in Table 1.

For the NUTS calculations, ALGEBRA is run on the output to calculate 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, Microsoft Excel is used to plot the breakthrough curves for each replicate/vector/isotope combination. A visual basic macro (Appendix A) is used to automate the plotting process.

Table 1 – List of the major codes used in the CRA PA.

Code	Version	Code Function
ALGEBRACDB	2.35	Data processor
BLOTADB	1.37	Plotting
BRAGFLO	5.00	Brine and gas flow
GENMESH	6.08	Grid generation
ICSET	2.22	Sets initial conditions
LHS	2.41	Latin hypercube sampler
MATSET	9.10	Sets material parameters
NUTS	2.05a	Salado transport
PANEL	4.02	Salado transport
POSTBRAG	4.00	BRAGFLO postprocessor
POSTLHS	4.07	LHS postprocessor
PREBRAG	7.00	BRAGFLO preprocessor
PRELHS	2.30	LHS preprocessor
SPLAT	1.02	Plotting
SUMMARIZE	2.20	Data interpolation

2.3.3. Data Flow

As mentioned above, NUTS requires input from BRAGFLO, and its own input file. The NUTS binary output file is used by ALGEBRA, which in turn produces output used by SUMMARIZE. The output from SUMMARIZE is imported into Microsoft Excel and plotted using the macro in Appendix A. The flow chart in Figure 1 illustrates the relationship between the major codes used in this analysis.

2.4. Type of Model Runs

Three types of model runs are performed using NUTS; screening runs, isotope runs (ISO), and time intrusion runs (TI). This section describes each type of run.

2.4.1. Screening Runs

Full transport calculations are computationally intensive and can consume large amounts of computer time. The NUTS screening runs are used to filter out those scenario-vector combinations that have no potential to release radionuclides to the Culebra and/or across the land withdrawal boundary (LWB), increasing computational efficiency. A screening

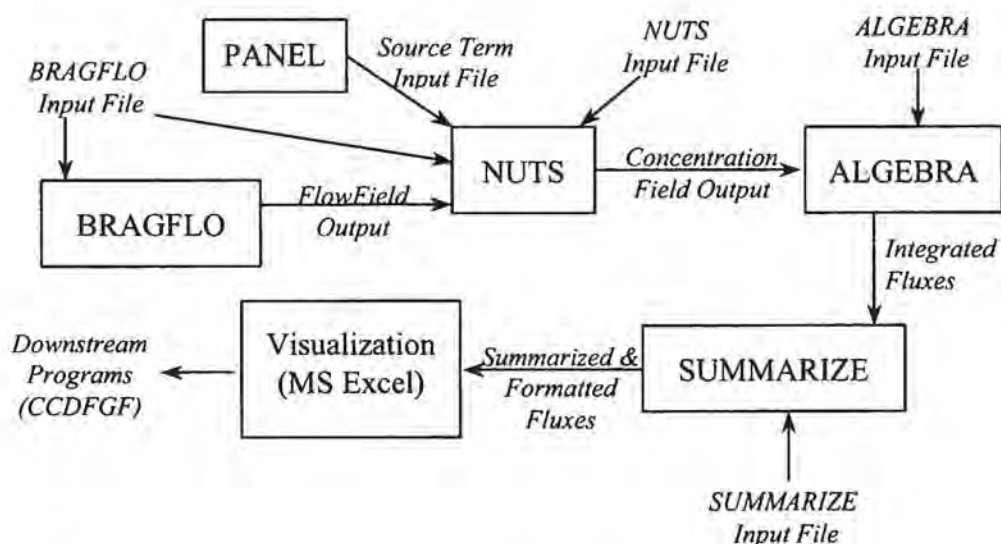


Figure 1 – Relationship and data flow for major codes used in the NUTS analysis.

run calculates the transport over 10,000 years of a temporally continuous conservative tracer (constant concentration, Dirichlet boundary condition) with an initial concentration of 1kg/m^3 in all waste disposal areas. A vector is considered ‘screened-in’ if the cumulative tracer mass-flux that enters the “accessible environment” (outside the LWB or to the Culebra via the borehole and/or shaft) exceeds 10^{-7} kg . The magnitude of the initial condition and the screening cutoff concentration are considered conservative. The development and assumptions concerning these two values can be found in Stockman et al. (1996). Vectors that are not screened-in are not included in the ISO or TI calculations, where specific isotopes and more complicated chemistry are modeled. For this analysis replicates one, two, and three (R1, R2, and R3) screened-in 134, 146, and 135 vectors out of the possible 500 (each), respectively. A list of the screened-in vectors is shown in **Error! Reference source not found.**

A FORTRAN program called SCREEN_BL.FOR is used to post-process the output from the SUMMARIZE screening runs and to list which runs violate the screening criteria and where the breach occurs (borehole, markerbeds, shaft). It also totals the number of ‘screened in’ vectors for each scenario. SCREEN_BL.FOR is reproduced in Appendix B.

Table 2 - Screened-in vectors for each scenario/replicate combination.

Replicate	Scenario	Vector Number
R1	S1	82
	S2	2, 3, 4, 6, 7, 8, 9, 10, 11, 17, 20, 21, 23, 25, 28, 30, 31, 32, 33, 37, 38, 42, 43, 44, 45, 46, 47, 48, 54, 56, 57, 58, 60, 62, 63, 66, 67, 69, 71, 73, 75, 76, 77, 78, 79, 80, 81, 82, 83, 84, 86, 88, 90, 91, 93, 94, 95, 96, 97, 98
	S3	2, 3, 4, 6, 7, 8, 9, 10, 11, 17, 20, 21, 23, 25, 28, 30, 31, 32, 33, 37, 43, 44, 45, 46, 47, 54, 56, 57, 58, 60, 63, 66, 73, 76, 77, 78, 79, 80, 81, 82, 84, 86, 88, 90, 91, 94, 95, 96, 97, 98
	S4	7, 9, 17, 20, 23, 31, 46, 66, 84, 91, 97
	S5	7, 9, 17, 20, 22, 23, 31, 46, 66, 84, 91, 97
R2	S1	No vectors screened-in
	S2	1, 4, 5, 7, 8, 9, 10, 14, 15, 17, 18, 19, 21, 22, 23, 24, 25, 26, 30, 34, 35, 37, 38, 39, 41, 42, 43, 44, 45, 46, 47, 50, 54, 56, 57, 58, 61, 62, 63, 64, 65, 67, 68, 69, 70, 71, 74, 76, 77, 80, 82, 83, 84, 85, 86, 87, 89, 90, 91, 94, 96, 97, 98, 99, 100
	S3	1, 4, 5, 7, 9, 10, 14, 15, 17, 18, 19, 21, 22, 23, 24, 25, 26, 30, 34, 35, 37, 39, 41, 42, 43, 44, 45, 46, 47, 50, 57, 58, 61, 62, 63, 64, 65, 67, 68, 69, 70, 71, 76, 77, 82, 83, 84, 87, 89, 90, 94, 97, 98, 99, 100
	S4	1, 9, 10, 22, 24, 26, 63, 64, 77, 83, 84, 89, 99, 100
	S5	1, 9, 10, 22, 24, 26, 63, 64, 83, 84, 89, 99, 100
R3	S1	No vectors screened-in
	S2	1, 2, 5, 7, 9, 13, 14, 15, 16, 17, 21, 22, 23, 24, 26, 28, 29, 30, 31, 32, 33, 34, 35, 39, 41, 43, 45, 46, 48, 49, 50, 51, 52, 53, 54, 55, 57, 60, 63, 64, 66, 67, 69, 70, 72, 74, 75, 77, 80, 81, 82, 83, 86, 88, 90, 91, 94, 96, 97, 98, 100
	S3	1, 5, 13, 14, 15, 16, 17, 21, 22, 23, 24, 26, 28, 29, 30, 31, 32, 33, 34, 35, 39, 40, 43, 45, 46, 48, 49, 50, 51, 52, 53, 54, 55, 57, 60, 63, 64, 66, 69, 70, 72, 74, 75, 80, 81, 82, 83, 86, 88, 90, 97, 100
	S4	22, 26, 28, 31, 54, 55, 57, 64, 72, 74, 83, 88
	S5	22, 26, 28, 31, 54, 55, 57, 64, 72, 74, 88

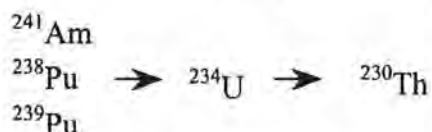
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2.4.2. Isotope (ISO) Runs

Because NUTS is a computationally intensive code that requires long run times, and because decreasing the number of isotopes it mobilizes can substantially decrease its run time, the possible isotopes and decay chains were 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 are combined in ways that would introduce little or no loss of release information in terms of normalized "EPA units". Combinations of similar isotopes are referred to as 'lumped isotopes'. EPA units are a measure of normalized releases, nR , calculated as:

$$nR = \sum \frac{Q_i}{L_i} \left(\frac{1 \times 10^6 \text{ curries}}{C} \right) \quad (1)$$

where Q_i is the 10,000-year cumulative release in curries of radionuclide i , L_i is the release limit for radionuclide i (as specified by CFR 40, Part 194), and C is the total transuranic inventory in the WIPP in curries. All values of EPA units quoted and used in this report are calculated by the ALGEBRA code and are contained in the appropriate ALGEBRA output files stored in the CMS (see Table 3, Page 16, below). The final conclusion of the decay chain analysis is that five "lumped" isotopes are modeled based on the following simplified decay chains:



These are the same isotopes modeled for the CCA, justified by the fact that the available isotopes in the waste packages have not changed between the CCA and the CRA. A complete justification for the use of these five isotopes can be found in Stockman et al. (1996).

For this analysis, only ${}^{241}\text{Am}$, ${}^{239}\text{Pu}$, ${}^{234}\text{U}$, and ${}^{230}\text{Th}$ are examined individually in the output since the half-life of ${}^{238}\text{Pu}$ is 87.7 years and will have decayed to negligible amounts in the time frames of interest. Total activity releases presented below do include the contribution from ${}^{238}\text{Pu}$. 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-S5) as calculated by BRAGFLO.

2.4.3. Time Intrusion (TI) Runs

The NUTS TI runs are for simulating intrusion times that are earlier and later than the 350 and 1000 year intrusions modeled in the ISO runs. This is done by shifting the initial conditions from the BRAGFLO runs to the appropriate time. For instance, the BRAGFLO results for E1 and E2 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 1000, 3000, 5000, 7000, and 9000 yrs. For times greater than 1000 years, 'shifted intrusion-time' calculations are performed that assume an undisturbed scenario until the time of intrusion and then the 1000-year intrusion flow-field after the intrusion.

This approach is justified by the fact that previous BRAGFLO simulations for intrusion times greater than 1000 years have shown that undisturbed conditions reach steady-state prior to the intrusion time. In addition, repository performance is most sensitive to gas-pressure relief and brine inflow (from the high-pressure brine pocket and/or marker beds) that occurs at or soon after intrusion. However, it is not sensitive to the kinds of changes (e.g. fracturing) that occur prior to intrusion (Stockman et al., 1996; Stein and Zelinski, 2003). Thus, the flow-field after intrusion is much more dependent on an intrusion event occurring rather than the conditions before the intrusion.

2.5. Modeling Grid

The grid used for the NUTS calculations is the same as used for the BRAGFLO calculations. The extent of the modeling domain is 46,630 m in the horizontal (x) direction by 940 m in the vertical (y) direction, which is the same as for the CCA calculations. The domain is discretized into 68 x 33 (x,y) non-uniform grid cells with higher resolution in the repository area and lower resolution towards the edges of the modeling domain. The grid is more refined and includes a more detailed representation of the panel closures and waste regions than was used for the CCA calculations. The changes made to the grid were accepted by the Salado Flow Peer Review panel in February 2003 (Caporuscio et al., 2003). The grid is illustrated in Figure 2. A full description of the grid can be found in Stein and Zelinski (2003).

2.6. Computational Environment

Calculations for the Salado Flow and Transport simulations are performed on ES-40, ES-45, and/or 8400 Compaq ALPHA computers running Open VMS Version 7.3-1 (WIPP PA, 2003a-c). Each job is executed using scripts, with run-time input files and output files residing in an access controlled environment on the cluster. The runs utilized the WIPP PA Software Configuration Management System (SCMS) to assure control of the various PA codes and associated files. The SCMS in turn is implemented by the Compaq Corporation Code Management System (CMS – WIPP PA, 2003d).

This section documents the input and output files used for NUTS, ALGEBRA, and SUMMARIZE for the Salado Flow and Transport simulations as well as the library locations within the CMS where the final versions are archived.

There are three sets of input files for all three programs; one each for the screening, ISO, and TI runs. Each set of input files are numbered according to the run type, replicate, scenario, and vector numbers. The CMS libraries, the included files, and the file descriptions are shown in Table 3. A sample input file for each program is listed in Appendix C, D, and E.

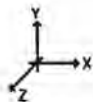
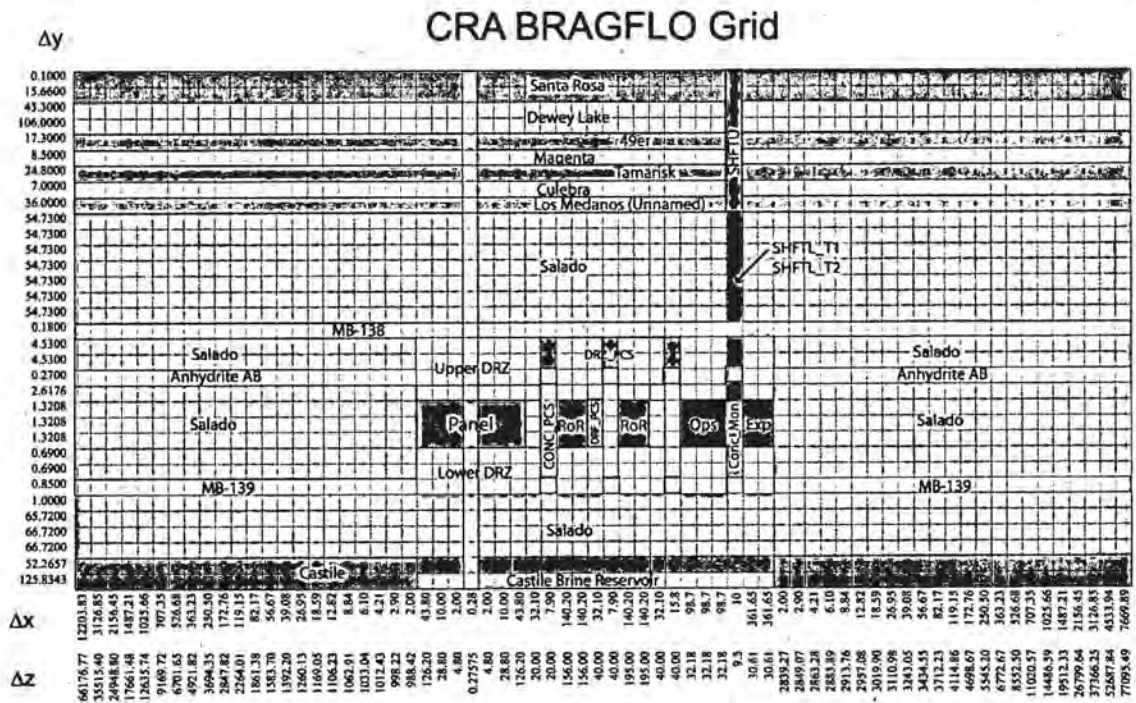


Figure 2 – Computational grid used for the BRAGFLO and NUTS runs for the Salado Flow and transport calculations. MB refers to the marker beds, DRZ is the disturbed rock zone surrounding the repository area, SHFTU is the upper shaft area, SHFTL is the lower shaft area. The green area within the DRZ is the repository area. The grayed cells (light colored) extending from the surface to the Castile Brine Reservoir shows the location of the borehole.

3. Other Data and Assumptions

This section looks at the major data inputs, modeling factors, and modeling assumptions for the NUTS CRA PA model. It is not intended to be a complete documentation of the inputs and workings of NUTS, but rather to give the reader a sufficient level of understanding to interpret and understand the results. For more detail, the reader is again referred to Stockman et al. (1996).

NUTS is designed to model mobilization and decay of the selected isotopes. For mobilization, the code requires the isotope inventory and element solubility. The isotope inventory is apportioned using volume or areal fractions, to the computational cell(s) of NUTS. This approach is equivalent to assuming a homogeneous waste inventory.

Radionuclide release from the repository to the Culebra depends on both the amount 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,

Table 3 – Library locations, file names, and description for the Salado Formation Flow and Transport simulations for NUTS, ALGEBRA, and SUMMARIZE.

CMS Library	File Name*	Description
LIBCRA1_NUT	NUT_CRA1_SCN_Rx_Sy.INP	NUTS screening runs input
	NUT_CRA1_ISO_Rx_Sy.INP	NUTS ISO runs input
	NUT_CRA1_INTz_Rx_Sy.INP**	NUTS TI runs input
	ALG_NUT_CRA1_SCN_Rx_Sy.INP	ALGEBRA screening runs input
	ALG_NUT_CRA1_POST_Sy.INP	ALGEBRA ISO runs input
	NUT_CRA1_SCN_Rx.OUT	Screening output from SCREEN_BL
LIBCRA1_NUTRxSy	NUT_CRA1_SCN_Rx_Sy_Vnnn.CDB	NUTS screening runs binary output
	NUT_CRA1_ISO_Rx_Sy_Vnnn.CDB	NUTS ISO runs binary output***
	NUT_CRA1_SCN_RxSyVnnn_STEP1.LOG	NUTS screening run log
	NUT_ISO_CRA1_RxSyVnnn_STEP1.LOG	NUTS ISO run log***
	ALG_NUT_CRA1_SCN_Rx_Sy_Vnnn.CDB	ALGEBRA screening runs binary output
	NUT_CRA1_INTz_Rx_Sy_Vnnn.CDB**	NUTS TI runs binary output***
	NUT_CRA1_INTz_RxSyVnnn_STEP1_2.LOG**	NUTS TI run log***
LIBCRA1_ALG	ALG_NUT_CRA1_POST_ISO_Rx_Sy_Vnnn.CDB	ALGEBRA ISO runs binary output***
	ALG_NUT_CRA1_POST_INTz_Rx_Sy_Vnnn.CDB**	ALGEBRA TI runs binary output***
LIBCRA1_SUM	SUM_NUT_CRA1_SCN_Rx_Sy.INP	SUMMARIZE screening runs input
	SUM_NUT_CRA1_SCN_Rx_Sy.DAT	SUMMARIZE screening runs output
	SUM_NUT_CRA1_Rx_Sy.INP	SUMMARIZE ISO runs input***
	SUM_NUT_CRA1_Rx_Sy.TBL	SUMMARIZE ISO runs output***
	SUM_NUT_CRA1_Rx_Sy_Tz.INP**	SUMMARIZE TI runs input***
	SUM_NUT_CRA1_Rx_Sy_Tz.TBL**	SUMMARIZE TI runs output***
<p>*File naming convention: Rx refers to the replicate number (x=1, 2, or 3), Sy refers to the scenario number (y=1 to 5), Tz refers to the intrusion time (z=100, 3000, 5000, 7000, or 9000), Vnnn refers to the vector number (nnn = 001, 002, ..., 099, 100)</p> <p>**TI files are only applicable to scenarios 2 to 5</p> <p>***These files are generated only for vectors that are 'screened-in'</p>		

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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) meaning the concentration in the brine and on the colloids is always at equilibrium. However, the isotope inventory changes with time due to decay and ingrowth, so the equilibrium is not steady-state.

The key processes modeled with NUTS are advective transport, decay, precipitation, solubility limits, and interior sources, all in a single porosity, continuous matrix. No dispersion is modeled. The initial condition for each run is to assume no contamination present within the model domain, with the exception of the source term in the waste panel area.

4. Results

This section presents the results from the NUTS simulations for transport of the four radioisotopes within the Salado formation for scenarios S1 to S5 as discussed above. As mentioned, there are five isotopes that are modeled but since ^{238}Pu is only a small fraction of the inventory within the repository and due to its short half-life (87.7 years) it is not included in the final analysis.

4.1. Summary of Potential Pathways

To provide a more complete picture of the results a conceptualization of the physical processes is given here. A complete analysis of the BRAGFLO results is given by Stein and Zelinski (2003).

When brine enters the disposal region, gas is generated by anoxic corrosion of iron and biodegradation of organic materials, and radioisotopes are released 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 has to 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 as is shown below, the most important pathway is a human intrusion into and possibly through the repository. Under this scenario, brine may be released up the 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 (Stein, 2003b). 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, Figure 2).

The dynamics of the brine movement are complex and highly dependent on the BRAGLO input parameters. Initially, brine may flow into the repository from anyone 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. Brine may be consumed by the oxidation of ferrous material in the waste containers and the waste itself, which has an effect on the solubility of the radioisotopes.

4.2. Screening Runs

The intent of the screening runs was to reduce the total number of 'complete' model simulations necessary by eliminating model vectors that have no possibility of transporting radionuclides beyond the repository boundary. To do this, a conservative tracer is modeled and the cumulative mass is monitored at several key points in the modeling domain. The key points are the borehole/Culebra intersection, the shaft/Culebra intersection, and the marker beds at the LWB. Vectors that show a cumulative mass tracer of 10^{-7} kg or more at those key points are deemed 'screened-in' and are then passed through to perform the full radionuclide transport simulations. The full process of the screening runs as well as the results are presented above in section 2.4.1.

4.3. ISO Runs

The ISO runs are for 350 and 1000-year E1 intrusions (scenarios S2 and S3), 350 and 1000-year E2 intrusions (scenarios S4 and S5), as well as the undisturbed case (scenario S1).

4.3.1. Undisturbed Scenario – S1

For replicates R1, R2, and R3, there are 1, 0, and 0 screened-in runs, respectively. The screenings detected the conservative contaminant at the LWB through the Marker Bed 139 South, with cumulative mass of 1.025×10^{-07} kg for R1S1v082. However, for the ISO case, the activity for the isotopes drops considerably with a total integrated flux of 2.89×10^{-15} EPA units.

The distance from the repository to where the integrated release becomes less than 1×10^{-7} EPA units can be calculated. Not surprisingly, ^{239}Pu penetrates the MB139S the furthest, moving 984.34 m from the repository boundary. All of the isotopes move through the marker bed a minimum of 677.48 m. As a comparison, the total distance from the repository to the LWB is 2400 m. The travel distance for each isotope for R1S1v082 is shown in Table 4.

Table 4 – Distance from the repository in meters along MB139S for the point where the integrated activity is less than 1×10^{-7} EPA units.

Vector #	Am-241	Pu-239	U-234	Th-230
R1S1v082	677.48	984.34	984.34	677.48

The small integrated activities at the LWB are almost certainly due to numerical dispersion due to the coarse grid between the repository and the LWB. Numerical dispersion in finite difference codes such as NUTS is due to the truncation of the Taylor series expansion that occurs when developing the algebraic representation of the initial governing equations. The net effect is an increase in the dispersion coefficient that is proportional to the grid cell size as well as the groundwater velocity. For the time-dependent, one-dimensional, advection-dispersion equation, the 'numerical dispersion coefficient', D_{nd} , is given by (de Marsily, 1986):

$$D_{nd} = \frac{u\Delta x}{2} \quad (2)$$

where u is the groundwater pore velocity and Δx is the cell size. D_{nd} will change depending on the formulation and dimensions of the problem, but will always be linked to the velocity and cell size. It should be mentioned that there are higher order terms that have been ignored in this example; the most notable is a 'source/sink' term that is equivalent to half the time step multiplied by the second order time derivative of the concentration. This term can impart oscillations in the solution if the time step is too large but does not add to the artificial spreading of the plume. Continuing, if we assume the 1×10^{-7} EPA units represents the advective front of the plume, the maximum average pore velocity through the marker bed is 0.098 m/yr (^{239}Pu moved 984.34 m in 10,000 yrs). For an average cell size of 78 m (cell size ranges from 2.0 m close to the repository to 363.23 m at the 984.34 m mark), this translates to a numerical dispersion coefficient of $3.84 \text{ m}^2/\text{yr}$, or an equivalent dispersivity of about 38 m, which is enough to account for the slight predicted activities at the LWB.

To further evaluate this slight release out the marker bed for vector R1S1v082, an ALGEBRA run was made to convert the ISO results to concentrations in curies per liter (see Appendix F: and Appendix G: for the input files). These concentrations were then extracted with SUMMARIZE and compared with the concentrations from the CCA (DOE, 2004). The concentrations from R1S1v082 are at least five orders of magnitude lower than the concentrations evaluated for undisturbed case of the CCA.

4.3.2. 350 Year E1 Intrusion – S2

Scenario S2 models an E1 intrusion, which penetrates the repository and the lower Castile formation, at 350 years. The S2 scenario is highly influenced by the conditions 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, S2 shows the highest number of screened in vectors as well as the highest outward fluxes of brine and radioisotopes.

The only pathway to show any contaminant movement at the LWB was up the borehole. No activity was shown through the marker beds or up the shaft at the Culebra interface. Thus, the analysis concentrates on the total activity in EPA units at the point where the borehole intersects the Culebra. The time series plots for each isotope, vector, and replicate are shown in Figure 10, Figure 11, and Figure 12. 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 isotope occurred in R1S2v007, which showed an integrated activity of 21.63 EPA units for ²⁴¹Am. For ²³⁹Pu, vector R3S2v028 showed the maximum with an integrated activity of 5.24 EPA units. ²³⁴U and ²³⁰Th were comparatively minor with maximums for each of 0.0066 and 0.00098 EPA units in vectors R2S2v009 and R2S2v007, respectively. On the average, ²⁴¹Am and ²³⁹Pu account for 68.1% and 31.4% of the total activity respectively with ²³⁴U and ²³⁰Th comprising the remaining 0.5%. The average percentage is calculated by summing the percent contribution of each isotope for each vector, and then dividing by the number of vectors. Mathematically, this is:

$$\frac{\sum_{i=1}^{N_{SI}} EPA_{ISO_i}}{N_{SI}} = \bar{P} \tag{3}$$

where EPA_{ISO_i} is the 10,000 year activity for a particular isotope, EPA_{T_i} is the 10,000 year total activity (including ²³⁸Pu), N_{SI} is the number of screened in vectors, \bar{P} is the average percentage of the total, and the i summation indicates the values are summed across all screened-in vectors. The releases in EPA units for each isotope and the total release are shown in Figure 3.

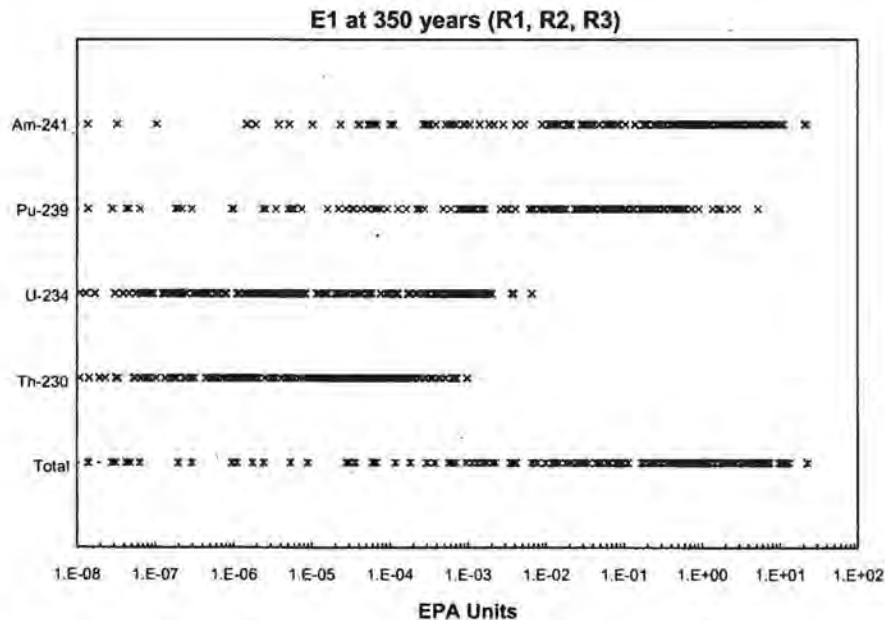


Figure 3 – Normalized Cumulative Release (EPA Units) to the Culebra from the borehole for each isotope and the total for Scenario 2: Borehole intrusion into the Castile brine pocket at 350 years.

4.3.3. 1000 Year E1 Intrusion – S3

The time difference between S2 and S3 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 S3 are highly influenced by the conditions in the pressurized Castile brine pocket and thus we see that S3 has similar characteristics to the S2 scenario, although the number of screened vectors and the maximum activities are slightly less.

Like S2, the only pathway with any activity is through the borehole. No activity was shown in the marker beds or the shaft for any of the vectors. The time series plots for each isotope, vector, and replicate are shown in Figure 13, Figure 14, and Figure 15. As can be seen in the figures, and like the S2 scenario, the releases for the S3 takes place over a short period of time. The maximum activity for any isotope occurred in RIS3v091, which showed an integrated activity of 4.84 EPA units for ^{241}Am . For ^{239}Pu , vector R3S3v028 showed the maximum with an integrated activity of 4.94 EPA units. ^{234}U and ^{230}Th were comparatively minor with maximums for each of 0.00591 and 0.00086 showing in vector R2S3v009. On the average, ^{241}Am and ^{239}Pu account for 48.24% and 50.87% of the total activity respectively with ^{234}U and ^{230}Th comprising the remaining 0.89%. The releases in EPA units for each isotope and the total release are shown in Figure 4.

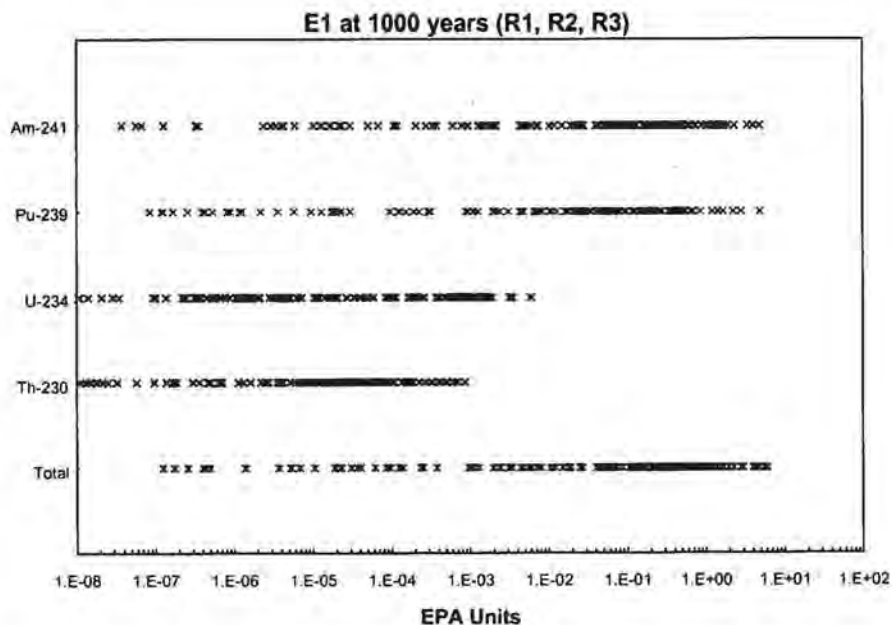


Figure 4 – Normalized Cumulative Release (EPA Units) to the Culebra from the borehole for each isotope and the total for Scenario 3: Borehole intrusion into the Castile brine pocket at 1000 years.

The difference in the activity distribution between the S2 and S3 scenarios is attributed to the time lag for the S3 intrusion. At early times, the release tends to be dominated by Am-241, 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.

4.3.4. 350 Year E2 Intrusion – S4

For most vectors associated with an E2 intrusion, BRAGFLO predicts nonzero or very little brine flow from the repository to the Culebra. All other pathways are zero or minimal. Figure 16, Figure 17, and Figure 18 show the time-series plots for each vector across all replicates. Since the E2 releases are not dominated by a physical process like the brine pocket pressure release associated with an E1 intrusion, the plots appear more 'disorganized' in that the standard deviation of the release times is much higher. This also creates a difference in the distribution of the contribution to the total activity. On the average, ^{241}Am contributes 33.16% to the total and ^{239}Pu contributes 66.50%. Like the S3 scenario, this is due to the longer time periods associated with the transport process in the E1 intrusion scenarios. The maximum activities for ^{241}Am , ^{239}Pu , ^{234}U , and ^{230}Th are 2.58, 0.172, 0.000149, and 0.0000328 EPA units, respectively. The releases in EPA units for each isotope and the total release are shown in Figure 5.

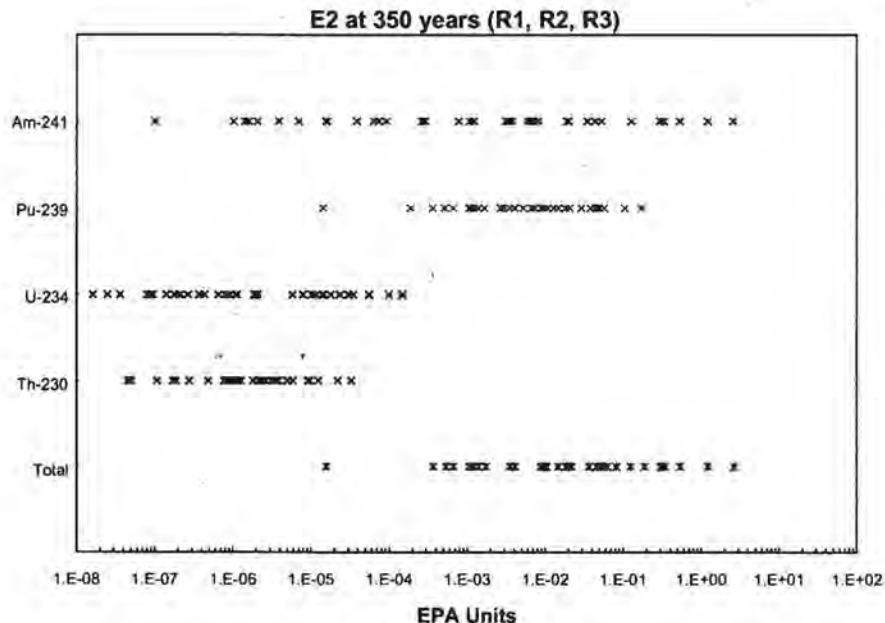


Figure 5 – Normalized Cumulative Release (EPA Units) to the Culebra from the borehole for each isotope and the total for Scenario 4: Borehole intrusion into the repository at 350 years.

4.3.5. 1000 year E2 Intrusion – S5

Like the 350 year E2 intrusion, the 1000 year intrusion 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.

Figure 19, Figure 20, and Figure 21 show the time-series plots for each vector across all replicates. Again, the plots appear more 'disorganized' than the E1 intrusion plots. For S5, ^{241}Am contributes 17.92% to the total and ^{239}Pu contributes 81.69%. The 1000 year intrusion time allows for more decay of the ^{241}Am and shift to a higher percentage of the total for ^{239}Pu . The maximum activities for ^{241}Am , ^{239}Pu , ^{234}U , and ^{230}Th are 0.074, 0.141, 0.000138, and 0.00003 EPA units, respectively. The releases in EPA units for each isotope and the total release are shown in Figure 6.

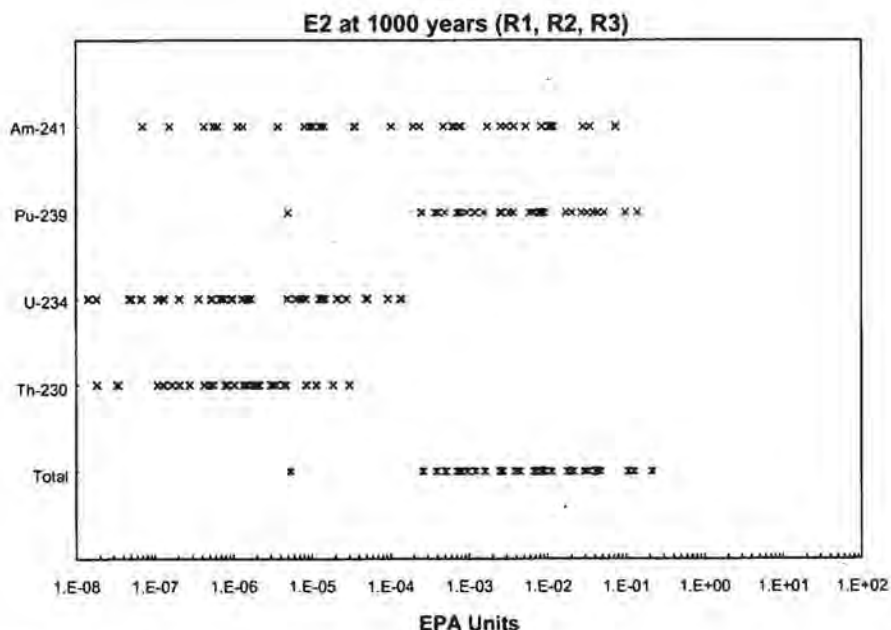


Figure 6 – Normalized Cumulative Release (EPA Units) to the Culebra from the borehole for each isotope and the total for Scenario 5: Borehole intrusion into the repository at 1000 years.

4.4. 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 5 shows the maximum normalized release in EPA units for each scenario/intrusion time combination. Note that the total activity also includes a small contribution from ^{238}Pu , which is not listed for reasons discussed above. The time series plots for each isotope at each time/vector/replicate combination are presented in Appendix H.

Combining the ISO and TI runs into one figure, the domination ^{241}Am and ^{239}Pu in relation to the total activity is clearly seen (Figure 7). The decay of ^{241}Am is evident in the straight line decrease in activity over time on the logarithmic y-axis. The differential between the E1 intrusions (solid lines) and the E2 intrusions (dashed lines) can also be seen

As the time of intrusion increases, the number of vectors showing a zero release also increases. The increase in zero release vectors with increasing intrusion time is approximately linear, as illustrated in Figure 8. Extrapolating forwards, this indicates that for an E1 intrusion, approximately 12.9% of the screened in vectors will show zero release for intrusions at 10,000 years. For the E2 intrusion, no vectors will show a release if an intrusion occurs after about 9440 years.

Table 5 – Maximum normalized release (EPA units) of each isotope at the Borehole/Culebra interface at each time interval of intrusion. Note that the total activity also includes a small contribution from ^{238}Pu , which is not listed for reasons discussed above.

	Am-241	Pu-239	U-234	Th-230	Total
E1 – 100 yrs	2.80E+01	5.34E+00	6.64E-03	9.82E-04	2.90E+01
3000 yrs	5.42E-01	4.12E+00	5.52E-03	9.19E-04	4.15E+00
5000 yrs	4.80E-02	3.29E+00	5.01E-03	9.55E-04	3.29E+00
7000 yrs	2.96E-03	2.46E+00	4.33E-03	9.64E-04	2.46E+00
9000 yrs	7.28E-04	1.33E+00	2.80E-03	1.05E-03	1.33E+00
E2 – 100 yrs	2.93E+00	1.79E-01	1.55E-04	3.39E-05	2.99E+00
3000 yrs	5.10E-03	8.93E-02	9.65E-05	2.11E-05	9.11E-02
5000 yrs	4.53E-04	4.03E-02	5.50E-05	1.20E-05	4.05E-02
7000 yrs	2.16E-05	2.72E-02	1.45E-05	3.13E-06	2.72E-02
9000 yrs	3.02E-07	1.19E-02	1.30E-06	2.04E-07	1.19E-02

^{241}Am shows the highest maximum activity (28.0 EPA units) of all the isotopes across all ISO and TI runs for a 100 year intrusion and is the isotope with the highest release for 45 of the 185 screened in vectors for the 100 year intrusion time across all replicates. For a 350 year intrusion, ^{241}Am is highest in 14 vectors. For intrusion times greater than 350 years, ^{239}Pu shows the highest activity across all replicates. In terms of the average percentage of total activity, ^{239}Pu provides the highest contribution for all intrusion times with the exception of an E1 intrusion at 100 years, where ^{241}Am is the highest. As mentioned above, this is due to the decay of ^{241}Am combined with the long half-life of ^{239}Pu . For those vectors where brine outflow from the repository was large at small time, ^{241}Am is the dominant isotope. This trend is listed numerically in Table 6.

5. Sensitivity Analysis

Sensitivity analysis allows for determining which input parameters have the most influence on the output of a model. Here we present the results of several types of analysis that help determine the most influential parameters. By understanding which parameters are most influential to the model output, one can determine the main source of uncertainty as well as where to concentrate future efforts to help reduce that uncertainty.

A good tool for examining the relationship between model inputs and model outputs is regression analysis. In this approach, a model of the form

Table 6 – Percentage of total activity after 10,000 years for each isotope. The percentages for the E1-100 and 350 year scenarios do not add to 100% due to a small contribution from ²³⁸Pu.

	Am-241	Pu-239	U-234	Th-230
E1-100 yrs	68.60%	30.64%	0.29%	0.17%
350 yrs	68.09%	31.39%	0.26%	0.15%
1000 yrs	48.24%	50.87%	0.24%	0.65%
3000 yrs	9.49%	89.92%	0.48%	0.11%
5000 yrs	1.61%	97.45%	0.73%	0.21%
7000 yrs	0.46%	98.23%	1.06%	0.26%
9000 yrs	0.25%	98.42%	1.17%	0.16%
E2-100 yrs	34.63%	65.01%	0.28%	0.05%
350 yrs	33.16%	66.50%	0.29%	0.05%
1000 yrs	17.92%	81.69%	0.34%	0.05%
3000 yrs	4.25%	95.34%	0.36%	0.06%
5000 yrs	1.00%	98.66%	0.28%	0.06%
7000 yrs	0.21%	99.48%	0.28%	0.03%
9000 yrs	0.05%	99.76%	0.17%	0.02%

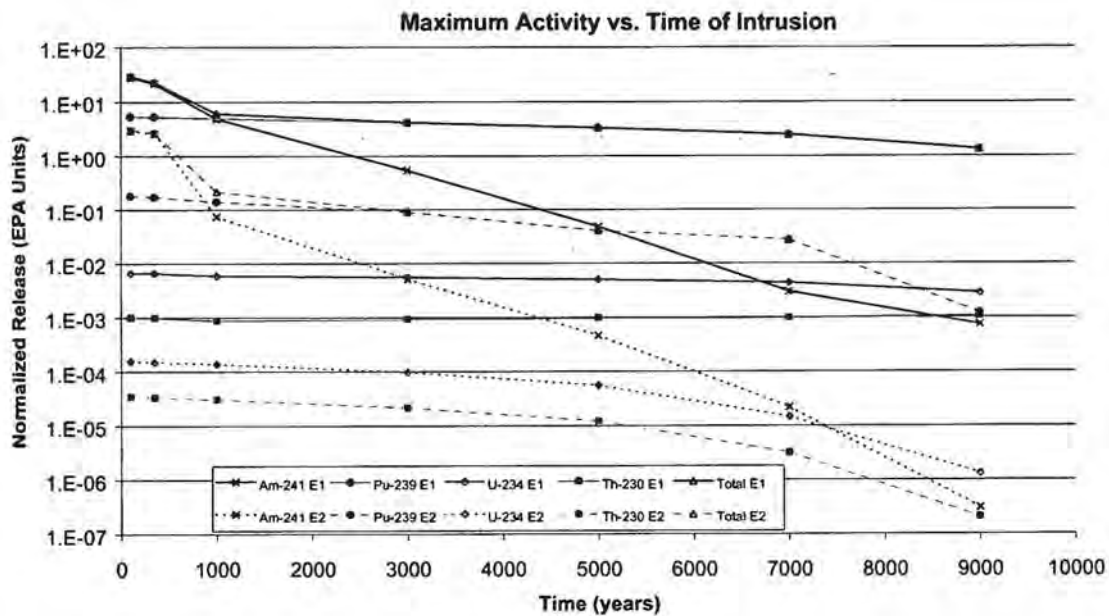


Figure 7 – Cumulative activity in EPA units after 10,000 years versus intrusion time. Each data point represents the maximum cumulative activity across all replicate/vector combinations.

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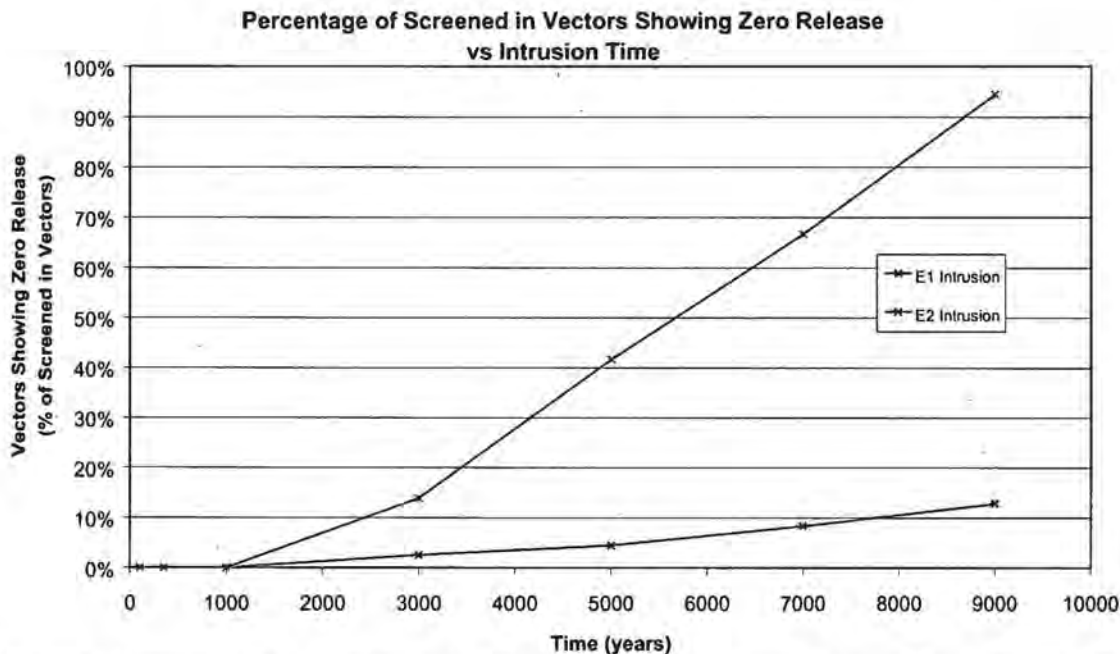


Figure 8 – Percentage of screened-in vectors showing zero release versus intrusion time. For the E1 intrusion at 100 and 350 years, there are 185 total screened in vectors; for 1000 plus years, 157 vectors. For the E2 intrusion, 37 vectors were screened-in for the 100 and 350 year intrusion and 38 screened-in for the balance of intrusion times.

$$y = b_0 + \sum_{j=1}^n b_j x_j \quad (4)$$

is developed where y is the model output parameter (dependent variable), x_j are the model input parameters (independent variables), b_j are the coefficients that must be determined, and n is the number of independent variables included in the model. The coefficient b_0 is the dependent variable intercept. For cases where the independent variables are uncorrelated, the coefficients, b_j , can be used to indicate the importance of the independent variables with respect to the dependent variable.

When many independent variables are involved, as is the case here, the inclusion of all of them is not necessarily needed nor desired. Typically, only a relatively few number of independent variables are needed to produce a satisfactory regression model. In addition, if some of the independent variables are correlated, this can render the regression coefficients unstable and result in the inability to determine the most sensitive parameters. Here, the variable pairs [BPPRM, BPCOMP], [HALPRM, HALCOMP], and [ANHPRM, ANHCOMP] show a -0.732, -0.987, and -0.937 correlation, respectively. These three pairs refer to the permeability and compressibility of the Castile, Salado (Halite), and Anhydrite material.

To circumvent these issues, three steps are taken in this regression analysis. First is the use of stepwise regression rather than multiple regression described by equation 4. With stepwise regression, a sequence of regression models is constructed; with each model adding the single input variable that has the largest impact on the uncertainty of the

output (i.e. the variable that has the highest correlation with the output). Thus, the first regression model will be of the form:

$$y = b_0 + b_1x_1 \quad (5)$$

where x_1 is the input variable that has the highest correlation with y . The second regression model is:

$$y = b_0 + b_1x_1 + b_2x_2 \quad (6)$$

where x_2 is the input variable that accounts for the balance of the uncertainty in y not explained by x_1 . Construction of the regression model continues in this manner until a user defined point of diminishing return is reached, usually determined by the use of the t -test. An explanation of the stepwise regression and the independent variable selection criteria as applied to the CCA is given in Helton et al. (1998).

The second step in determining parameter sensitivity is to perform a rank transformation of the input and output parameters prior to conducting the stepwise regression. A rank transformation ranks each value of a parameter based on its magnitude in relation to the other instances of that parameter. Thus, for each parameter, the vector with the lowest value is given a value of '1', the next highest vector a value of '2', and so on. This is done across all replicate/vector combinations. The benefit of performing the rank transformation is it helps reduce any non-linearity effects that may exist between the independent variables and the dependent variables. It also helps with the inclusion of 'flag-type' parameters. Flag-type parameters are parameters whose value has no physical basis or are not directly utilized as model input. The input parameter, ANHBCVGP, which determines the relative permeability model for the South Marker Bed 139, is an example of this.

We do not include those independent variables that are highly correlated with other independent variables. As mentioned, there are only three pairs that fall into this category, [BPPRM, BPCOMP], [HALPRM, HALCOMP], and [ANHPRM, ANHCOMP]. For this analysis, the variables BPCOMP, HALCOMP, and ANHCOMP are not included. In addition, the variable BPINTPRS, which is the brine pocket internal pressure, is not included for the E2 intrusion scenarios since the brine pocket is not modeled in these cases.

To help increase the accuracy of the regression, all three replicates are grouped as one. This provides a longer record for describing the independent/dependent variable relationship. Thus, unless otherwise noted, all stats for this section are based on the entire replicate/vector group. Each scenario is separately modeled.

5.1. Stepwise Regression

The dependent variable used for this regression analysis is the total integrated flux after 10,000 years in EPA units in the borehole at the Culebra interface. The integrated flux refers to the total integrated activity after the 10,000-year modeling time.

Both the E1 and E2 disturbed scenarios are examined; the E1 at two different intrusion times of 350 and 5000 years and the E2 at 350 years. The file-names of the files included in the analysis are given in Table 7. For E2 intrusions greater than 350 years as well as

for the undisturbed scenario (S1), there are an insufficient number of data points to provide a meaningful analysis. Two times are chosen for the E1 intrusion to help determine if the sensitivity of the model changes with time of intrusion. The regressed scenarios are referred to as Case 1 (E1 intrusion at 350 years), Case 2 (E1 intrusion at 5000 years), and Case 3 (E2 intrusion at 350 years).

Table 7 – File names for inclusion in the regression analysis, located in CMS library LIBCRA1_SUM. 'Rx' indicates all three replicate files are used for the regression.

Time	E1	E2
350 years	SUM_NUT_CRA1_Rx_S2.TBL	SUM_NUT_CRA1_Rx_S4.TBL
5000 years	SUM_NUT_CRA1_Rx_S3_T5000.TBL	NA

Table 8 lists the most influential dependent variables, their associated coefficients, and the R^2 value indicating the goodness of fit for a four-step regression for each Case. Figure 9 shows the regression model output versus the NUTS output data, providing a visual comparison of how well the regression model fits the transformed data.

Table 8 – Stepwise regression analysis on rank-transformed data for selected scenarios across all replicates.

	β_0	Var ₁	β_1	Var ₁	β_2	Var ₁	β_3	Var ₁	β_4
Case 1	10.936	BHPERM	0.973	BPINTPRS	0.174	WGRCOR	-0.144	WMICDFLG	-0.209
R^2			80.75		83.11		84.89		86.13
Case 2	-2.498	BHPERM	0.924	BPINTRS	0.124	WGRCOR	-0.082	SHUPRM	0.065
R^2			79.23		80.6		81.30		81.7
Case 3	4.112	BHPERM	0.58	WRGSSAT	0.30	SHUPRM	-0.25	HALPRM	0.25
R^2			43.36		50.66		54.65		60.10

The parameter BHPERM has the greatest influence over the amount of release in the borehole at the Culebra interface for all three cases. BHPERM is the permeability of the borehole and shows a strong positive correlation with the total activity. It explains 80.75%, 79.23 and 43.36% of the variability in the output variable for Case 1, 2, and 3, respectively. A higher permeability in the borehole leads to a more open pathway for migration of brine into the repository and the subsequent migration of radioisotopes out of the repository, so this relationship is expected.

For Cases 1 and 2, the second most influential parameter is BPINTPRS. BPINTPRS is the Castile brine-pocket internal pressure. An increase in this value results in higher brine flows into the repository when the brine pocket is penetrated in the E1 intrusions, leading to a higher ability to mobilize contaminants. The third most influential parameter for Cases 1 and 2 is WGRCOR. WGRCOR is the corrosion rate of steel. Steel in this context refers to the steel in the containers and within the waste. Both Cases show a slight negative correlation because steel corrosion consumes brine and produces gas, resulting in higher pressures and lower brine inflow. Both the increased consumption of brine and the decreased brine inflow results in lower saturations and thus a lower ability to mobilize radioisotopes. WGRCOR becomes less influential with time because the source of steel is consumed resulting in lower gas production and brine consumption. In

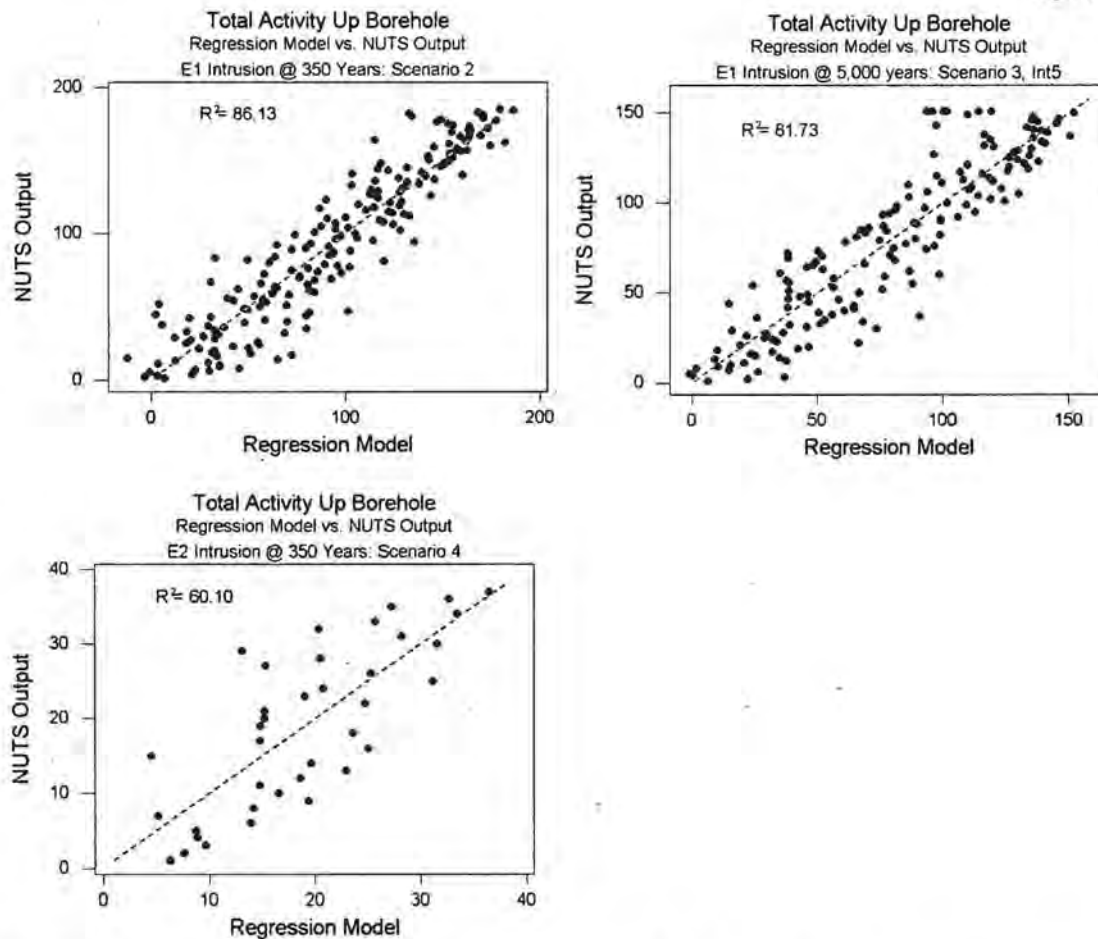


Figure 9 – Nuts output versus regression model results for an E1 intrusion at 350 and 5000 years and an E2 intrusion at 350 years.

comparison to BHPERM, BPINTPRS and WGRCOR have relatively minor influence accounting for approximately 2% each of the total variability.

The second most influential parameter for Case 3 is WRGSSAT. WRGSSAT is the residual gas saturation level in the waste emplacement area. WRGSSAT is able to explain approximately 7.3% of the output variability. The third most influential parameter is SHUPRM, which is the permeability of the upper shaft. There is a slight negative correlation to this parameter since an increase in the shaft permeability will lower pressures in the repository before an intrusion would occur, and result in lower releases. Overall, the fit for the E2 scenario accounts for 60.10% of the total variability.

The sensitivity parameters are all BRAGFLO input variables and control the flow of brine into and out of the repository. For that reason, the reader is directed to Stein and Zelinski (2003) for further discussion.

6. Summary

This analysis package describes the transport calculations that are part of the "Salado Flow and Transport Calculations for the Compliance Recertification Application (CRA)

of the Waste Isolation Pilot Plant (WIPP)" as described in Analysis Plan AP-99 (Stein, 2003a). Specifically, it covers the calculations to determine the mobilization and subsequent migration of radioisotopes throughout the repository, shaft system, Salado formation, and possible human intrusion boreholes. These calculations are part of the Performance Assessment (PA) that estimates releases from the repository for the regulatory period of 10,000 years after closure, which is required for the CRA.

To represent possible future states of the repository and to predict possible releases through the Salado, six modeling scenarios are defined. The six scenarios are:

- **S1:** Undisturbed performance (no human intervention or intrusion into the repository during 10,000 years)
- **S2:** An intrusion borehole at 350 years that penetrates both the repository and an underlying pressurized brine reservoir in the Castile formation (E1-type intrusion)
- **S3:** An intrusion borehole at 1000 years that penetrates both the repository and an underlying pressurized brine reservoir in the Castile formation (E1-type intrusion)
- **S4:** An intrusion borehole at 350 years that penetrates the repository but does not encounter a pressurized brine reservoir (E2-type intrusion)
- **S5:** An intrusion borehole at 1000 years that penetrates the repository but does not encounter a pressurized brine reservoir (E2-type intrusion)
- **S6:** A multiple intrusion scenario, which includes an E2 intrusion followed by and E1 intrusion at a later date

Scenario S6 is addressed in a separate analysis (Garner, 2003) and is not discussed in this report.

To address the uncertainty in many of the input parameters used in the PA calculations, three replicates of 100 sets of Latin Hypercube sampled parameters (each unique set is called a vector) are defined. The analysis is composed of three types of modeling runs: the screening runs, the ISO runs, and the TI runs. The screening runs are used to screen out those vectors that have no possibility of radioactive release to the accessible environment. This is accomplished by performing transport simulations on all vectors using a continuous 1 kg/m^3 source of a conservative tracer as the contaminant and calculating the cumulative mass crossing into the accessible environment. Those vectors that show cumulative mass greater than $1 \times 10^{-7} \text{ kg}$ are 'screened-in' and are used for the more detailed ISO and TI runs.

Unlike the screening runs, the ISO and TI runs (ISO refers to isotope runs and TI refers to time-intrusion runs) model specific isotopes and decay chains. To help reduce computational overhead the possible isotopes and decay chains were 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 are combined in ways that introduce little or no loss of release information in terms of normalized "EPA units". EPA units are a relative unit that is proportional to the ratio of the cumulative release of an isotope to the release limit for that isotope. Combinations of similar isotopes are referred to as 'lumped isotopes'. This

analysis models 5 lumped isotopes: ^{241}Am , ^{238}Pu , ^{239}Pu , ^{234}U , and ^{230}Th . ISO runs are performed on scenarios S1 through S5 and directly utilize the 350 and 1000 year intrusion time flow-fields from the brine and gas flow code, BRAGFLO (Stein and Zelinski, 2003). The TI runs are used to examine the sensitivity of the results to different borehole intrusion times. Intrusion times of 100, 3000, 5000, 7000, and 9000 years are modeled in the TI runs using 'time-shifted' flow-field inputs from BRAGFLO. Time shifting means applying a flow-field based on one intrusion time to a different intrusion time by extending or shortening the pre-intrusion condition as necessary. This prevents the need of re-running the computationally intensive flow model for each intrusion time. Justification for this approach is discussed in section 2.4.3.

The transport and decay of radionuclides are calculated using the computer code NUTS (NUclide Transport System), version 2.05a. NUTS is a five-point finite difference code designed to model multi-dimensional, multi-component, and radioactive-contaminant transport. The key processes modeled here are advective transport, decay, precipitation, solubility limits, and interior sources, all in a single porosity, continuous matrix. No dispersion is modeled.

Three potential pathways for migration of radioisotopes in dissolved brine are considered in this analysis. The first, and the most important pathway, is a human intrusion into and possibly 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.

The dynamics of the brine movement are complex and highly dependent on the BRAGLO input parameters. Initially, brine may flow into the repository from anyone 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. Brine may be consumed by the oxidation of ferrous material in the waste containers and the waste itself, which has an effect on the solubility of the radioisotopes.

The screening runs produced 415 'screened-in' vectors out of a possible 1500 (three replicates of 100 vectors across 5 scenarios). Results of the ISO and TI runs show that there is effectively no releases out the marker beds or up the shaft. The only release for either of these two pathways was found in scenario S1, where only a trivial amount of activity was detected in the marker beds (total activity of 2.89×10^{-15} EPA units) and no activity indicated at the shaft/Culebra interface.

The E1 intrusions (S2 and S3) produced the highest releases, with a maximum total activity at the borehole/Culebra intersection of 28.26 EPA units occurring with a 100 year intrusion time. For perspective, the average for all vectors at the 100 year intrusion time is 1.42 EPA units and the median is 0.237 EPA units. No releases are predicted in the

marker beds for the E1 intrusions, and a maximum total activity at the shaft/Culebra intersection was calculated to be 8.74×10^{-23} EPA units. As the intrusion time increases, the maximum total release tends to decrease. For example, at an intrusion time of 5000 years, the maximum total activity for an E1 intrusion is predicted to be 2.89 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 2.12 EPA units (100 year intrusion time). This too declines with increasing intrusion times, with 0.049 EPA units predicted at a 5000 year intrusion time. Like the other scenarios, little or no activity is predicted in the marker beds or at the shaft/Culebra intersection.

For all scenarios, the permeability in the borehole is the parameter most strongly correlated with the total activity at the borehole/Culebra interface. For the E1 intrusions, this correlation is quite strong, accounting for over 80% of the output variability at the 350 year intrusion time. However, the correlation becomes less pronounced (43.36%) for the E2 intrusions. This is due to the E2 intrusion being more reliant on brine inflow into the repository prior to borehole penetration. With an E1 penetration, brine is supplied directly from the Castile brine pocket, meaning other sources of brine are not as important. Scenarios 2 and 3 (E1 intrusion) are secondarily sensitive to the brine pocket pressure (BPINTPRS) showing a positive correlation to this parameter. Scenarios 4 and 5 (E2 intrusion) are secondarily sensitive to the residual gas saturation in the waste emplacement area, also showing a positive correlation.

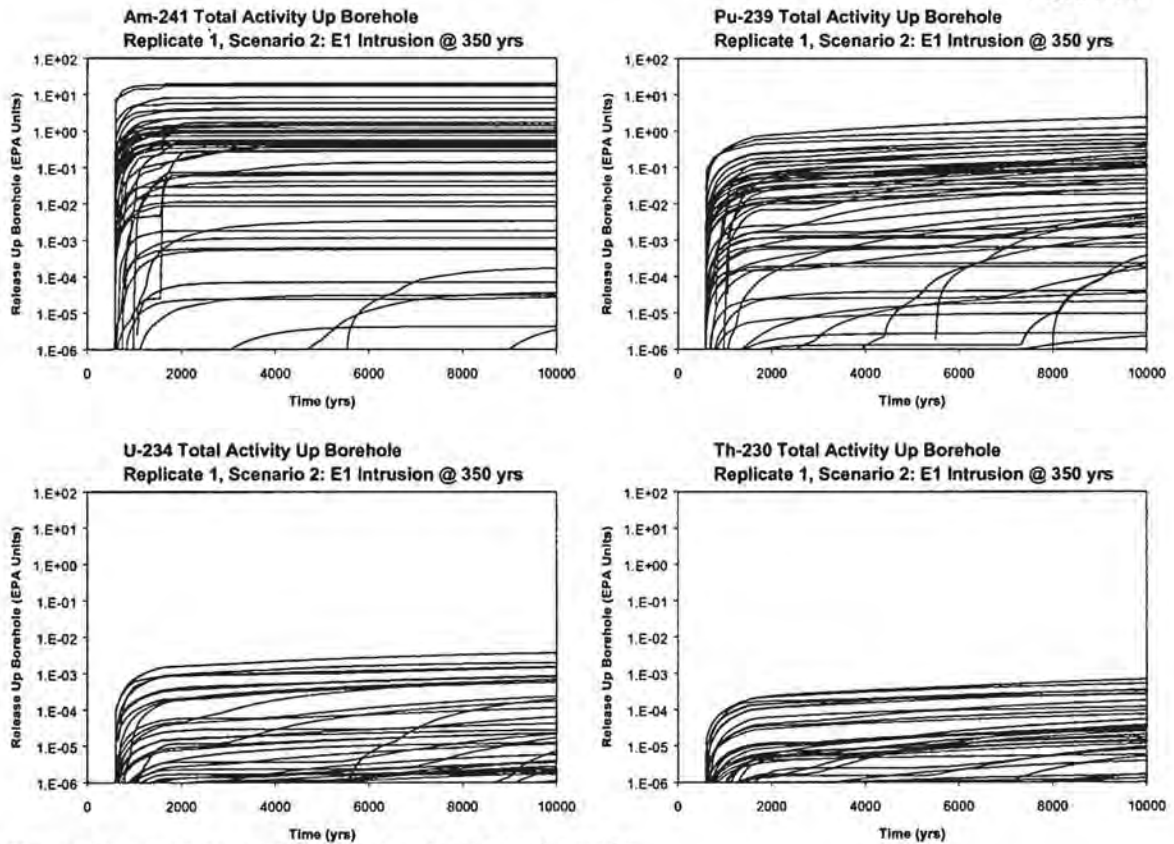


Figure 10 – Activity up borehole in EPA Units for R1S2.

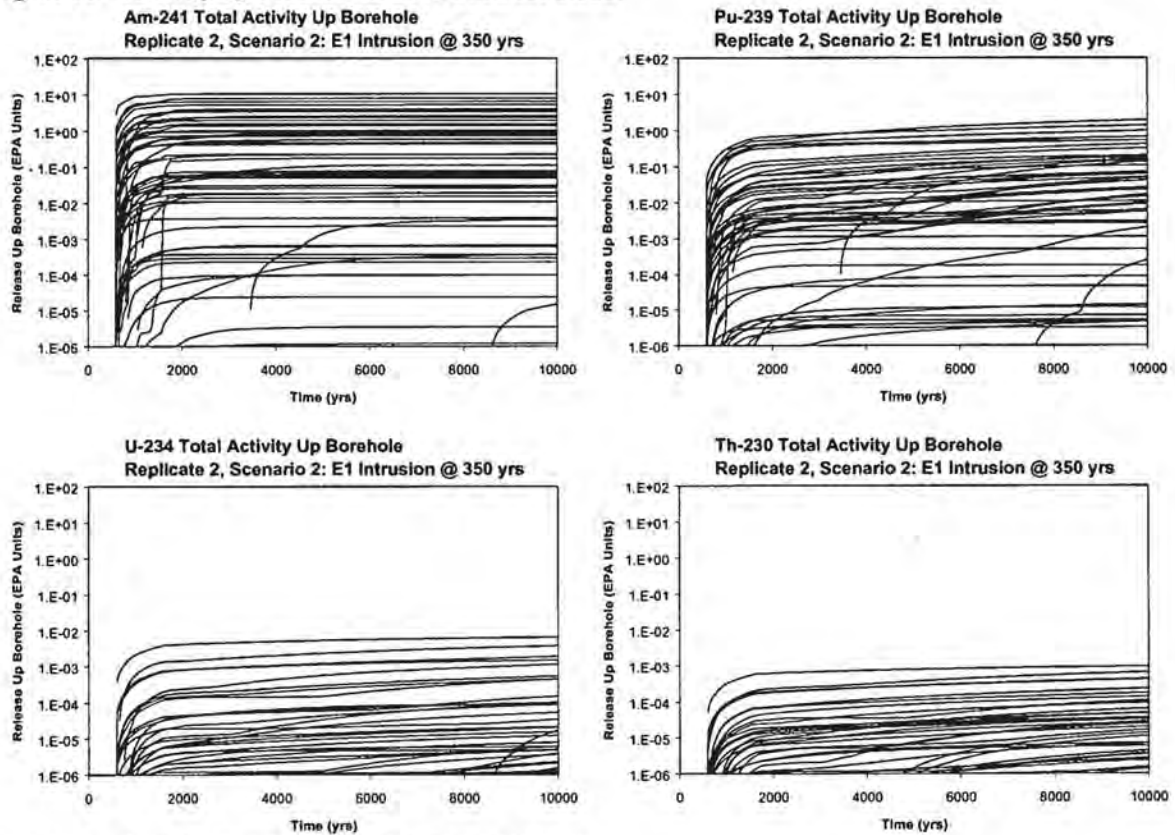


Figure 11 – Activity up borehole in EPA Units for R2S2.

Information Only

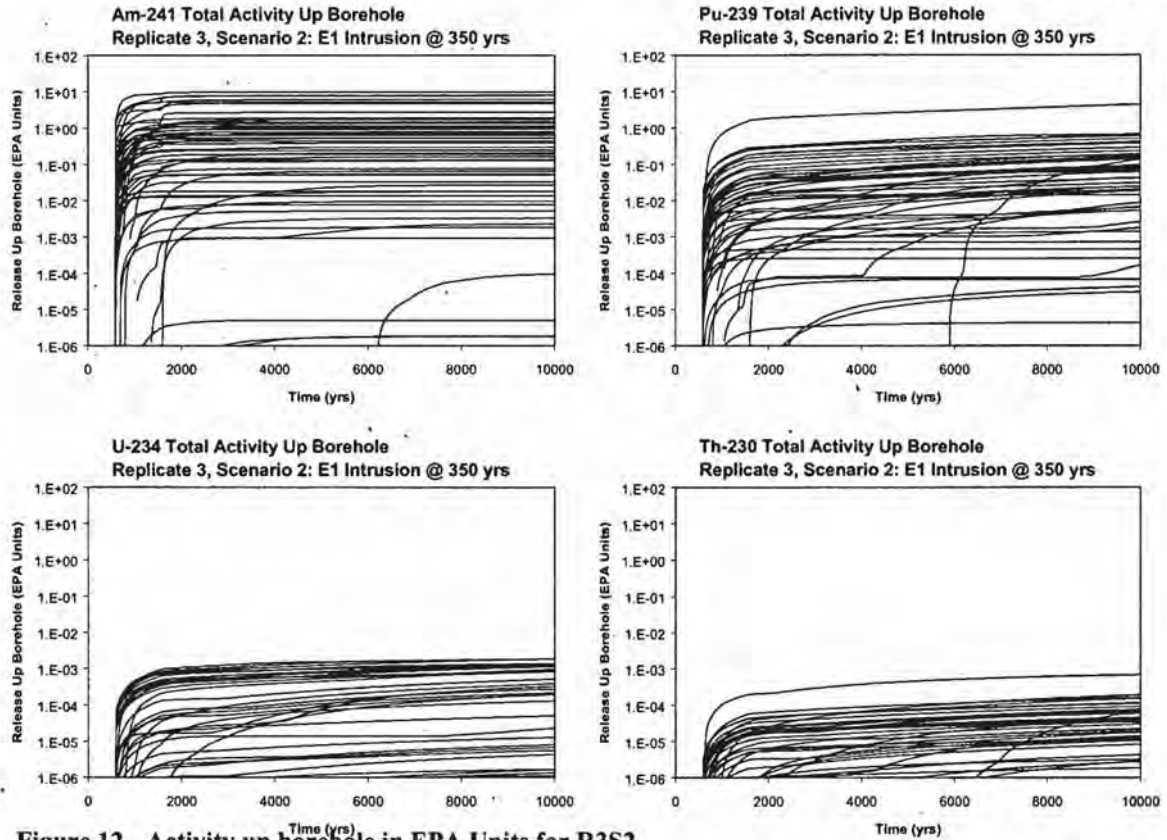


Figure 12 - Activity up borehole in EPA Units for R3S2.

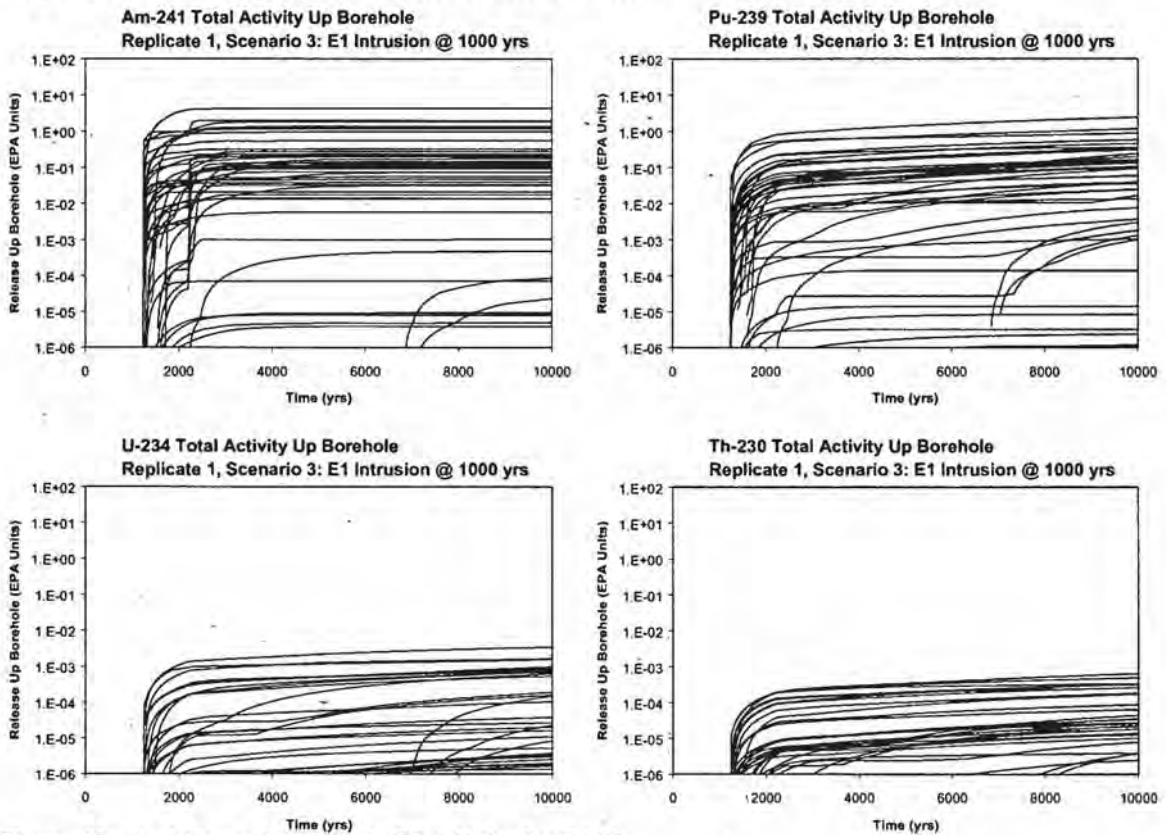


Figure 13 - Activity up borehole in EPA Units for R1S3.

Information Only

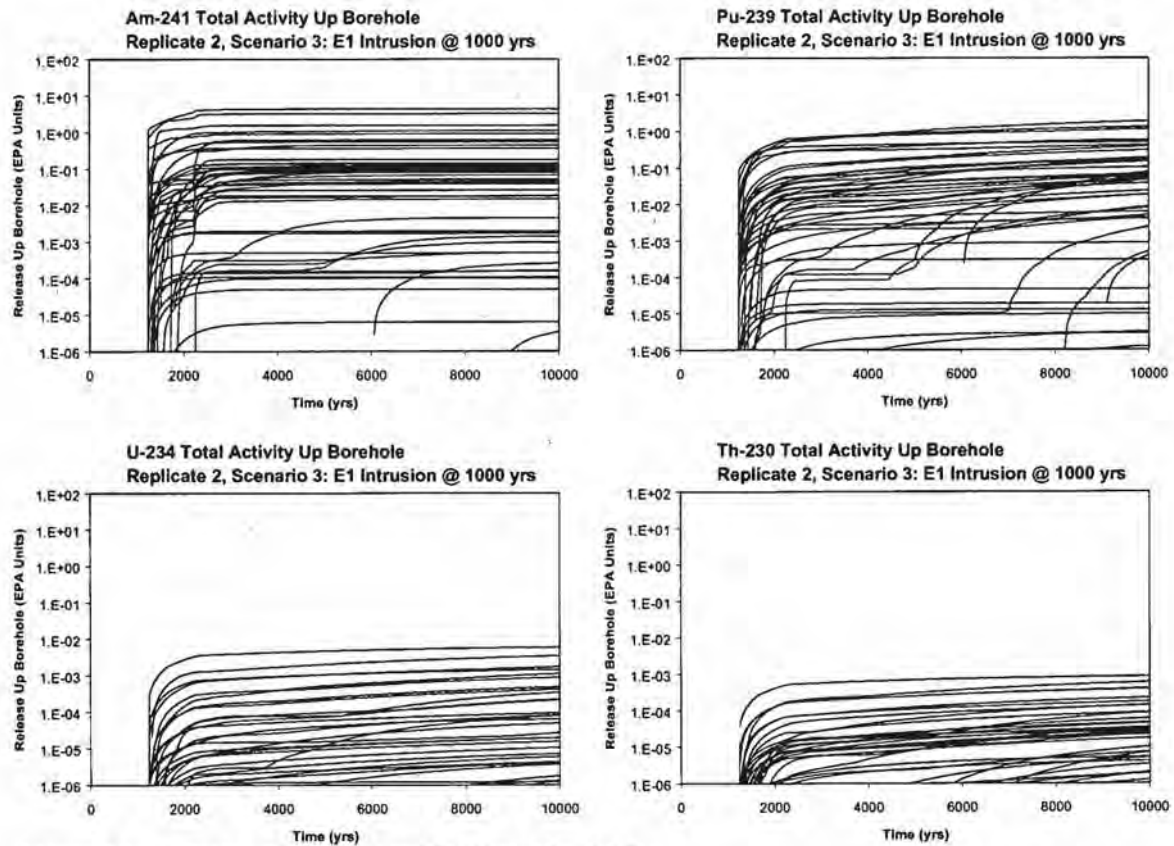


Figure 14 - Activity up borehole in EPA Units for R2S3.

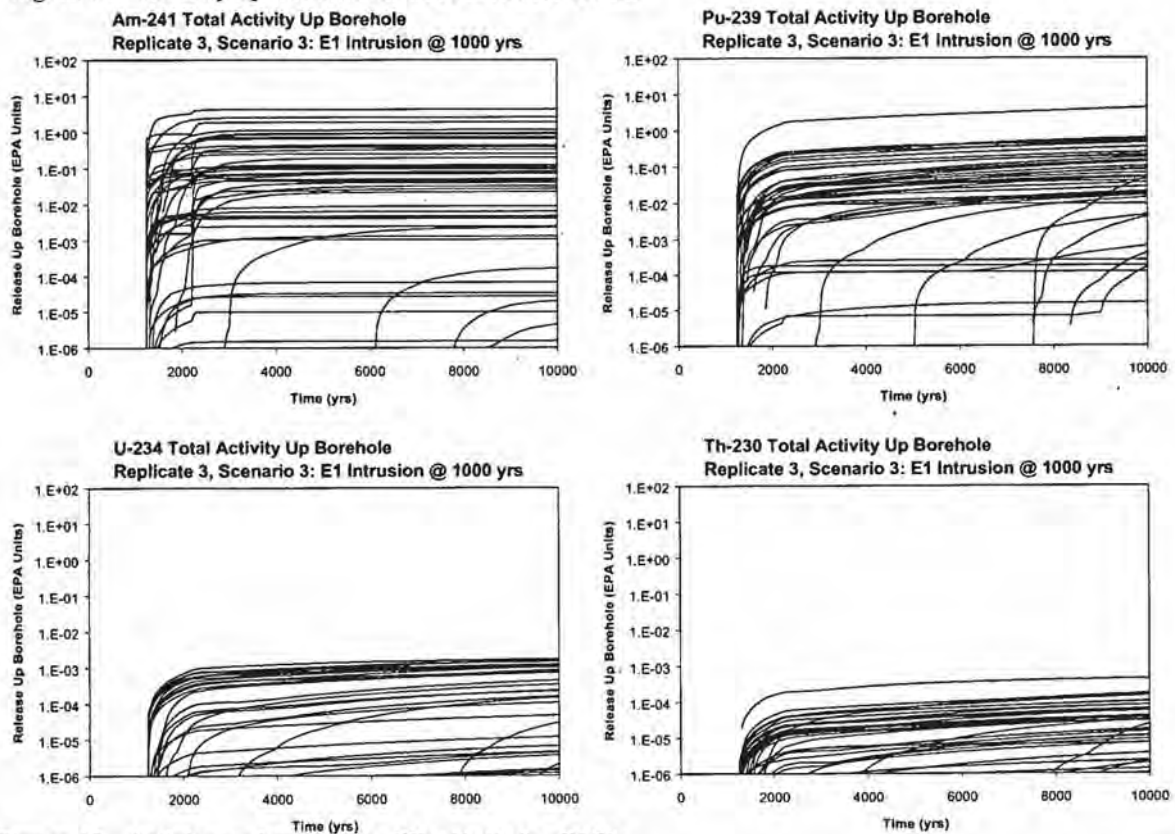


Figure 15 - Activity up borehole in EPA Units for R3S3.

Information Only

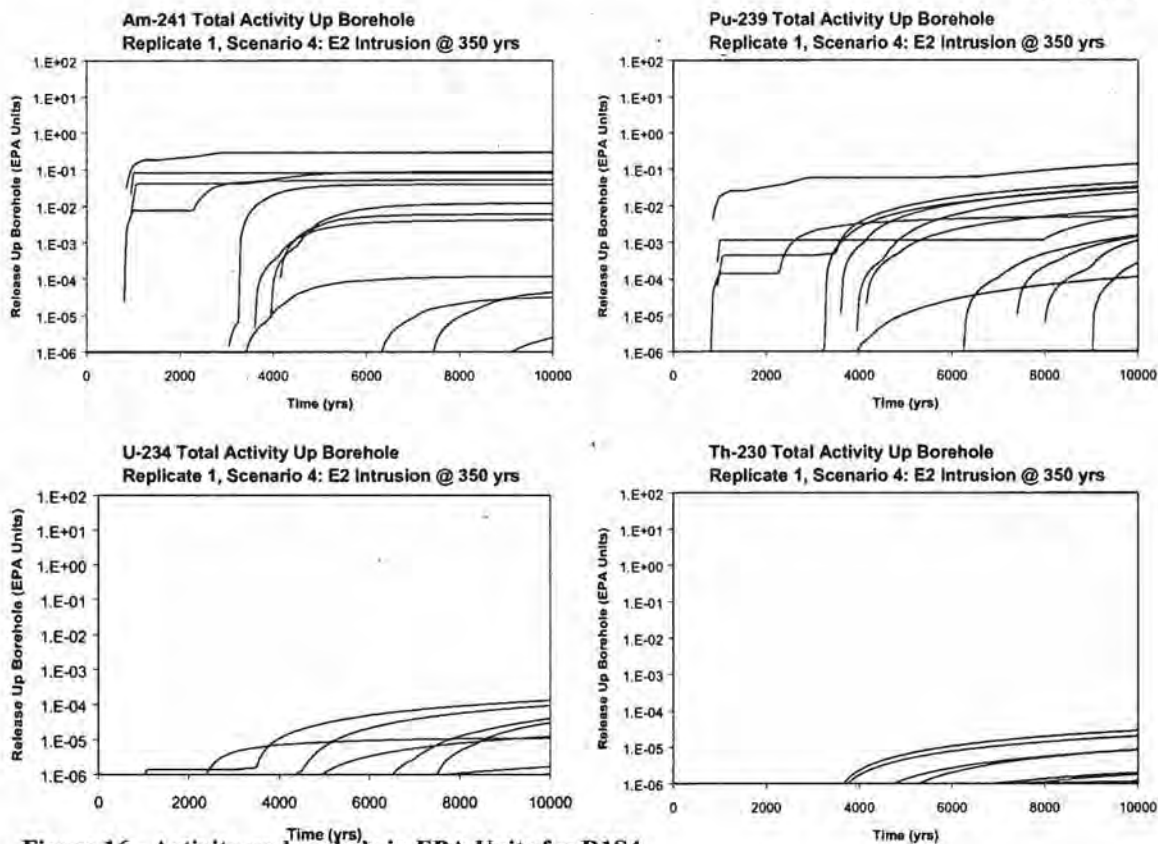


Figure 16 - Activity up borehole in EPA Units for R1S4.

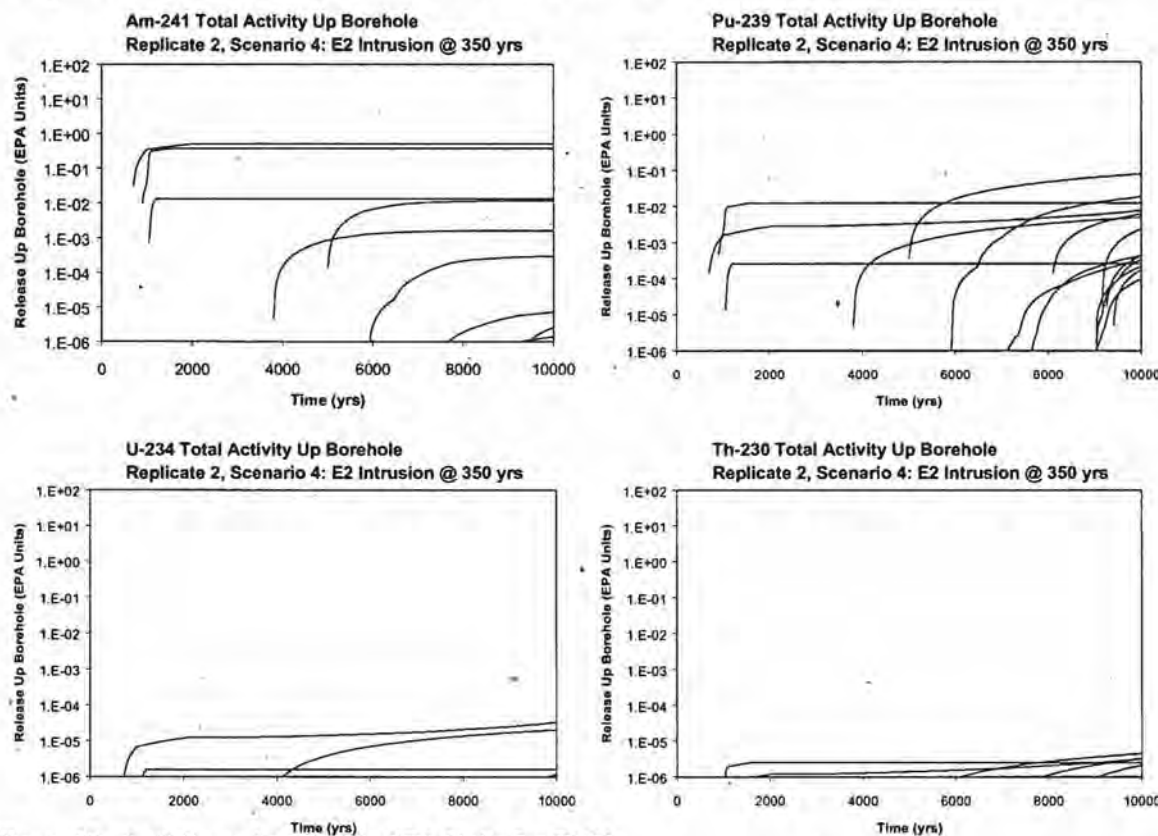


Figure 17 - Activity up borehole in EPA Units for R2S4.

Information Only

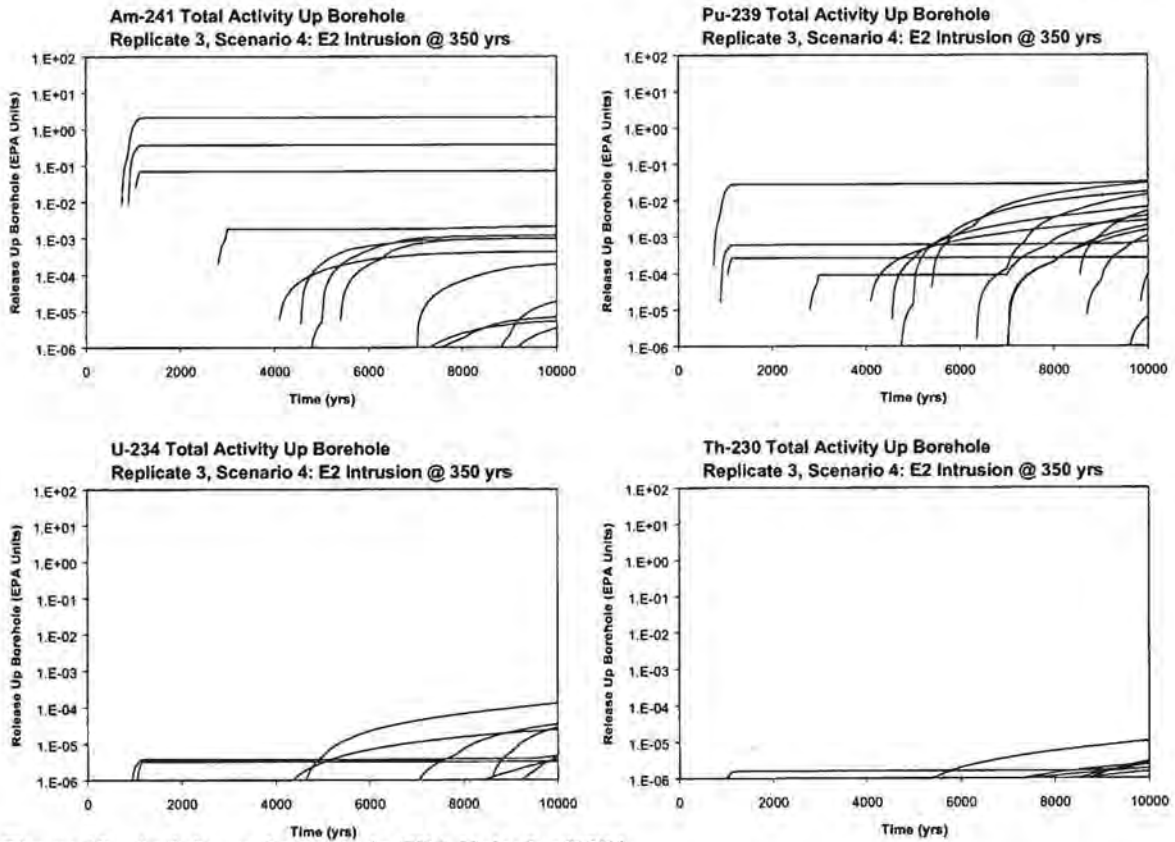


Figure 18 - Activity up borehole in EPA Units for R3S4.

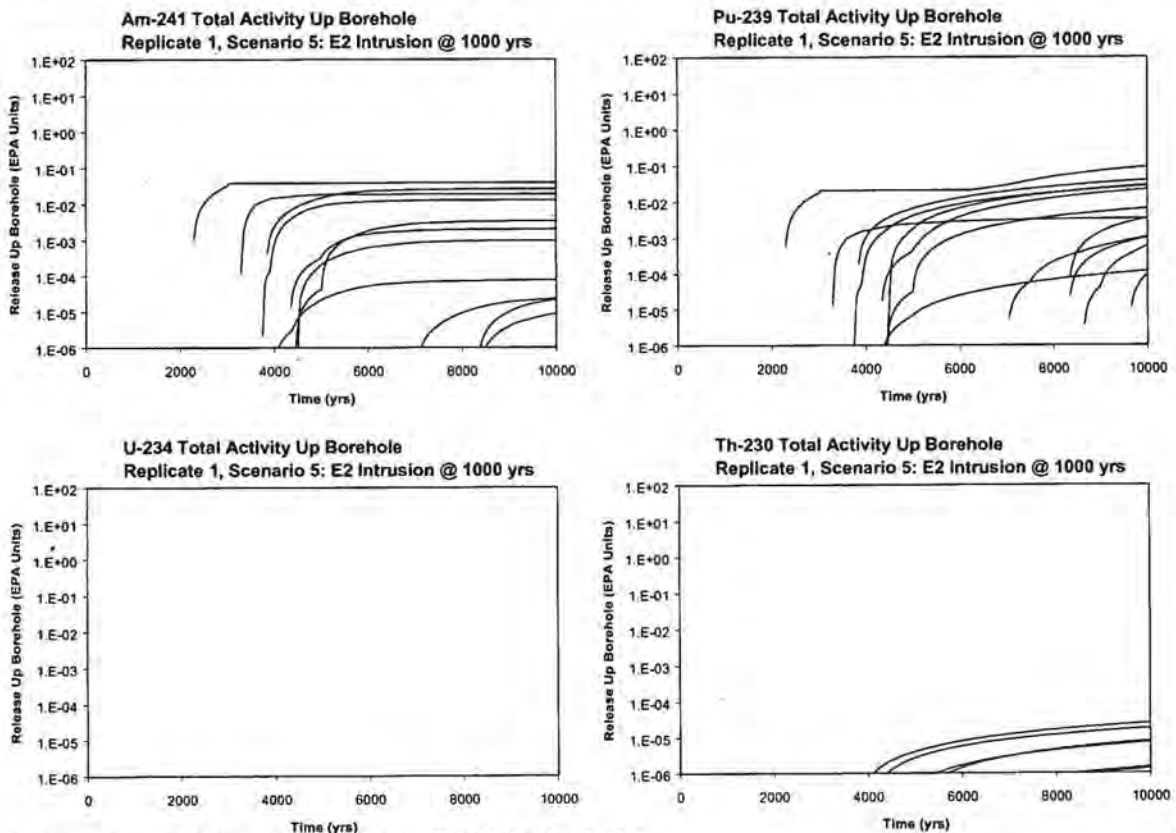


Figure 19 - Activity up borehole in EPA Units for R1S5.

Information Only

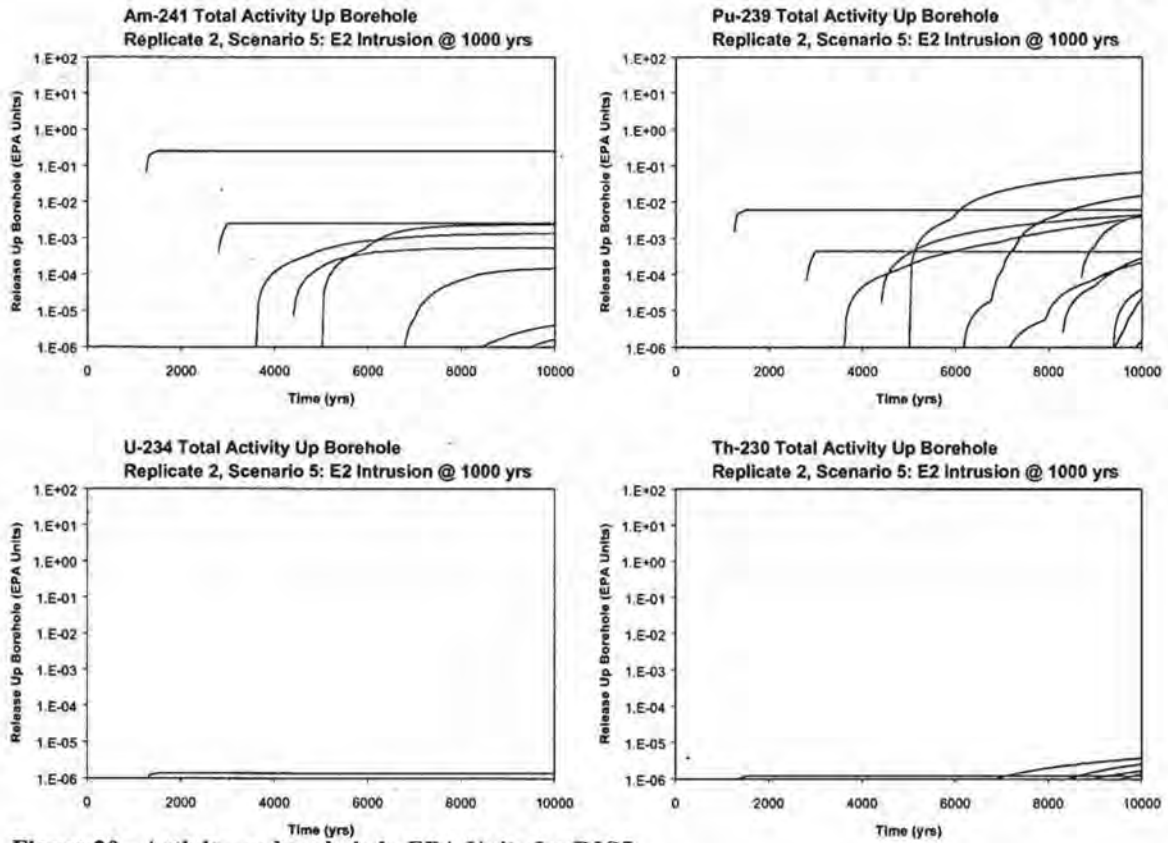


Figure 20 - Activity up borehole in EPA Units for R2S5.

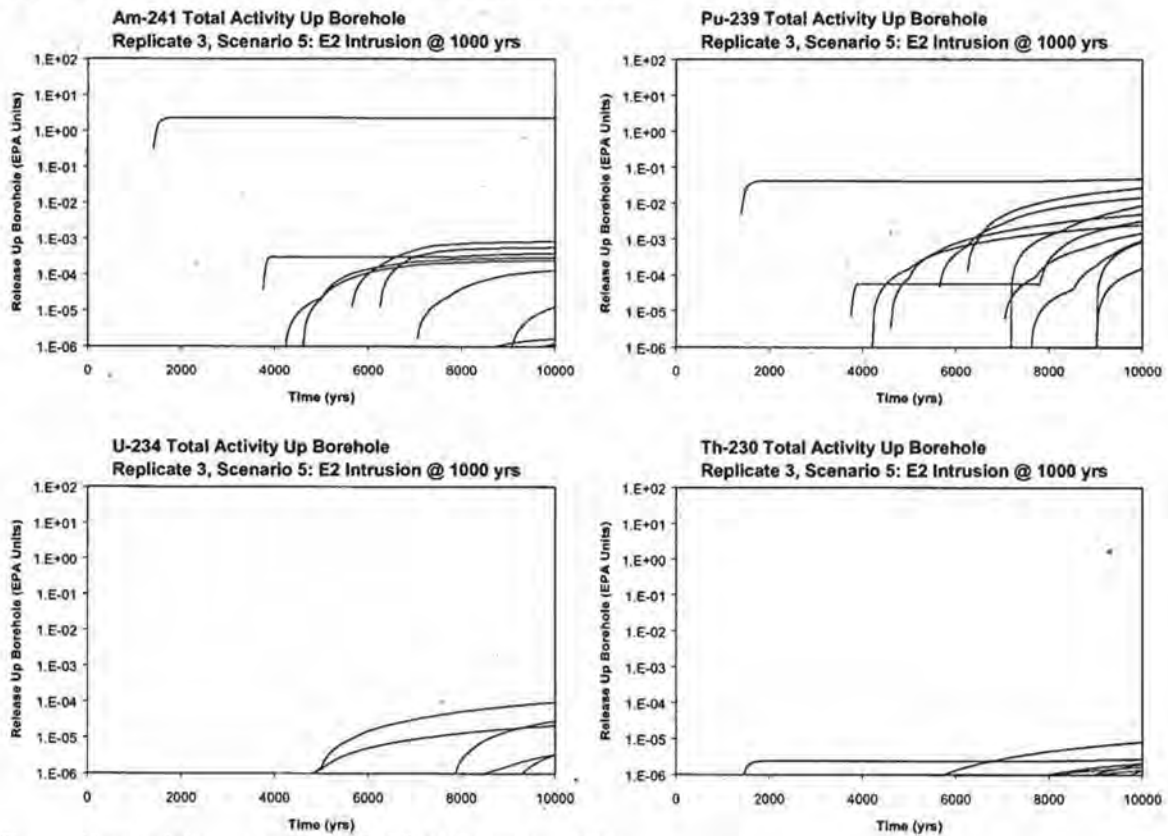




Figure 21 - Activity up borehole in EPA Units for R3S5.

Information Only

References

- Caporuscio, F., Gibbons, J., and Oswald, E. 2003. *Waste Isolation Pilot Plant: Salado Flow Conceptual Models Final Peer Review Report*. Report prepared for the U.S. Department of Energy, Carlsbad Area Office, Office of Regulatory Compliance. ERMS# 526879.
- De Marsily, G. 1986, *Quantitative Hydrogeology: Groundwater Hydrology for Engineers*. Academic Press, San Diego, CA.
- DOE/WIPP, 2004, *Title 40 CFR part 191, subparts B and C Compliance Recertification Application*, 2004-3231.
- Garner, J. 2003. "Analysis Package for PANEL: Compliance Recertification Application" AP-99. Carlsbad, NM: Sandia National Laboratories. ERMS# .
- Hansen, C. 2003. "Analysis Plan for Calculation of CCDF's" Compliance Recertification Application" AP-102. Carlsbad, NM: Sandia National Laboratories. ERMS# 530149.
- Helton, J.C., Bean, J.E., Berglund, J.W., Davis, F.J., Garner, J.W., Johnson, J.D., MacKinnon, R.J., Miller, J., O'Brien, D.G., Ramsey, J.L., Schreiber, J.D., Shinta, A., Smith, L.N., Stoelzel, D.M., Stockman, C., and Vaughn, P. 1998. *Uncertainty and Sensitivity Analysis Results Obtained in the 1996 Performance Assessment for the Waste Isolation Pilot Plant*. SAND98-0365. Albuquerque, NM: Sandia National Laboratories.
- Helton, J.C., and Marietta, M.G. 2000. "The 1996 performance assessment for the Waste Isolation Pilot Plant," *Reliability Engineering & System Safety*. Vol. 69, no. 1-3, 1-3.
- Stein, J. 2003a. "Analysis Plan for Calculations of Salado Flow and Transport: Compliance Recertification Application." AP-99. Carlsbad, NM: Sandia National Laboratories. ERMS# 526891.
- Stein, J.S. 2003b. "Analysis Package for Direct Brine Releases: Compliance Recertification Application." Carlsbad, NM: Sandia National Laboratories. ERMS# 530163.
- Stein, J.S., and Zelinski, W. 2003. "Analysis Package for BRAGFLO: Compliance Recertification Application." Carlsbad, NM: Sandia National Laboratories. ERMS# .
- Stockman, C., Shinta, A., and Garner, J. 1996. "Analysis Package for the Salado Transport Calculations (Task 2) of the Performance Assessment Analysis Supporting the Compliance Certification Application." Carlsbad, NM: Sandia National Laboratories. WPO# 40515.
- WIPP PA (Performance Assessment). 2003a. "Analysis Report for the 8400 Regression Test." Sandia National Laboratories. Sandia WIPP Central Files Records Package # 525278.

WIPP PA (Performance Assessment). 2003b. "Analysis Report for the ES45 Regression Test." Sandia National Laboratories. Sandia WIPP Central Files Records Package # 525278.

WIPP PA (Performance Assessment). 2003c. "Analysis Report for the ES40 Regression Test." Sandia National Laboratories. Sandia WIPP Central Files Records Package # 525278.

WIPP PA (Performance Assessment). 2003d. "Execution of the Performance Assessment for the Compliance Recertification Application (CRA1)." Sandia National Laboratories. Sandia WIPP Central Files Records Package # 530170

Information Only

Appendix A: Plotting script for time-series activity plots.

Sub Plot_Ti()

```
' Plot_Ti Macro
' Macro recorded by Thomas Lowry
'
' Keyboard Shortcut: Ctrl+a
'

Const realization As String = 1 'Replicate #
Const fsTitle As Integer = 18 'Font size of chart title
Const fsAxis As Integer = 16 'Font size of axis titles
Const fsLabel As Integer = 16 'Font size of axis labels
Dim scenario As Integer 'Scenario #
Dim iSeries As Integer 'Series counter
Dim intn As String 'Undisturbed, E1 or E2
Dim inTime As String 'Intrusion time
Dim fName As String 'File name
Dim cTitle As String 'Chart title
Dim dSheet As String 'Name of data sheet
Dim cSheet As String 'Name of chart sheet
Dim oldSheet As Integer 'Name of previous sheet
Dim wBook As String 'Name of data file workbook
Dim pBook As String 'Name of permanent workbook
Dim nukes 'Array of nuclide names
Dim cSeries 'Array of number of vectors
Dim sTime As String 'Intrusion time for scenarios 3 & 5

pBook = "Chart_macro.xls"
cSeries = Array(0, 1, 60, 47, 13, 13)
nukes = Array("Am-241", "Pu-239", "U-234", "Th-230")
oldSheet = 1

For scenario = 1 To 5 'Loop through each scenario
    If scenario = 2 Or scenario = 4 Then
        inTime = 350
    ElseIf scenario = 3 Or scenario = 5 Then
        inTime = 1000
    End If

    If scenario = 2 Or scenario = 3 Then
        intn = "E1"
    ElseIf scenario = 4 Or scenario = 5 Then
```

Information Only

```

    intn = "E2"
Else
    intn = "Undisturbed Case"
End If

```

```

For inukes = 0 To 3 'Loop through each nuclide

```

```

'Set file names, etc.

```

```

    fName = "C:\Documents and Settings\slowry\My Documents\WIPP\NUTS\ISO Runs\R" _
        & realization & "\r" & realization & "_s" & scenario & "_" & _
        nukes(inukes) & ".txt"
    dSheet = "r" & realization & "_s" & scenario & "_" & nukes(inukes)
    cSheet = dSheet & "_ch"
    wBook = dSheet & ".txt"
    If scenario = 1 Then
        cTitle = nukes(inukes) & " Total Activity Up Borehole " & Chr(10) & "Replicate " _
            & realization & ", Scenario " & scenario & ": " & intn
    Else
        cTitle = nukes(inukes) & " Total Activity Up Borehole " & Chr(10) & "Replicate " _
            & realization & ", Scenario " & scenario & ": " & intn & " Intrusion @ " & inTime & "

```

```

yrs"

```

```

    End If

```

```

'Open data file and import data to new workbook of same name

```

```

    Workbooks.OpenText fileName:=fName _
        , Origin:=xlWindows, StartRow:=1, DataType:=xlFixedWidth, FieldInfo:= _
        Array(Array(0, 1), Array(6, 1), Array(19, 1), Array(32, 1), Array(45, 1), Array(58, 1), _
        Array(71, 1), Array(84, 1), Array(97, 1), Array(110, 1), Array(123, 1), Array(136, 1), _
        Array(149, 1), Array(162, 1), Array(175, 1), Array(188, 1), Array(201, 1), Array(214, 1), _
        Array(227, 1), Array(240, 1), Array(253, 1), Array(266, 1), Array(279, 1), Array(292, 1), _
        Array(305, 1), Array(318, 1), Array(331, 1), Array(344, 1), Array(357, 1), Array(370, 1), _
        Array(383, 1), Array(396, 1), Array(409, 1), Array(422, 1), Array(435, 1), Array(448, 1), _
        Array(461, 1), Array(474, 1), Array(487, 1), Array(500, 1), Array(513, 1), Array(526, 1), _
        Array(539, 1), Array(552, 1), Array(565, 1), Array(578, 1), Array(591, 1), Array(604, 1), _
        Array(617, 1), Array(630, 1), Array(643, 1), Array(656, 1), Array(669, 1), Array(682, 1), _
        Array(695, 1), Array(708, 1), Array(721, 1), Array(734, 1), Array(747, 1), Array(760, 1), _
        Array(773, 1), Array(786, 1), Array(799, 1), Array(812, 1))

```

```

'Add scatter chart

```

```

    Charts.Add
    ActiveChart.ChartType = xlXYScatterSmoothNoMarkers
    ActiveChart.SetSourceData Source:=Sheets(dSheet).Range( _
        "A1:BI199"), PlotBy:=xlColumns
    ActiveChart.Location Where:=xlLocationAsNewSheet, Name:=cSheet

```

Information Only

'Set chart and axis titles

With ActiveChart

```
.HasTitle = True
.chartTitle.Characters.Font.Size = fsTitle
.chartTitle.Characters.Text = cTitle
.Axes(xlCategory, xlPrimary).HasTitle = True
.Axes(xlCategory, xlPrimary).AxisTitle.Characters.Font.Size = fsAxis
.Axes(xlCategory, xlPrimary).AxisTitle.Characters.Text = "Time (yrs)"
.Axes(xlValue, xlPrimary).HasTitle = True
.Axes(xlValue, xlPrimary).AxisTitle.Characters.Font.Size = fsAxis
.Axes(xlValue, xlPrimary).AxisTitle.Characters.Text = _
"Release Up Borehole (EPA Units)"
```

End With

'Change scale and format of y-axis

```
ActiveChart.Axes(xlValue).Select
With ActiveChart.Axes(xlValue)
.MinimumScale = 0.000001
.MaximumScale = 100
.MinorUnitIsAuto = True
.MajorUnitIsAuto = True
.Crosses = xlCustom
.CrossesAt = 0.000001
.ReversePlotOrder = False
.ScaleType = xlLogarithmic
.DisplayUnit = xlNone
.TickLabels.NumberFormat = "0.E+00"
.TickLabels.Font.Size = fsLabel
```

End With

'Change scale of x-axis

```
ActiveChart.Axes(xlCategory).Select
With ActiveChart.Axes(xlCategory)
.MinimumScaleIsAuto = True
.MaximumScale = 10000
.MinorUnitIsAuto = True
.MajorUnitIsAuto = True
.Crosses = xlAutomatic
.ReversePlotOrder = False
.ScaleType = xlLinear
.DisplayUnit = xlNone
.TickLabels.Font.Size = fsLabel
```

Information Only

End With

'Delete legend

ActiveChart.Legend.Select
Selection.Delete

'Put border around chart

ActiveChart.PlotArea.Select
With Selection.Border
.Weight = xlThin
.LineStyle = xlContinuous
.ColorIndex = 1
End With

'Change interior color to white (none)

Selection.Interior.ColorIndex = xlNone
ActiveChart.ChartArea.Select

'Loop through each data series and turn series black

For iSeries = 1 To cSeries(scenario)
On Error Resume Next
ActiveChart.SeriesCollection(iSeries).Select
With Selection.Border
.ColorIndex = 1
.Weight = xlThin
.LineStyle = xlContinuous
End With
With Selection
.MarkerBackgroundColorIndex = xlNone
.MarkerForegroundColorIndex = xlNone
.MarkerStyle = xlNone
.Smooth = True
.MarkerSize = 3
.Shadow = False
End With
Next iSeries

'Turn off gridlines

ActiveChart.PlotArea.Select
With ActiveChart.Axes(xlCategory)
.HasMajorGridlines = False
.HasMinorGridlines = False
End With

Information Only

Appendix B: Post-processing code for SUMMARIZE screening runs, SCREEN_BL.FOR.

```

PROGRAM SCREEN_BL
CHARACTER *10, CHAR1, CHAR2, DUMMY
OPEN (10, FILE='SUM_NUT_CRA1_SCN_R1_S1.DAT;1', STATUS='OLD',
&     BLANK='NULL')
OPEN (12, FILE='SUM_NUT_CRA1_SCN_R1_S2.DAT;1', STATUS='OLD')
OPEN (14, FILE='SUM_NUT_CRA1_SCN_R1_S3.DAT;1', STATUS='OLD')
OPEN (16, FILE='SUM_NUT_CRA1_SCN_R1_S4.DAT;1', STATUS='OLD')
OPEN (18, FILE='SUM_NUT_CRA1_SCN_R1_S5.DAT;1', STATUS='OLD')
OPEN (20, FILE='NUT_CRA1_SCN.OUT', STATUS='NEW')

C
CHAR1 = 'Borehole '
CHAR2 = 'Markerbeds'
DO 200 J = 0, 8, 2
  IUNIT1 = 10 + J
  IS      = 1 + J/2
  WRITE (20, 30) IS
30  FORMAT (2X, 'SCENARIO R1_S', I1, ':', /) .
  ICOUNT = 0
  DO 100 I = 1, 100
    IF (IS.EQ.1) THEN

READ (IUNIT1, *) IVECTOR1, TIME, SWASTE1C, SMB39S1C, SMBABS1C, SMB38N1C,
&     SMB38S1C, SMB39N1C, SMBABN1C, SCULBR1C, SHUP1C, SURFSH1C, SSHM1C,
&     BHUP1C, SURFBH1C, SSALAD1C
    ELSE

READ (IUNIT1, *) IVECTOR1, TIME, SWASTE1C, SMB39S1C, SMBABS1C, SMB38N1C,
&     SMB38S1C, SMB39N1C, SMBABN1C, SCULBR1C, SHUP1C, SURFSH1C, SSHM1C,
&     BHUP1C, SURFBH1C, SBHM1C, SSALAD1C
    ENDIF
    SUMMB = SMB38N1C+SMB38S1C+SMB39N1C+SMB39S1C+SMBABN1C+SMBABS1C
    IF (SUMMB .GT. 0.0000001) THEN
      ICOUNT = ICOUNT + 1
      WRITE (20, 50) IVECTOR1, CHAR2
50  FORMAT (2X, I5, 2X, A10)
    ENDIF
    IF (SHUP1C+BHUP1C .GT. 0.0000001) THEN
      ICOUNT = ICOUNT + 1
      WRITE (20, 50) IVECTOR1, CHAR1
    ENDIF
100 CONTINUE

```

```
With ActiveChart.Axes(xlValue)
    .HasMajorGridlines = False
    .HasMinorGridlines = False
End With
```

```
'Change size of chart and center chart on page
```

```
ActiveChart.PlotArea.Select
Selection.Width = 487
ActiveChart.PlotArea.Select
Selection.Left = 110
```

```
'Move title and left justify
```

```
ActiveChart.chartTitle.Select
Selection.Left = 161
Selection.Top = 34
With Selection
    .HorizontalAlignment = xlLeft
    .VerticalAlignment = xlCenter
    .Orientation = xlHorizontal
End With
ActiveChart.ChartArea.Select
```

```
'Move chart to permanent workbook
```

```
Sheets(Array(dSheet, cSheet)).Select
Sheets(Array(dSheet, cSheet)).Move Before:=Workbooks(pBook).Sheets(oldSheet)
```

```
oldSheet = oldSheet + 2
```

```
Next inukes
```

```
Next scenario
```

```
End Sub
```



```
      WRITE (20,120) ICOUNT
120    FORMAT (/2X,'TOTAL = ',I3,/)
200  CONTINUE
      END
```

Information Only

Appendix C: Sample NUTS screening input file for replicate 1, scenario 1.

```

** NUTS TITLE **
'NUTS 2.05A TRACER SCREENING TEST FOR CRA1 R1S1 (UNDISTURBED SCENARIO)'
** 1.# OF SITES,# OF MATERIAL,(2.SITE NAME,# COMP. TO BE MODELED)1,..,NSITES **
1,30
'WIPP_SITE' 1
**(1. SITE, 2.COMP., DAUGHTER, PARENT, GROUP NAMES)1,..,NSITES **
'WIPP_SITE'
'TWASTE' 'NONE' 'NONE' 'WASTE'
** 1.# OF ELEMENT,(2.ELEM. NAME, TEMP. DEPEND., TABLE LOOK-UP)1,..,NELEMENT **
1
'WASTE' .FALSE. .FALSE.
** COLLOIDAL TRANSPORT FLAG (T/F) **
.FALSE.
** PH DEPENDENT SOLUBILITY(IS PH REQUIRED (Y/N)) **
'N'
** ORDER OF THE METHOD **
1
** DEGREE OF IMPLICITNESS **
1.D0
** PRECIPITATE IMPLICITNESS; 1.T/F,IF IMPLICIT 2.# OF ITERATION,TOL. **
.FALSE.
** IS MATRIX ADSORPTION REQUIRED (Y/N) **
'N'
** DO YOU HAVE DISPERSION IN THE MATRIX (Y/N) **
'N'
** DOES MATRIX HAVE SYMMETRIC DISPERSION (T/F): ANSWER IF DISPERSION IS Y **
** DO YOU HAVE INJECTION/PRODUCTION IN THE MATRIX (Y/N) **
'N'
** DO YOU HAVE DIRICHLET B.CS. IN THE MATRIX (F/T) **
.TRUE.
** IS CONCENTRATION INITIALIZED MANUALLY IN THE MATRIX (F/T) **
.FALSE.
** OPEN NUTS UNDISTURBED CDB FOR INTRUSION TIME OTHER THAN 350,1000 YRS **
.FALSE.
** PRINT FLAGS OF MATRIX VARIABLES IN A BINARY FILE **
0,0,0,0,0,0,1,0,0,0,0,0,0,0
** TEMP. DEPEND. OF Kd (ENTER DATA IF ADSORP. IS (Y) AND TEMP. DEPEND.) **
** PRINTING FREQUENCY IN A BINARY FILE **
1,1.D14
** DO YOU HAVE EXTERNAL NUCLIDE SOURCE? (T/F) **
.FALSE.
** MINIMUM LIMITS OF TIME TO BE SET IF ZERO ENCOUNTERED **
1.D-18
** INTRUSION TIME, ITERPOLATED INTRUSION TIME, TOLERANCE **
*** END MATERIAL MAP AND START NUCLIDES PROPERTIES ***
** IF NOT TEMP. DEPEND. (ELEMENT NAME, SOLUBILITY LIMIT) 1,..,NELEMENT **
'WASTE' -2.D0
** (COMP. NAME, MOL.(ATOMIC) WT., INITIAL INVENTS., HALF LIFE)1,..,NUCLIDE **
'TWASTE' .1D0 0.D0 0.D0 0.D0

```

Information Only


```

** GROUND WATER PH INPUT **
** STANDARD BR. DENS. IF NOT BRAGFLO RUN (READ ASCII FILE FOR FLUX FIELD) **
** MOLECULAR DIFFUSION OF EACH COMPONENT **
** ROCK GRAIN DENSITY INPUT (REQUIRED ONLY IF SORPTION OR SOIL BASE CONC.) **
** WASTE MATRIX INPUT (1.# OF ISO,2.NAME, LOC. IN THE INPUT, WASTE SITE #) **
1
'TWASTE' 1 1
*** (1.SITE NAME, NUMBER OF GRIDS IN THE SITE 2.INDECES)1...NSITES ***
'WIPP_SITE' 33
 23,10,1 24,10,1 25,10,1 26,10,1 27,10,1 28,10,1 29,10,1
32,10,1 33,10,1 35,10,1 37,10,1
 23,11,1 24,11,1 25,11,1 26,11,1 27,11,1 28,11,1 29,11,1
32,11,1 33,11,1 35,11,1 37,11,1
 23,12,1 24,12,1 25,12,1 26,12,1 27,12,1 28,12,1 29,12,1
32,12,1 33,12,1 35,12,1 37,12,1
** MATRIX ADSORPTION INPUT **
** MATRIX DISPERSION INPUT **
** MATRIX SOURCE INPUT (INJECTED NUCLIDES IF ANY) **
** MATRIX DIR. B.CS. INPUT (REP.= 'GENERAL', ANYWHERE= 'NOT_GENERAL') **
1 'NOT_GENERAL'
'TWASTE' 1 33
 23,10,1 24,10,1 25,10,1 26,10,1 27,10,1 28,10,1 29,10,1
32,10,1 33,10,1 35,10,1 37,10,1
 23,11,1 24,11,1 25,11,1 26,11,1 27,11,1 28,11,1 29,11,1
32,11,1 33,11,1 35,11,1 37,11,1
 23,12,1 24,12,1 25,12,1 26,12,1 27,12,1 28,12,1 29,12,1
32,12,1 33,12,1 35,12,1 37,12,1
'TWASTE'
1.D0 1.D0 1.D0 1.D0 1.D0 1.D0 1.D0 1.D0 1.D0 1.D0 1.D0 1.D0
1.D0 1.D0 1.D0 1.D0 1.D0 1.D0 1.D0 1.D0 1.D0 1.D0 1.D0 1.D0
1.D0 1.D0 1.D0 1.D0 1.D0 1.D0 1.D0 1.D0 1.D0 1.D0 1.D0 1.D0
** TIME DEPENDENT SOURCE IN THE MATRIX **
** MATRIX CONCENTRATION INITIALIZATION **
** COLLOID TRANSPORT VELOCITY SCALING FACTORS IN THE MATRIX **

```

Appendix D: Sample ALGEBRA screening input file for replicate 1, scenario 1.

```
! ALGEBRA INPUT FILE FOR NUTS SCREENING
! Modified for CRA grid by Thomas Lowry, 11-April-2003
!
ALLTIMES
!FIRST ISOTOP
!MASS FLUXES LEAVING THE WASTE REGION
! WASTE TOP LAYER
!
SWASTE1 =IFGT0 (FLUXJM1 [E:1165], FLUXJM1 [E:1165], 0.)
SWASTE1 = SWASTE1 + IFGT0 (FLUXJM1 [E:1166], FLUXJM1 [E:1166], 0.)
SWASTE1 = SWASTE1 + IFGT0 (FLUXJM1 [E:1167], FLUXJM1 [E:1167], 0.)
SWASTE1 = SWASTE1 + IFGT0 (FLUXJM1 [E:1168], FLUXJM1 [E:1168], 0.)
SWASTE1 = SWASTE1 + IFGT0 (FLUXJM1 [E:1169], FLUXJM1 [E:1169], 0.)
SWASTE1 = SWASTE1 + IFGT0 (FLUXJM1 [E:1170], FLUXJM1 [E:1170], 0.)
SWASTE1 = SWASTE1 + IFGT0 (FLUXJM1 [E:1171], FLUXJM1 [E:1171], 0.)
SWASTE1 = SWASTE1 + IFGT0 (FLUXJM1 [E:1172], FLUXJM1 [E:1172], 0.)
SWASTE1 = SWASTE1 + IFGT0 (FLUXJM1 [E:1469], FLUXJM1 [E:1469], 0.)
SWASTE1 = SWASTE1 + IFGT0 (FLUXJM1 [E:1197], FLUXJM1 [E:1297], 0.)
SWASTE1 = SWASTE1 + IFGT0 (FLUXJM1 [E:1198], FLUXJM1 [E:1298], 0.)
SWASTE1 = SWASTE1 + IFGT0 (FLUXJM1 [E:1199], FLUXJM1 [E:1299], 0.)
SWASTE1 = SWASTE1 + IFGT0 (FLUXJM1 [E:1475], FLUXJM1 [E:1475], 0.)
SWASTE1 = SWASTE1 + IFGT0 (FLUXJM1 [E:1209], FLUXJM1 [E:1209], 0.)
SWASTE1 = SWASTE1 + IFGT0 (FLUXJM1 [E:1210], FLUXJM1 [E:1210], 0.)
SWASTE1 = SWASTE1 + IFGT0 (FLUXJM1 [E:1211], FLUXJM1 [E:1211], 0.)
SWASTE1 = SWASTE1 + IFGT0 (FLUXJM1 [E:1481], FLUXJM1 [E:1481], 0.)
!
!WASTE LOWER LAYER
!
SWASTE1 = SWASTE1 + IFGT0 (-FLUXJM1 [E:1407], -FLUXJM1 [E:1407], 0.)
SWASTE1 = SWASTE1 + IFGT0 (-FLUXJM1 [E:1408], -FLUXJM1 [E:1408], 0.)
SWASTE1 = SWASTE1 + IFGT0 (-FLUXJM1 [E:1409], -FLUXJM1 [E:1409], 0.)
SWASTE1 = SWASTE1 + IFGT0 (-FLUXJM1 [E:1410], -FLUXJM1 [E:1410], 0.)
SWASTE1 = SWASTE1 + IFGT0 (-FLUXJM1 [E:1411], -FLUXJM1 [E:1411], 0.)
SWASTE1 = SWASTE1 + IFGT0 (-FLUXJM1 [E:1412], -FLUXJM1 [E:1412], 0.)
SWASTE1 = SWASTE1 + IFGT0 (-FLUXJM1 [E:1413], -FLUXJM1 [E:1413], 0.)
SWASTE1 = SWASTE1 + IFGT0 (-FLUXJM1 [E:1455], -FLUXJM1 [E:1455], 0.)
SWASTE1 = SWASTE1 + IFGT0 (-FLUXJM1 [E:1466], -FLUXJM1 [E:1466], 0.)
SWASTE1 = SWASTE1 + IFGT0 (-FLUXJM1 [E:1428], -FLUXJM1 [E:1428], 0.)
SWASTE1 = SWASTE1 + IFGT0 (-FLUXJM1 [E:1429], -FLUXJM1 [E:1429], 0.)
SWASTE1 = SWASTE1 + IFGT0 (-FLUXJM1 [E:1458], -FLUXJM1 [E:1458], 0.)
SWASTE1 = SWASTE1 + IFGT0 (-FLUXJM1 [E:1472], -FLUXJM1 [E:1472], 0.)
SWASTE1 = SWASTE1 + IFGT0 (-FLUXJM1 [E:1434], -FLUXJM1 [E:1434], 0.)
SWASTE1 = SWASTE1 + IFGT0 (-FLUXJM1 [E:1435], -FLUXJM1 [E:1435], 0.)
SWASTE1 = SWASTE1 + IFGT0 (-FLUXJM1 [E:1461], -FLUXJM1 [E:1461], 0.)
SWASTE1 = SWASTE1 + IFGT0 (-FLUXJM1 [E:1478], -FLUXJM1 [E:1478], 0.)
!
! WASTE LEFT LAYER
!
```

Information Only


```
SWASTE1 = SWASTE1 + IFGT0(-FLUXIM1[E:1421],-FLUXIM1[E:1421],0.)
SWASTE1 = SWASTE1 + IFGT0(-FLUXIM1[E:1414],-FLUXIM1[E:1414],0.)
SWASTE1 = SWASTE1 + IFGT0(-FLUXIM1[E:1407],-FLUXIM1[E:1407],0.)
```

```
!
```

```
! WASTE RIGHT LAYER
```

```
!
```

```
SWASTE1 = SWASTE1 + IFGT0(FLUXIM1[E:1446],FLUXIM1[E:1446],0.)
SWASTE1 = SWASTE1 + IFGT0(FLUXIM1[E:1443],FLUXIM1[E:1443],0.)
SWASTE1 = SWASTE1 + IFGT0(FLUXIM1[E:1440],FLUXIM1[E:1440],0.)
```

```
!
```

```
!MASS FLUXES REACHING CULEBRA LOWER BOUNDARY
```

```
!
```

```
SCULBR1 = IFGT0(FLUXJM1[E:1825],FLUXJM1[E:1825],0.)
SCULBR1 = SCULBR1 + IFGT0(FLUXJM1[E:1826],FLUXJM1[E:1826],0.)
SCULBR1 = SCULBR1 + IFGT0(FLUXJM1[E:1827],FLUXJM1[E:1827],0.)
SCULBR1 = SCULBR1 + IFGT0(FLUXJM1[E:1828],FLUXJM1[E:1828],0.)
SCULBR1 = SCULBR1 + IFGT0(FLUXJM1[E:1829],FLUXJM1[E:1829],0.)
SCULBR1 = SCULBR1 + IFGT0(FLUXJM1[E:1830],FLUXJM1[E:1830],0.)
SCULBR1 = SCULBR1 + IFGT0(FLUXJM1[E:1831],FLUXJM1[E:1831],0.)
SCULBR1 = SCULBR1 + IFGT0(FLUXJM1[E:1832],FLUXJM1[E:1832],0.)
SCULBR1 = SCULBR1 + IFGT0(FLUXJM1[E:1833],FLUXJM1[E:1833],0.)
SCULBR1 = SCULBR1 + IFGT0(FLUXJM1[E:1834],FLUXJM1[E:1834],0.)
SCULBR1 = SCULBR1 + IFGT0(FLUXJM1[E:1835],FLUXJM1[E:1835],0.)
SCULBR1 = SCULBR1 + IFGT0(FLUXJM1[E:1836],FLUXJM1[E:1836],0.)
SCULBR1 = SCULBR1 + IFGT0(FLUXJM1[E:1837],FLUXJM1[E:1837],0.)
SCULBR1 = SCULBR1 + IFGT0(FLUXJM1[E:1838],FLUXJM1[E:1838],0.)
SCULBR1 = SCULBR1 + IFGT0(FLUXJM1[E:1839],FLUXJM1[E:1839],0.)
SCULBR1 = SCULBR1 + IFGT0(FLUXJM1[E:1840],FLUXJM1[E:1840],0.)
SCULBR1 = SCULBR1 + IFGT0(FLUXJM1[E:1841],FLUXJM1[E:1841],0.)
SCULBR1 = SCULBR1 + IFGT0(FLUXJM1[E:1842],FLUXJM1[E:1842],0.)
SCULBR1 = SCULBR1 + IFGT0(FLUXJM1[E:1843],FLUXJM1[E:1843],0.)
SCULBR1 = SCULBR1 + IFGT0(FLUXJM1[E:1844],FLUXJM1[E:1844],0.)
SCULBR1 = SCULBR1 + IFGT0(FLUXJM1[E:1845],FLUXJM1[E:1845],0.)
SCULBR1 = SCULBR1 + IFGT0(FLUXJM1[E:1846],FLUXJM1[E:1846],0.)
SCULBR1 = SCULBR1 + IFGT0(FLUXJM1[E:1847],FLUXJM1[E:1847],0.)
SCULBR1 = SCULBR1 + IFGT0(FLUXJM1[E:1848],FLUXJM1[E:1848],0.)
SCULBR1 = SCULBR1 + IFGT0(FLUXJM1[E:1849],FLUXJM1[E:1849],0.)
SCULBR1 = SCULBR1 + IFGT0(FLUXJM1[E:1850],FLUXJM1[E:1850],0.)
SCULBR1 = SCULBR1 + IFGT0(FLUXJM1[E:1851],FLUXJM1[E:1851],0.)
SCULBR1 = SCULBR1 + IFGT0(FLUXJM1[E:1852],FLUXJM1[E:1852],0.)
SCULBR1 = SCULBR1 + IFGT0(FLUXJM1[E:1853],FLUXJM1[E:1853],0.)
SCULBR1 = SCULBR1 + IFGT0(FLUXJM1[E:1854],FLUXJM1[E:1854],0.)
SCULBR1 = SCULBR1 + IFGT0(FLUXJM1[E:1855],FLUXJM1[E:1855],0.)
SCULBR1 = SCULBR1 + IFGT0(FLUXJM1[E:1856],FLUXJM1[E:1856],0.)
SCULBR1 = SCULBR1 + IFGT0(FLUXJM1[E:1857],FLUXJM1[E:1857],0.)
SCULBR1 = SCULBR1 + IFGT0(FLUXJM1[E:1858],FLUXJM1[E:1858],0.)
SCULBR1 = SCULBR1 + IFGT0(FLUXJM1[E:1859],FLUXJM1[E:1859],0.)
SCULBR1 = SCULBR1 + IFGT0(FLUXJM1[E:1860],FLUXJM1[E:1860],0.)
SCULBR1 = SCULBR1 + IFGT0(FLUXJM1[E:1861],FLUXJM1[E:1861],0.)
SCULBR1 = SCULBR1 + IFGT0(FLUXJM1[E:1489],FLUXJM1[E:1489],0.)
SCULBR1 = SCULBR1 + IFGT0(FLUXJM1[E:1862],FLUXJM1[E:1862],0.)
SCULBR1 = SCULBR1 + IFGT0(FLUXJM1[E:1863],FLUXJM1[E:1863],0.)
```

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```
SCULBR1 = SCULBR1 + IFGT0 (FLUXJM1 [E:1864], FLUXJM1 [E:1864], 0.)
SCULBR1 = SCULBR1 + IFGT0 (FLUXJM1 [E:1865], FLUXJM1 [E:1865], 0.)
SCULBR1 = SCULBR1 + IFGT0 (FLUXJM1 [E:1866], FLUXJM1 [E:1866], 0.)
SCULBR1 = SCULBR1 + IFGT0 (FLUXJM1 [E:1867], FLUXJM1 [E:1867], 0.)
SCULBR1 = SCULBR1 + IFGT0 (FLUXJM1 [E:1868], FLUXJM1 [E:1868], 0.)
SCULBR1 = SCULBR1 + IFGT0 (FLUXJM1 [E:1869], FLUXJM1 [E:1869], 0.)
SCULBR1 = SCULBR1 + IFGT0 (FLUXJM1 [E:1870], FLUXJM1 [E:1870], 0.)
SCULBR1 = SCULBR1 + IFGT0 (FLUXJM1 [E:1871], FLUXJM1 [E:1871], 0.)
SCULBR1 = SCULBR1 + IFGT0 (FLUXJM1 [E:1872], FLUXJM1 [E:1872], 0.)
SCULBR1 = SCULBR1 + IFGT0 (FLUXJM1 [E:1873], FLUXJM1 [E:1873], 0.)
SCULBR1 = SCULBR1 + IFGT0 (FLUXJM1 [E:1874], FLUXJM1 [E:1874], 0.)
SCULBR1 = SCULBR1 + IFGT0 (FLUXJM1 [E:1875], FLUXJM1 [E:1875], 0.)
SCULBR1 = SCULBR1 + IFGT0 (FLUXJM1 [E:1876], FLUXJM1 [E:1876], 0.)
SCULBR1 = SCULBR1 + IFGT0 (FLUXJM1 [E:1877], FLUXJM1 [E:1877], 0.)
SCULBR1 = SCULBR1 + IFGT0 (FLUXJM1 [E:1878], FLUXJM1 [E:1878], 0.)
SCULBR1 = SCULBR1 + IFGT0 (FLUXJM1 [E:1879], FLUXJM1 [E:1879], 0.)
SCULBR1 = SCULBR1 + IFGT0 (FLUXJM1 [E:1880], FLUXJM1 [E:1880], 0.)
!
!MASS FLUXES INTO MB139 SOUTH MARKER BED
!
SMB139S1 = IFGT0 (-FLUXJM1 [E:278], -FLUXJM1 [E:278], 0.)
SMB139S1 = SMB139S1 + IFGT0 (FLUXJM1 [E:1246], FLUXJM1 [E:1246], 0.)
SMB139S1 = SMB139S1 + IFGT0 (-FLUXIM1 [E:1247], -FLUXIM1 [E:1247], 0.)
SMB139S1 = SMB139S1 + IFGT0 (FLUXIM1 [E:1246], FLUXIM1 [E:1246], 0.)
!
!MASS FLUXES INTO MB139 NORTH MARKER BED
!
SMB139N1 = IFGT0 (-FLUXJM1 [E:421], -FLUXJM1 [E:421], 0.)
SMB139N1 = SMB139N1 + IFGT0 (FLUXJM1 [E:1283], FLUXJM1 [E:1283], 0.)
SMB139N1 = SMB139N1 + IFGT0 (FLUXIM1 [E:1283], FLUXIM1 [E:1283], 0.)
SMB139N1 = SMB139N1 + IFGT0 (-FLUXIM1 [E:1284], -FLUXIM1 [E:1284], 0.)
!
!
!MASS FLUXES INTO SOUTH MBAAB MARKER BED
!
SMBABS1 = IFGT0 (-FLUXJM1 [E:548], -FLUXJM1 [E:548], 0.)
SMBABS1 = SMBABS1 + IFGT0 (FLUXJM1 [E:1295], FLUXJM1 [E:1295], 0.)
SMBABS1 = SMBABS1 + IFGT0 (FLUXIM1 [E:1295], FLUXIM1 [E:1295], 0.)
SMBABS1 = SMBABS1 + IFGT0 (-FLUXIM1 [E:1296], -FLUXIM1 [E:1296], 0.)
!
!MASS FLUXES INTO NORTH MBAAB MARKER BED
!
SMBABN1 = IFGT0 (-FLUXJM1 [E:603], -FLUXJM1 [E:603], 0.)
SMBABN1 = SMBABN1 + IFGT0 (FLUXJM1 [E:1332], FLUXJM1 [E:1332], 0.)
SMBABN1 = SMBABN1 + IFGT0 (FLUXIM1 [E:1332], FLUXIM1 [E:1332], 0.)
SMBABN1 = SMBABN1 + IFGT0 (-FLUXIM1 [E:1333], -FLUXIM1 [E:1333], 0.)
!
!MASS FLUXES INTO SOUTH MB138 MARKER BED
!
SMB138S1 = IFGT0 (-FLUXJM1 [E:638], -FLUXJM1 [E:638], 0.)
SMB138S1 = SMB138S1 + IFGT0 (FLUXJM1 [E:1344], FLUXJM1 [E:1344], 0.)
SMB138S1 = SMB138S1 + IFGT0 (FLUXIM1 [E:1344], FLUXIM1 [E:1344], 0.)
```


SMB138S1 = SMB138S1 + IFGT0(-FLUXIM1[E:1345],-FLUXIM1[E:1345],0.)

!

!MASS FLUXES INTO NORTH MB139 MARKER BED

!

SMB138N1 = IFGT0(-FLUXJM1[E:945],-FLUXJM1[E:945],0.)

SMB138N1 = SMB138N1 + IFGT0(FLUXJM1[E:1400],FLUXJM1[E:1400],0.)

SMB138N1 = SMB138N1 + IFGT0(FLUXIM1[E:1400],FLUXIM1[E:1400],0.)

SMB138N1 = SMB138N1 + IFGT0(-FLUXIM1[E:1401],-FLUXIM1[E:1401],0.)

!

!POINTS OF INTEREST

!

SHUP1 = IFGT0(FLUXJM1[E:1489],FLUXJM1[E:1489],0.)

BHUP1 = IFGT0(FLUXJM1[E:1845],FLUXJM1[E:1845],0.)

SURFBH1 = IFGT0(FLUXJM1[E:2155],FLUXJM1[E:2155],0.)

SURFSH1 = IFGT0(FLUXJM1[E:1496],FLUXJM1[E:1496],0.)

!

!MASS FLUXES REACHING BOREHOLE IN CULEBRA

!BOREHOLE COMMENTED OUT FOR SCENARIO 1 (UNDISTURBED SCENARIO)

!T.Lowry 4-18-03

!SBHM1 = BHUP1 + IFGT0(-FLUXJM1[E:2155],-FLUXJM1[E:2155],0.)

!SBHM1 = SBHM1 + IFGT0(FLUXIM1[E:1845],FLUXIM1[E:1845],0.)

!SBHM1 = SBHM1 + IFGT0(-FLUXIM1[E:1846],-FLUXIM1[E:1846],0.)

!SBHM1 = SBHM1 + IFGT0(FLUXIM1[E:1711],FLUXIM1[E:1711],0.)

!SBHM1 = SBHM1 + IFGT0(-FLUXIM1[E:1712],-FLUXIM1[E:1712],0.)

!SBHM1 = SBHM1 + IFGT0(FLUXIM1[E:1912],FLUXIM1[E:1912],0.)

!SBHM1 = SBHM1 + IFGT0(-FLUXIM1[E:1913],-FLUXIM1[E:1913],0.)

!SBHM1 = SBHM1 + IFGT0(FLUXIM1[E:1778],FLUXIM1[E:1778],0.)

!SBHM1 = SBHM1 + IFGT0(-FLUXIM1[E:1779],-FLUXIM1[E:1779],0.)

!SBHM1 = SBHM1 + IFGT0(FLUXIM1[E:1979],FLUXIM1[E:1979],0.)

!SBHM1 = SBHM1 + IFGT0(-FLUXIM1[E:1980],-FLUXIM1[E:1980],0.)

!SBHM1 = SBHM1 + IFGT0(FLUXIM1[E:2021],FLUXIM1[E:2021],0.)

!SBHM1 = SBHM1 + IFGT0(-FLUXIM1[E:2022],-FLUXIM1[E:2022],0.)

!SBHM1 = SBHM1 + IFGT0(FLUXIM1[E:2113],FLUXIM1[E:2113],0.)

!SBHM1 = SBHM1 + IFGT0(-FLUXIM1[E:2114],-FLUXIM1[E:2114],0.)

!

!MASS FLUXES REACHING SHAFT IN CULEBRA

!

SSHM1 = SHUP1 + IFGT0(-FLUXJM1[E:1496],-FLUXJM1[E:1496],0.)

SSHM1 = SSHM1 + IFGT0(FLUXIM1[E:1489],FLUXIM1[E:1489],0.)

SSHM1 = SSHM1 + IFGT0(-FLUXIM1[E:1862],-FLUXIM1[E:1862],0.)

SSHM1 = SSHM1 + IFGT0(FLUXIM1[E:1490],FLUXIM1[E:1490],0.)

SSHM1 = SSHM1 + IFGT0(-FLUXIM1[E:1728],-FLUXIM1[E:1728],0.)

SSHM1 = SSHM1 + IFGT0(FLUXIM1[E:1491],FLUXIM1[E:1491],0.)

SSHM1 = SSHM1 + IFGT0(-FLUXIM1[E:1929],-FLUXIM1[E:1929],0.)

SSHM1 = SSHM1 + IFGT0(FLUXIM1[E:1492],FLUXIM1[E:1492],0.)

SSHM1 = SSHM1 + IFGT0(-FLUXIM1[E:1795],-FLUXIM1[E:1795],0.)

SSHM1 = SSHM1 + IFGT0(FLUXIM1[E:1493],FLUXIM1[E:1493],0.)

SSHM1 = SSHM1 + IFGT0(-FLUXIM1[E:2038],-FLUXIM1[E:2038],0.)

SSHM1 = SSHM1 + IFGT0(FLUXIM1[E:1494],FLUXIM1[E:1494],0.)

SSHM1 = SSHM1 + IFGT0(-FLUXIM1[E:2063],-FLUXIM1[E:2063],0.)

SSHM1 = SSHM1 + IFGT0(FLUXIM1[E:1495],FLUXIM1[E:1495],0.)

SSHM1 = SSHM1 + IFGT0(-FLUXIM1[E:2172],-FLUXIM1[E:2172],0.)

Information Only

!

!MASS FLUXES REACHING SALADO UPPER BOUNDARY

!

SSALAD1 = IFGT0 (FLUXJM1 [E:885], FLUXJM1 [E:885], 0.)
SSALAD1 = SSALAD1 + IFGT0 (FLUXJM1 [E:886], FLUXJM1 [E:886], 0.)
SSALAD1 = SSALAD1 + IFGT0 (FLUXJM1 [E:887], FLUXJM1 [E:887], 0.)
SSALAD1 = SSALAD1 + IFGT0 (FLUXJM1 [E:888], FLUXJM1 [E:888], 0.)
SSALAD1 = SSALAD1 + IFGT0 (FLUXJM1 [E:889], FLUXJM1 [E:889], 0.)
SSALAD1 = SSALAD1 + IFGT0 (FLUXJM1 [E:890], FLUXJM1 [E:890], 0.)
SSALAD1 = SSALAD1 + IFGT0 (FLUXJM1 [E:891], FLUXJM1 [E:891], 0.)
SSALAD1 = SSALAD1 + IFGT0 (FLUXJM1 [E:892], FLUXJM1 [E:892], 0.)
SSALAD1 = SSALAD1 + IFGT0 (FLUXJM1 [E:893], FLUXJM1 [E:893], 0.)
SSALAD1 = SSALAD1 + IFGT0 (FLUXJM1 [E:894], FLUXJM1 [E:894], 0.)
SSALAD1 = SSALAD1 + IFGT0 (FLUXJM1 [E:895], FLUXJM1 [E:895], 0.)
SSALAD1 = SSALAD1 + IFGT0 (FLUXJM1 [E:896], FLUXJM1 [E:896], 0.)
SSALAD1 = SSALAD1 + IFGT0 (FLUXJM1 [E:897], FLUXJM1 [E:897], 0.)
SSALAD1 = SSALAD1 + IFGT0 (FLUXJM1 [E:898], FLUXJM1 [E:898], 0.)
SSALAD1 = SSALAD1 + IFGT0 (FLUXJM1 [E:899], FLUXJM1 [E:899], 0.)
SSALAD1 = SSALAD1 + IFGT0 (FLUXJM1 [E:900], FLUXJM1 [E:900], 0.)
SSALAD1 = SSALAD1 + IFGT0 (FLUXJM1 [E:901], FLUXJM1 [E:901], 0.)
SSALAD1 = SSALAD1 + IFGT0 (FLUXJM1 [E:902], FLUXJM1 [E:902], 0.)
SSALAD1 = SSALAD1 + IFGT0 (FLUXJM1 [E:903], FLUXJM1 [E:903], 0.)
SSALAD1 = SSALAD1 + IFGT0 (FLUXJM1 [E:904], FLUXJM1 [E:904], 0.)
SSALAD1 = SSALAD1 + IFGT0 (FLUXJM1 [E:905], FLUXJM1 [E:905], 0.)
SSALAD1 = SSALAD1 + IFGT0 (FLUXJM1 [E:906], FLUXJM1 [E:906], 0.)
SSALAD1 = SSALAD1 + IFGT0 (FLUXJM1 [E:907], FLUXJM1 [E:907], 0.)
SSALAD1 = SSALAD1 + IFGT0 (FLUXJM1 [E:908], FLUXJM1 [E:908], 0.)
SSALAD1 = SSALAD1 + IFGT0 (FLUXJM1 [E:909], FLUXJM1 [E:909], 0.)
SSALAD1 = SSALAD1 + IFGT0 (FLUXJM1 [E:910], FLUXJM1 [E:910], 0.)
SSALAD1 = SSALAD1 + IFGT0 (FLUXJM1 [E:911], FLUXJM1 [E:911], 0.)
SSALAD1 = SSALAD1 + IFGT0 (FLUXJM1 [E:912], FLUXJM1 [E:912], 0.)
SSALAD1 = SSALAD1 + IFGT0 (FLUXJM1 [E:913], FLUXJM1 [E:913], 0.)
SSALAD1 = SSALAD1 + IFGT0 (FLUXJM1 [E:914], FLUXJM1 [E:914], 0.)
SSALAD1 = SSALAD1 + IFGT0 (FLUXJM1 [E:915], FLUXJM1 [E:915], 0.)
SSALAD1 = SSALAD1 + IFGT0 (FLUXJM1 [E:916], FLUXJM1 [E:916], 0.)
SSALAD1 = SSALAD1 + IFGT0 (FLUXJM1 [E:917], FLUXJM1 [E:917], 0.)
SSALAD1 = SSALAD1 + IFGT0 (FLUXJM1 [E:918], FLUXJM1 [E:918], 0.)
SSALAD1 = SSALAD1 + IFGT0 (FLUXJM1 [E:919], FLUXJM1 [E:919], 0.)
SSALAD1 = SSALAD1 + IFGT0 (FLUXJM1 [E:920], FLUXJM1 [E:920], 0.)
SSALAD1 = SSALAD1 + IFGT0 (FLUXJM1 [E:921], FLUXJM1 [E:921], 0.)
SSALAD1 = SSALAD1 + IFGT0 (FLUXJM1 [E:922], FLUXJM1 [E:922], 0.)
SSALAD1 = SSALAD1 + IFGT0 (FLUXJM1 [E:923], FLUXJM1 [E:923], 0.)
SSALAD1 = SSALAD1 + IFGT0 (FLUXJM1 [E:924], FLUXJM1 [E:924], 0.)
SSALAD1 = SSALAD1 + IFGT0 (FLUXJM1 [E:925], FLUXJM1 [E:925], 0.)
SSALAD1 = SSALAD1 + IFGT0 (FLUXJM1 [E:926], FLUXJM1 [E:926], 0.)
SSALAD1 = SSALAD1 + IFGT0 (FLUXJM1 [E:1503], FLUXJM1 [E:1503], 0.)
SSALAD1 = SSALAD1 + IFGT0 (FLUXJM1 [E:1077], FLUXJM1 [E:1077], 0.)
SSALAD1 = SSALAD1 + IFGT0 (FLUXJM1 [E:1078], FLUXJM1 [E:1078], 0.)
SSALAD1 = SSALAD1 + IFGT0 (FLUXJM1 [E:1079], FLUXJM1 [E:1079], 0.)
SSALAD1 = SSALAD1 + IFGT0 (FLUXJM1 [E:1080], FLUXJM1 [E:1080], 0.)
SSALAD1 = SSALAD1 + IFGT0 (FLUXJM1 [E:1081], FLUXJM1 [E:1081], 0.)
SSALAD1 = SSALAD1 + IFGT0 (FLUXJM1 [E:1082], FLUXJM1 [E:1082], 0.)

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```

SSALAD1 = SSALAD1 + IFGT0(FLUXJM1[E:1083],FLUXJM1[E:1083],0.)
SSALAD1 = SSALAD1 + IFGT0(FLUXJM1[E:1084],FLUXJM1[E:1084],0.)
SSALAD1 = SSALAD1 + IFGT0(FLUXJM1[E:1085],FLUXJM1[E:1085],0.)
SSALAD1 = SSALAD1 + IFGT0(FLUXJM1[E:1086],FLUXJM1[E:1086],0.)
SSALAD1 = SSALAD1 + IFGT0(FLUXJM1[E:1087],FLUXJM1[E:1087],0.)
SSALAD1 = SSALAD1 + IFGT0(FLUXJM1[E:1088],FLUXJM1[E:1088],0.)
SSALAD1 = SSALAD1 + IFGT0(FLUXJM1[E:1089],FLUXJM1[E:1089],0.)
SSALAD1 = SSALAD1 + IFGT0(FLUXJM1[E:1090],FLUXJM1[E:1090],0.)
SSALAD1 = SSALAD1 + IFGT0(FLUXJM1[E:1091],FLUXJM1[E:1091],0.)
SSALAD1 = SSALAD1 + IFGT0(FLUXJM1[E:1092],FLUXJM1[E:1092],0.)
SSALAD1 = SSALAD1 + IFGT0(FLUXJM1[E:1093],FLUXJM1[E:1093],0.)
SSALAD1 = SSALAD1 + IFGT0(FLUXJM1[E:1094],FLUXJM1[E:1094],0.)
SSALAD1 = SSALAD1 + IFGT0(FLUXJM1[E:1095],FLUXJM1[E:1095],0.)
SSALAD1 = SSALAD1 + IFGT0(FLUXJM1[E:1096],FLUXJM1[E:1096],0.)
SSALAD1 = SSALAD1 + IFGT0(FLUXJM1[E:1097],FLUXJM1[E:1097],0.)
SSALAD1 = SSALAD1 + IFGT0(FLUXJM1[E:1098],FLUXJM1[E:1098],0.)
SSALAD1 = SSALAD1 + IFGT0(FLUXJM1[E:1099],FLUXJM1[E:1099],0.)
SSALAD1 = SSALAD1 + IFGT0(FLUXJM1[E:1100],FLUXJM1[E:1100],0.)
SSALAD1 = SSALAD1 + IFGT0(FLUXJM1[E:1101],FLUXJM1[E:1101],0.)
!
! INTEGRATION OF MASSES
!
SWASTE1C = intright(SWASTE1)
SMB39S1C = iflt0(intright(SMB139S1)-1.e-7,0.,intright(SMB139S1))
SMBABS1C = iflt0(intright(SMBABS1)-1.e-7,0.,intright(SMBABS1))
SMB38N1C = iflt0(intright(SMB138N1)-1.e-7,0.,intright(SMB138N1))
SMB38S1C = iflt0(intright(SMB138S1)-1.e-7,0.,intright(SMB138S1))
SMB39N1C = iflt0(intright(SMB139N1)-1.e-7,0.,intright(SMB139N1))
SMBABN1C = iflt0(intright(SMBABN1)-1.e-7,0.,intright(SMBABN1))
SCULBR1C = iflt0(intright(SCULBR1)-1.e-7,0.,intright(SCULBR1))
SHUP1C   = iflt0(intright(SHUP1)-1.e-7,0.,intright(SHUP1))
SURFSH1C = iflt0(intright(SURFSH1)-1.e-7,0.,intright(SURFSH1))
SSHM1C   = iflt0(intright(SSHM1)-1.e-7,0.,intright(SSHM1))
BHUP1C   = iflt0(intright(BHUP1)-1.e-7,0.,intright(BHUP1))
SURFBH1C = iflt0(intright(SURFBH1)-1.e-7,0.,intright(SURFBH1))
!SBHM1C  = iflt0(intright(SBHM1)-1.e-7,0.,intright(SBHM1))
SSALAD1C = intright(SSALAD1)
!
DELETE ATTRIBUTE, PROPERTY, HISTORY, ELEMENT, NODAL
!
END

```

Appendix E: Sample SUMMARIZE screening input file for replicate 1, scenario 1.

*INPUT FILES

DIR = PAWORK:[ANALYSIS.CRA1.NUT.SCN.DATA.R1S1]

TEMPLATE = ALG_NUT_CRA1_SCN_R1_S1_V%%%

TYPE = CDB

*VECTORS

ID = %

VECTOR = 1 TO 100

*TIMES

READ = SECONDS

INPUT = YEARS

OUTPUT = YEARS

TIMES = 10000

*ITEM

TYPE = GLOBAL

NAME = SWASTE1C, SMB39S1C, SMBABS1C, SMB38N1C, SMB38S1C, SMB39N1C, SMBABN1C, SCULBR1C, SHUP1C, SURFSH1C, SSHM1C, BHUP1C, SURFBH1C, SSALAD1C

*OUTPUT

DRIVER = EXCEL

WRITE = TIME VS ITEM

NAME = SUM_NUT_CRA1_SCN_R1_S1.DAT

Appendix F: ALGEBRA input file for analysis of R1S1v082.

```

=====
! ALGEBRA file for post-processing NUTS (non-screening runs) output
! Reduced file for calculating concentration of isotopes at several
! locations as time histories in units of Curies/liter
!
! 8 July 1996
! Author: Joel D. Miller, SNL Org. 9363
=====
! Eliminate excess output
!
DELETE ALL
!
!*****
!*****
!
! Conversion factors (Curies per kilogram), where radionuclides are
! numbered
!
!      1 = Am-241
!      2 = Pu-239
!      3 = Pu-238
!      4 = U-234
!      5 = Th-230
!
A1 = 3431.154
A2 = 62.14574
A3 = 17115.25
A4 = 6.247269
A5 = 20.18264
!
! To convert from kg/m^3 to Ci/l, multiply by 0.001 m^3/l
!
!*****
!*****
!
! Isotope concentration (Ci/l) in shaft at top of Salado (El 1488)
!
! Param 1: Am-241 concn. in shaft at top of Salado (el.1488) -->
C1SH_661
! Param 2: Pu-239 concn. in shaft at top of Salado (el.1488) -->
C2SH_661

```

Information Only

```
! Param 3: Pu-238 concen. in shaft at top of Salado (el.1488) -->
C3SH_661
! Param 4: U--234 concen. in shaft at top of Salado (el.1488) -->
C4SH_661
! Param 5: Th-230 concen. in shaft at top of Salado (el.1488) -->
C5SH_661
!
! Isotope concentration (Ci/l) in shaft at Culebra Dolomite (El 1489)
!
! Param 6: Am-241 conc. in shaft at Culebra Dolomite (el.1489) -->
C1SH_662
! Param 7: Pu-239 conc. in shaft at Culebra Dolomite (el.1489) -->
C2SH_662
! Param 8: Pu-238 conc. in shaft at Culebra Dolomite (el.1489) -->
C3SH_662
! Param 9: U--234 conc. in shaft at Culebra Dolomite (el.1489) -->
C4SH_662
! Param 10: Th-230 conc. in shaft at Culebra Dolomite (el.1489) -->
C5SH_662
!
!*****
!
! Isotope concentration (Ci/l) in shaft at top of Salado (El 1488)
!
C1SH_661 = CM1[E:1488]*A1*0.001
C2SH_661 = CM2[E:1488]*A2*0.001
C3SH_661 = CM3[E:1488]*A3*0.001
C4SH_661 = CM4[E:1488]*A4*0.001
C5SH_661 = CM5[E:1488]*A5*0.001
!
! Isotope concentration (Ci/l) in shaft at Culebra Dolomite (El 1489)
!
C1SH_662 = CM1[E:1489]*A1*0.001
C2SH_662 = CM2[E:1489]*A2*0.001
C3SH_662 = CM3[E:1489]*A3*0.001
C4SH_662 = CM4[E:1489]*A4*0.001
C5SH_662 = CM5[E:1489]*A5*0.001
!
!*****
!*****
!
! Isotope concentration (Ci/l) at South L-W boundary in MB 138 (El
1344)
!
! Param 11: Am-241 concen. in MB 138 inside L-W bndry (el.1344) -->
C1LWM38S
```

Information Only


```
! Param 12: Pu-239 concen. in MB 138 inside L-W bndry (el.1344) -->
C2LWM38S
! Param 13: Pu-238 concen. in MB 138 inside L-W bndry (el.1344) -->
C3LWM38S
! Param 14: U--234 concen. in MB 138 inside L-W bndry (el.1344) -->
C4LWM38S
! Param 15: Th-230 concen. in MB 138 inside L-W bndry (el.1344) -->
C5LWM38S
!
! Isotope concentration (Ci/l) at South L-W bndry in Anhydrite A/B (El
1295)
!
! Param 16: Am-241 conc. in Anhyd.A/B inside L-W bndry (el.1295) -->
C1LWAABS
! Param 17: Pu-239 conc. in Anhyd.A/B inside L-W bndry (el.1295) -->
C2LWAABS
! Param 18: Pu-238 conc. in Anhyd.A/B inside L-W bndry (el.1295) -->
C3LWAABS
! Param 19: U--234 conc. in Anhyd.A/B inside L-W bndry (el.1295) -->
C4LWAABS
! Param 20: Th-230 conc. in Anhyd.A/B inside L-W bndry (el.1295) -->
C5LWAABS
!
! Isotope concentration (Ci/l) at South L-W boundary in MB 139 (El
1246)
!
! Param 21: Am-241 concen. in MB 139 inside L-W bndry (el.1246) -->
C1LWM39S
! Param 22: Pu-239 concen. in MB 139 inside L-W bndry (el.1246) -->
C2LWM39S
! Param 23: Pu-238 concen. in MB 139 inside L-W bndry (el.1246) -->
C3LWM39S
! Param 24: U--234 concen. in MB 139 inside L-W bndry (el.1246) -->
C4LWM39S
! Param 25: Th-230 concen. in MB 139 inside L-W bndry (el.1246) -->
C5LWM39S
!
!*****
!
! Isotope concentration (Ci/l) at South L-W boundary in MB 138 (El
1344)
!
C1LWM38S = CM1[E:1344]*A1*0.001
C2LWM38S = CM2[E:1344]*A2*0.001
C3LWM38S = CM3[E:1344]*A3*0.001
C4LWM38S = CM4[E:1344]*A4*0.001
C5LWM38S = CM5[E:1344]*A5*0.001
```

Information Only

!
! Isotope concentration (Ci/l) at South L-W bndry in Anhydrite A/B (El
1295)

!
C1LWMAAB = CM1[E:1295]*A1*0.001
C2LWMAAB = CM2[E:1295]*A2*0.001
C3LWMAAB = CM3[E:1295]*A3*0.001
C4LWMAAB = CM4[E:1295]*A4*0.001
C5LWMAAB = CM5[E:1295]*A5*0.001

!
! Isotope concentration (Ci/l) at South L-W boundary in MB 139 (El
1246).

!
C1LWM39S = CM1[E:1246]*A1*0.001
C2LWM39S = CM2[E:1246]*A2*0.001
C3LWM39S = CM3[E:1246]*A3*0.001
C4LWM39S = CM4[E:1246]*A4*0.001
C5LWM39S = CM5[E:1246]*A5*0.001

!
!*****
!*****

!
DELETE A1, A2, A3, A4, A5

!
!*****
!*****
END

Appendix G: SUMMARIZE input file for analysis of R1S1v082.

```
*input files
  name=      PA_NUTS_ISO_R1S1_CONC_V082
  disk=      U1
  directory=[JWGARNE.cra2.NUTS.MB]
  type=      CDB

*times
  read=      seconds
  input=     years
  output=    years
  times=     0 to 1400 by 50, 1400 to 10000 by 200

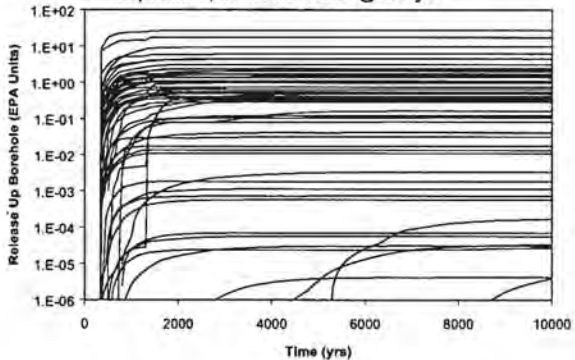
*items
  type= GLOBAL
!   name= C1SH_661, C2SH_661, C3SH_661, C4SH_661, C5SH_661, &
!         C1SH_662, C2SH_662, C3SH_662, C4SH_662, C5SH_662, &
!         C1LWM38S, C2LWM38S, C3LWM38S, C4LWM38S, C5LWM38S, &
!         C1LWMAAB, C2LWMAAB, C3LWMAAB, C4LWMAAB, C5LWMAAB, &
!         C1LWM39S, C2LWM39S, C3LWM39S, C4LWM39S, C5LWM39S
  name= C1LWM38S, C2LWM38S, C3LWM38S, C4LWM38S, C5LWM38S, &
        C1LWMAAB, C2LWMAAB, C3LWMAAB, C4LWMAAB, C5LWMAAB, &
        C1LWM39S, C2LWM39S, C3LWM39S, C4LWM39S, C5LWM39S

*output
  driver= EXCEL
  write=  time vs item
  name=   PA_NUTS_ISO_S1_CONC.TBL

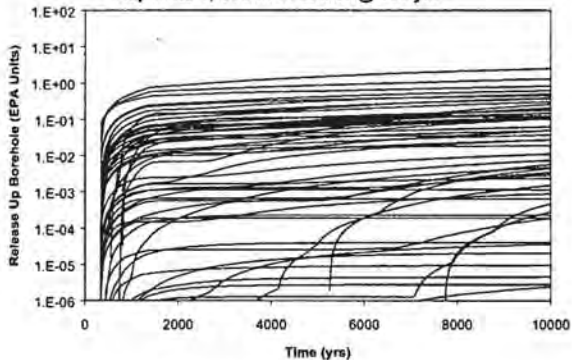
*end
```

Appendix H: TI Time Series Plots

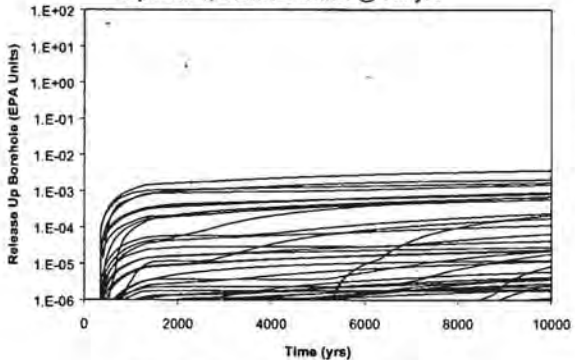
Am-241 Total Activity Up Borehole
Replicate 1, Scenario 2: Int1 @ 100 yrs



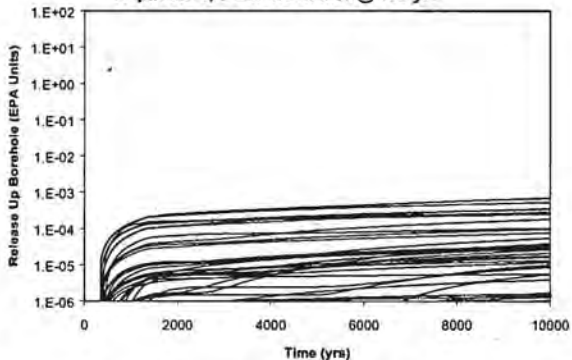
Pu-239 Total Activity Up Borehole
Replicate 1, Scenario 2: Int1 @ 100 yrs



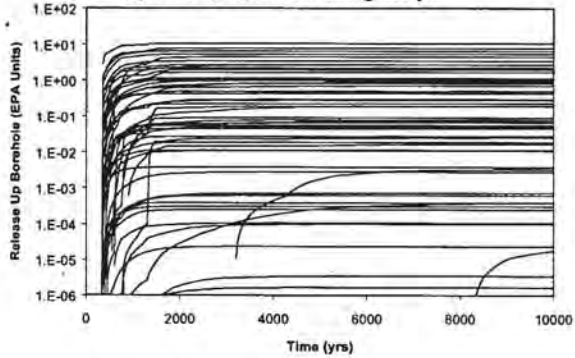
U-234 Total Activity Up Borehole
Replicate 1, Scenario 2: Int1 @ 100 yrs



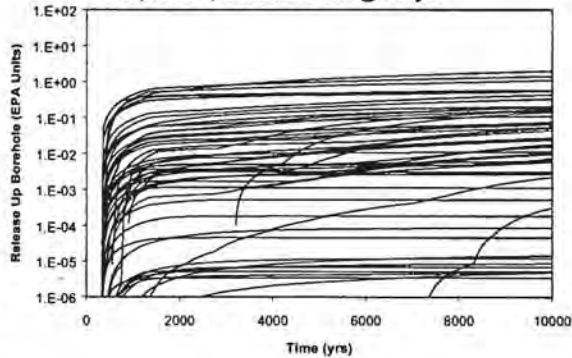
Th-230 Total Activity Up Borehole
Replicate 1, Scenario 2: Int1 @ 100 yrs



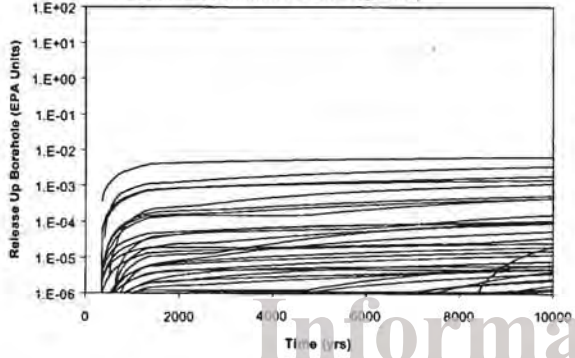
Am-241 Total Activity Up Borehole
Replicate 2, Scenario 2: Int1 @ 100 yrs



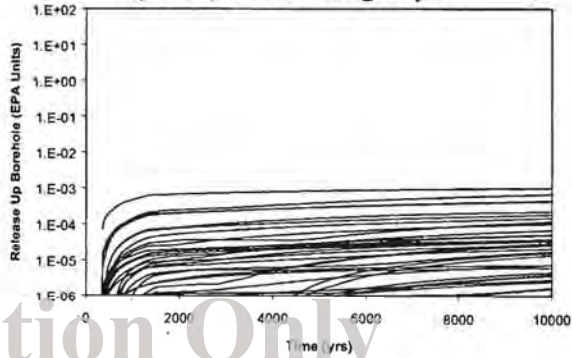
Pu-239 Total Activity Up Borehole
Replicate 2, Scenario 2: Int1 @ 100 yrs

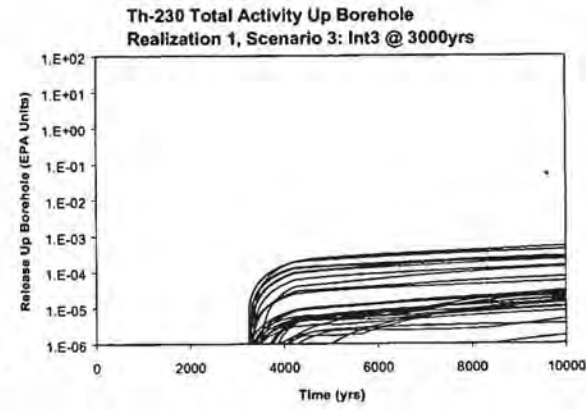
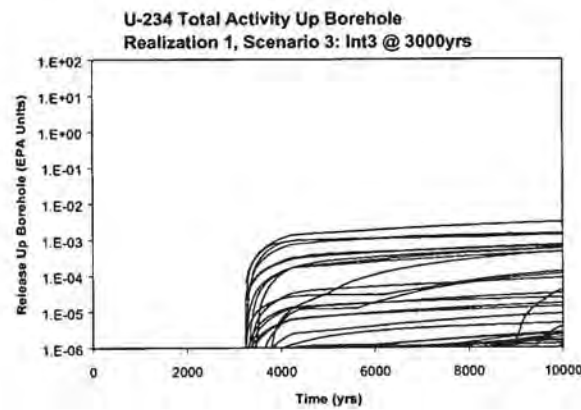
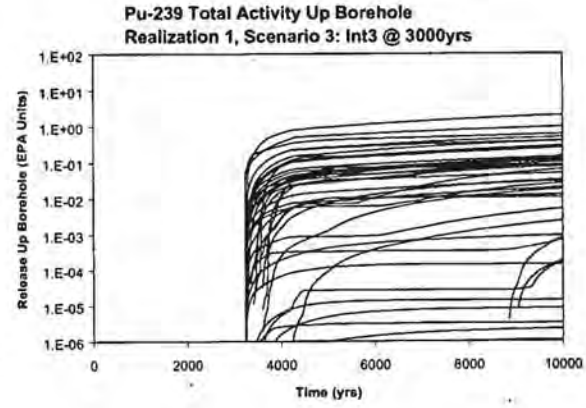
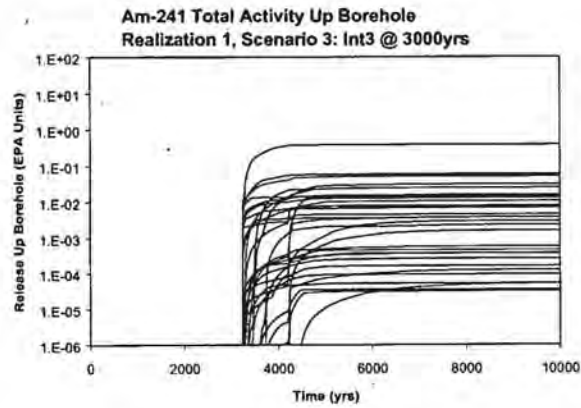
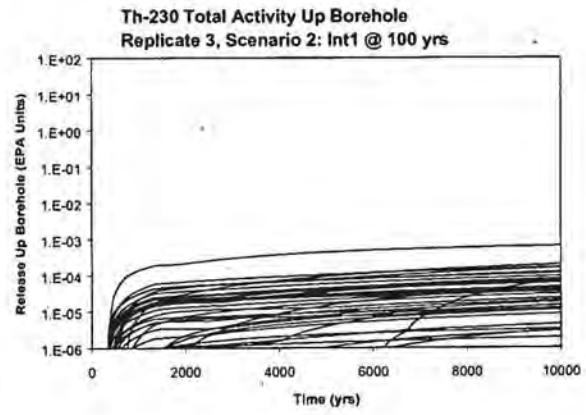
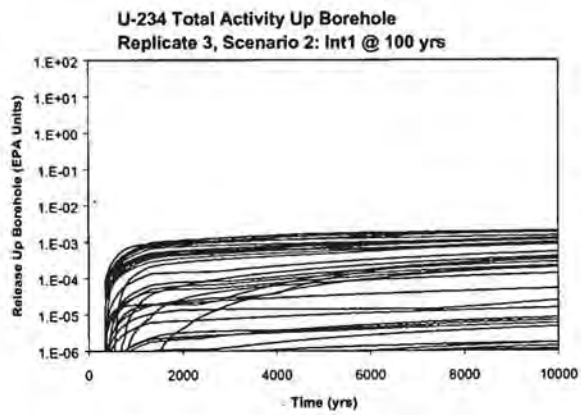
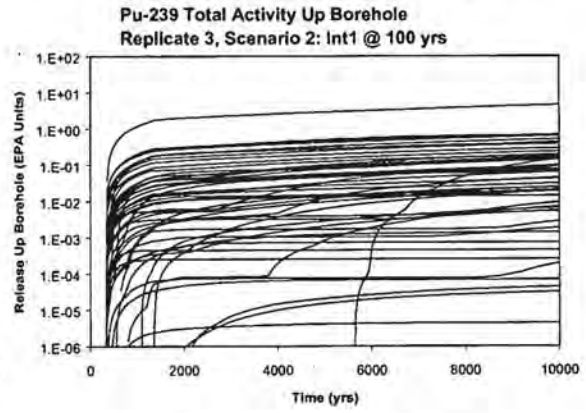
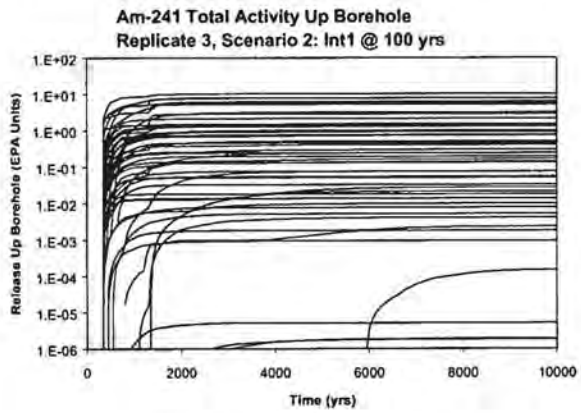


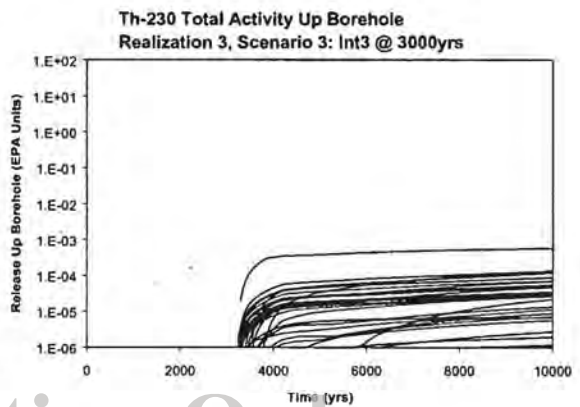
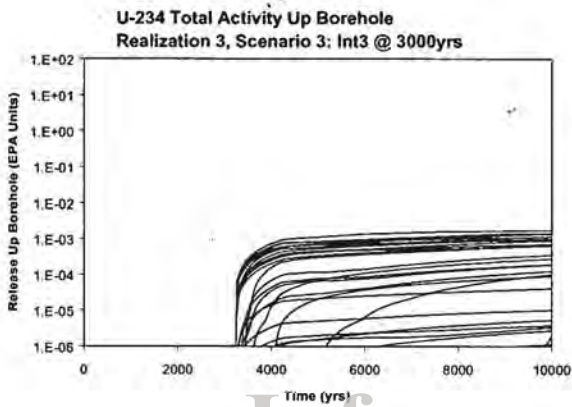
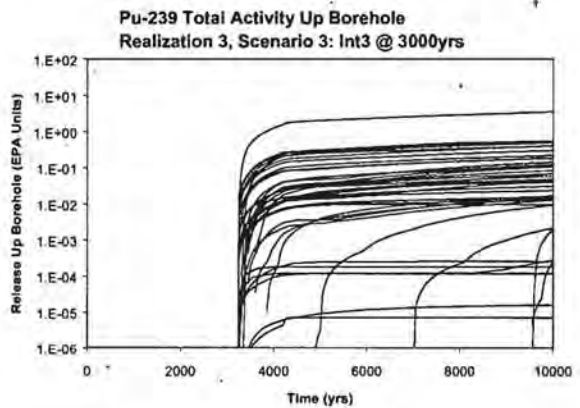
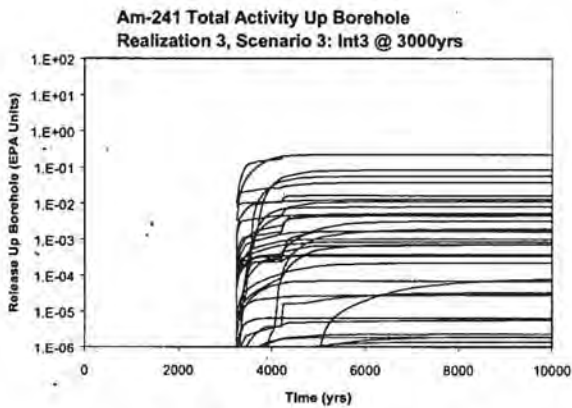
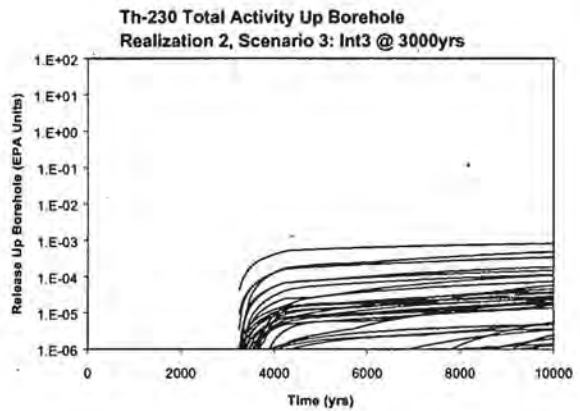
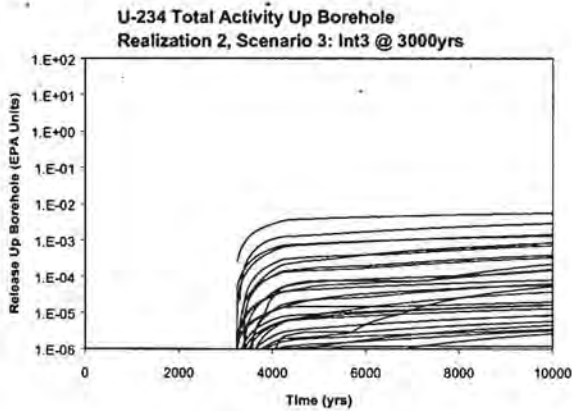
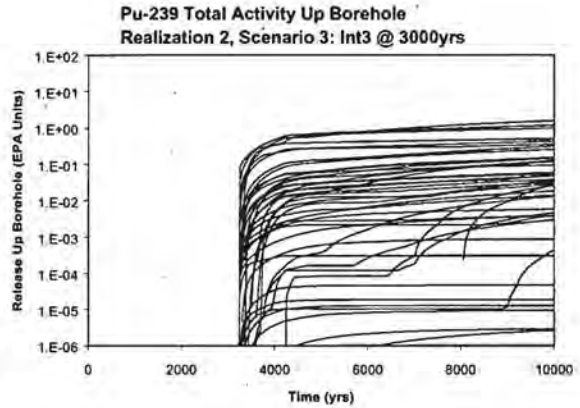
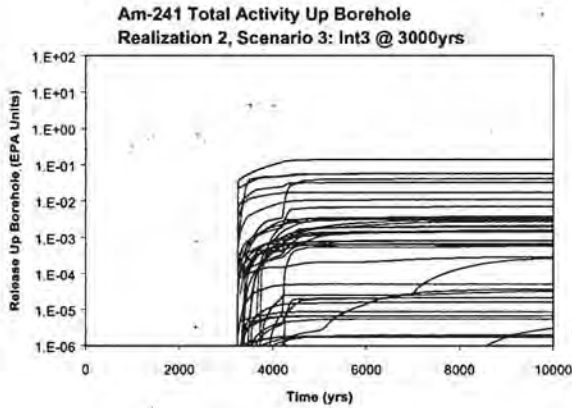
U-234 Total Activity Up Borehole
Replicate 2, Scenario 2: Int1 @ 100 yrs

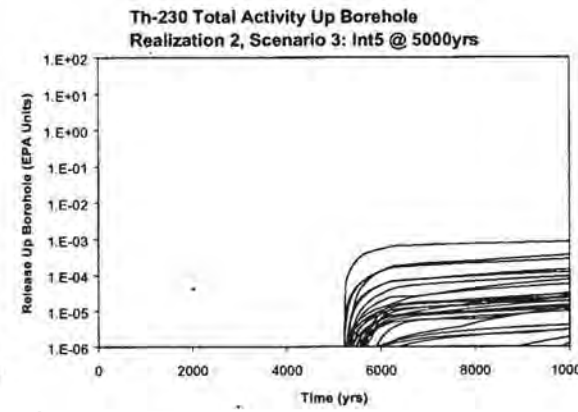
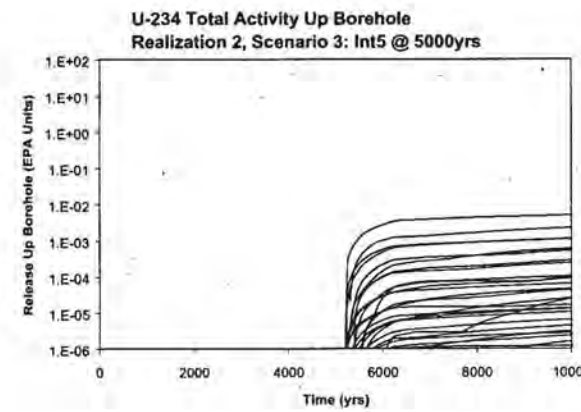
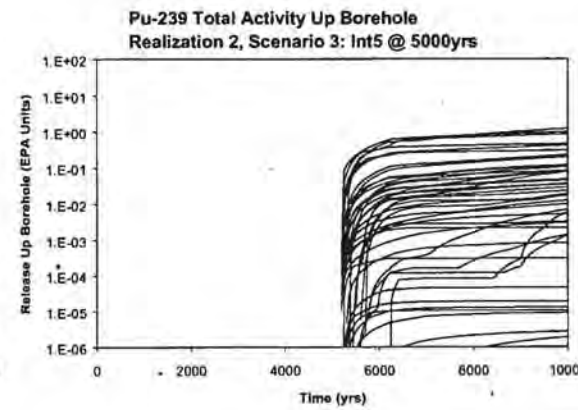
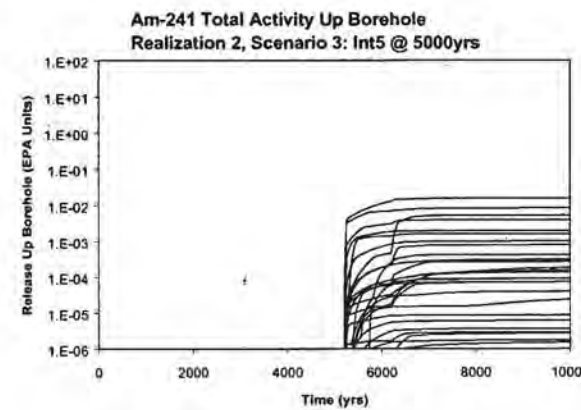
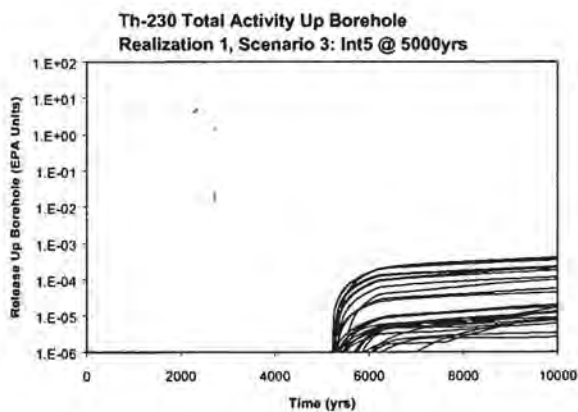
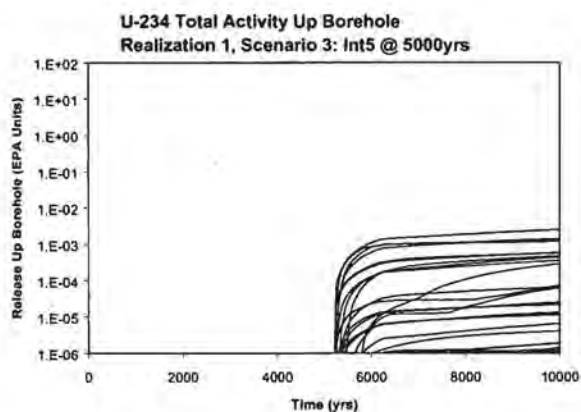
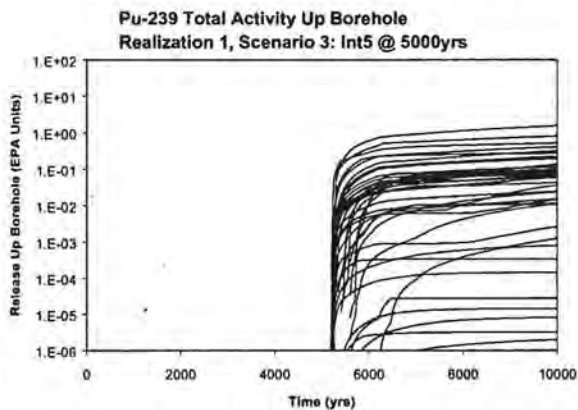
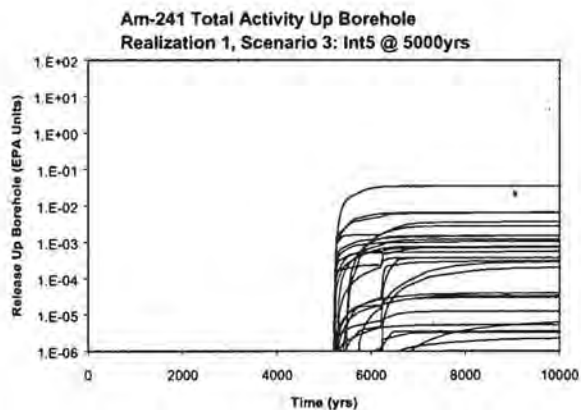


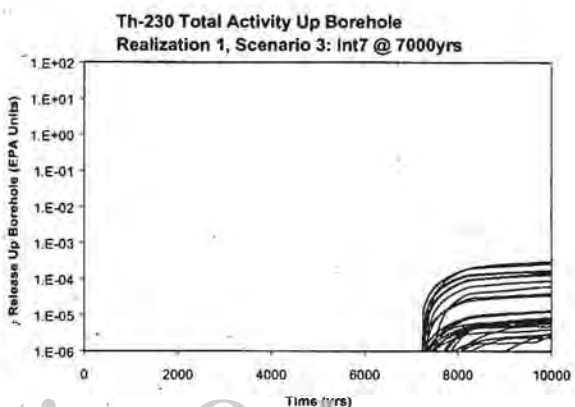
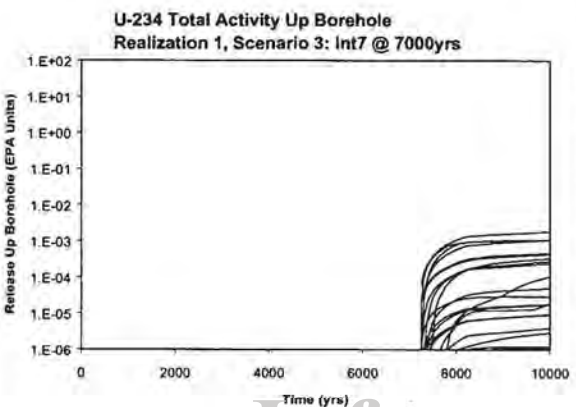
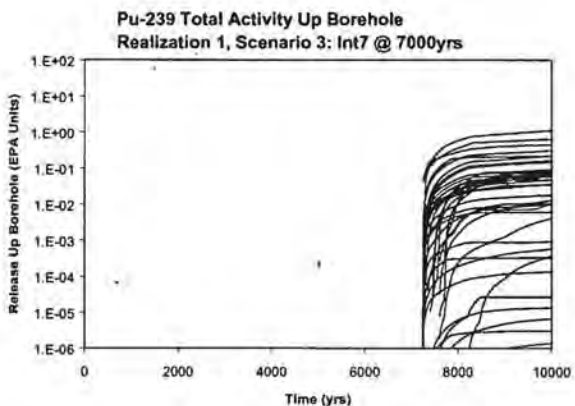
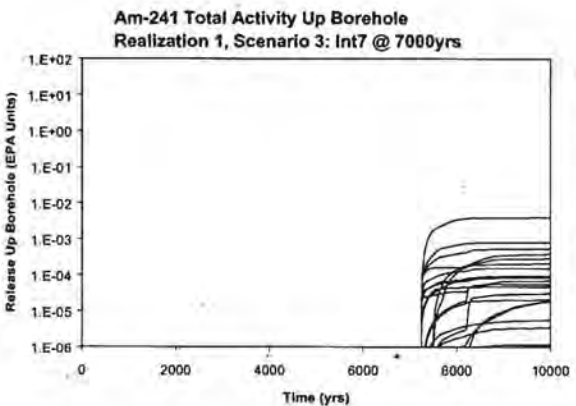
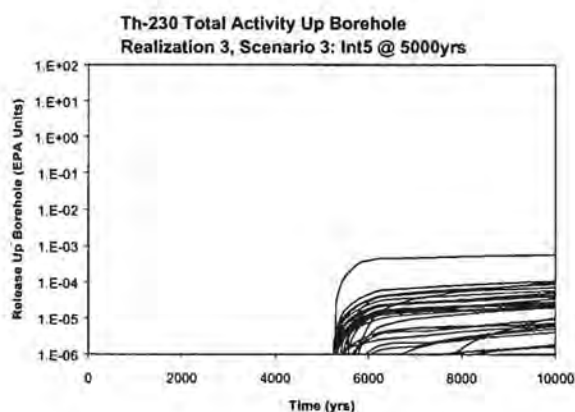
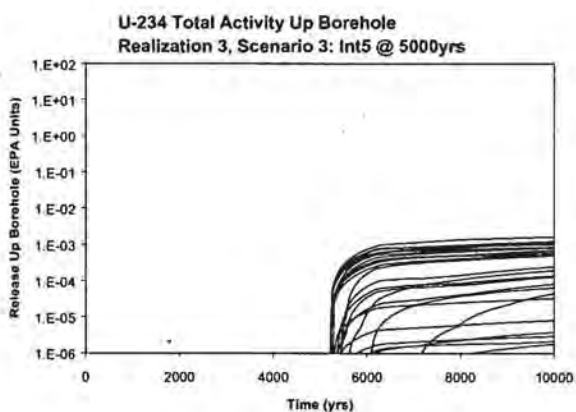
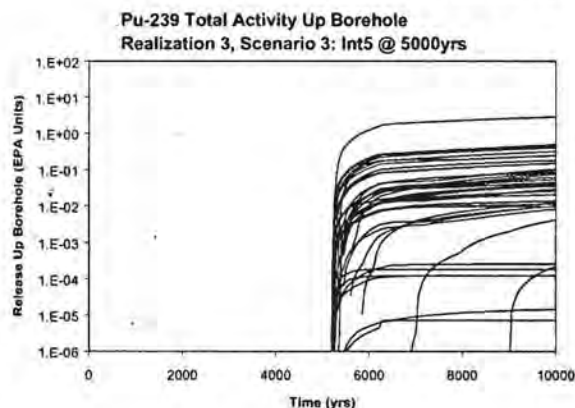
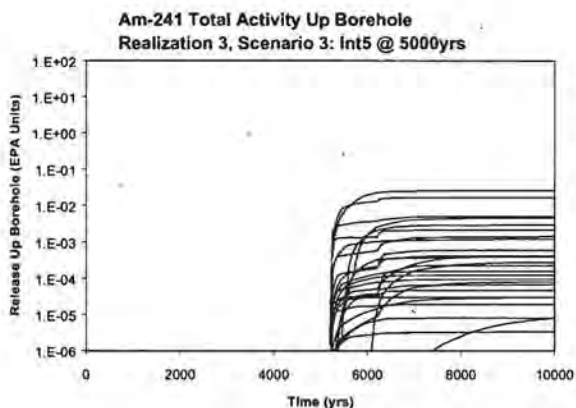
Th-230 Total Activity Up Borehole
Replicate 2, Scenario 2: Int1 @ 100 yrs

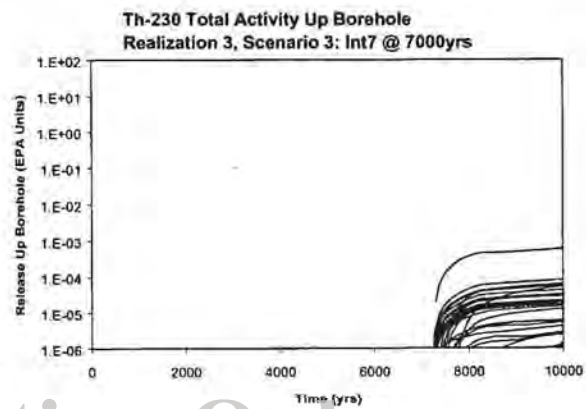
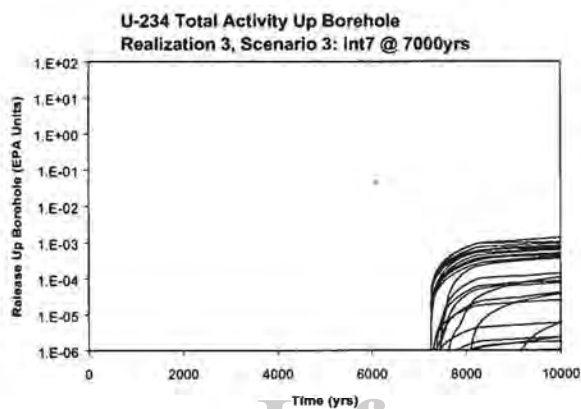
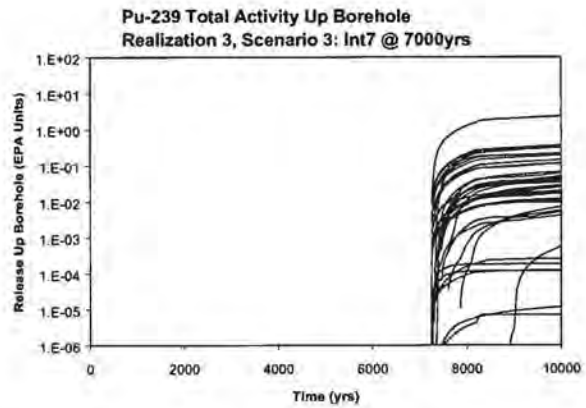
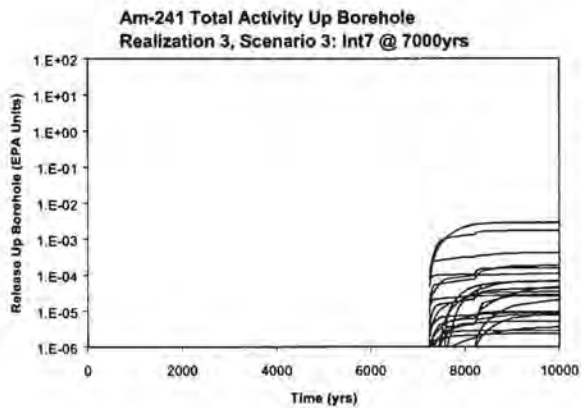
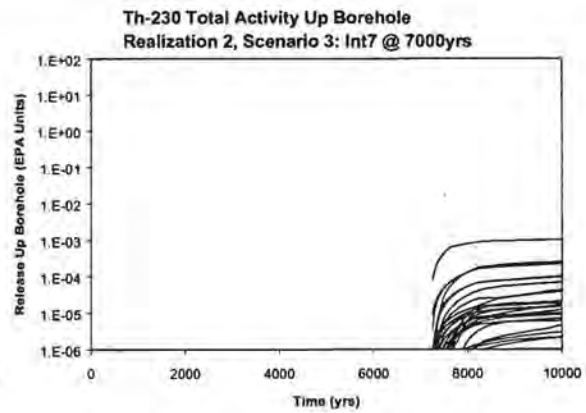
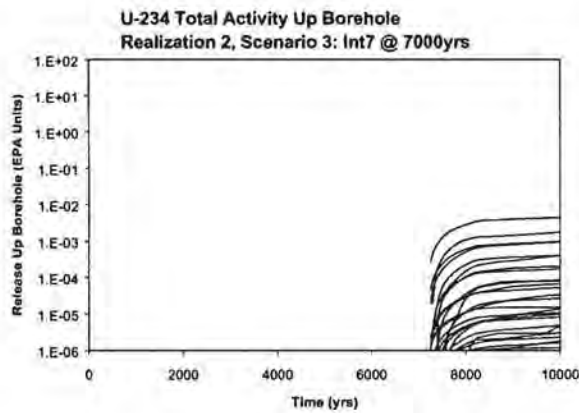
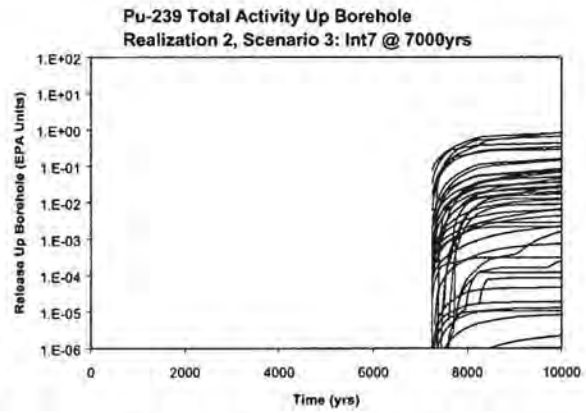
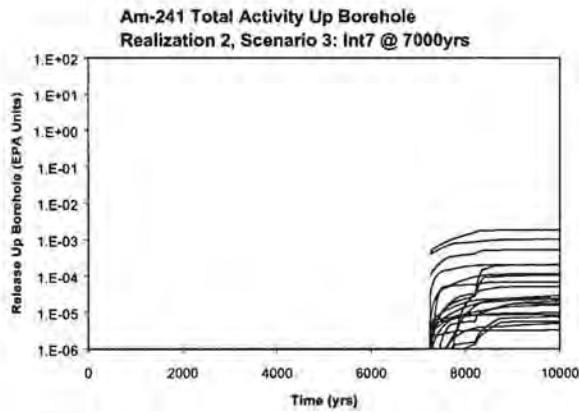


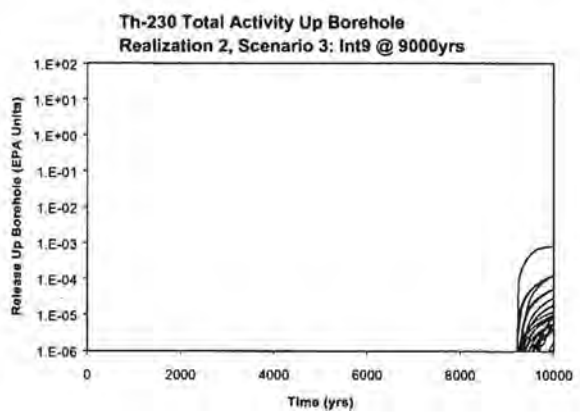
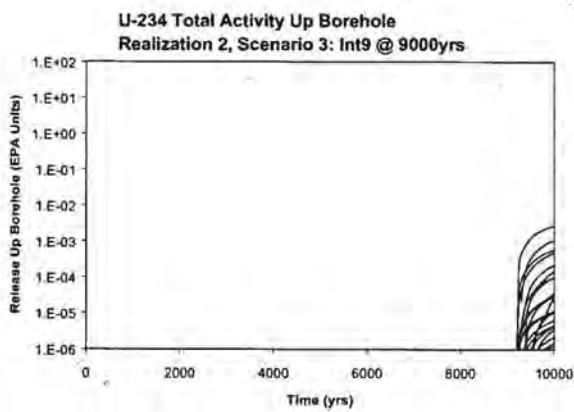
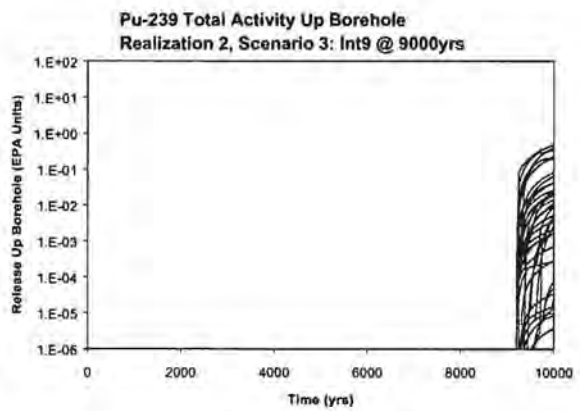
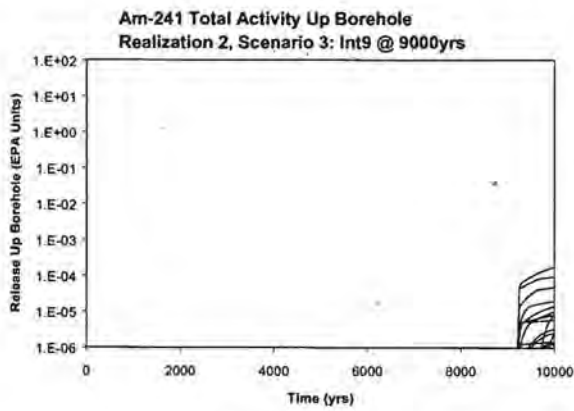
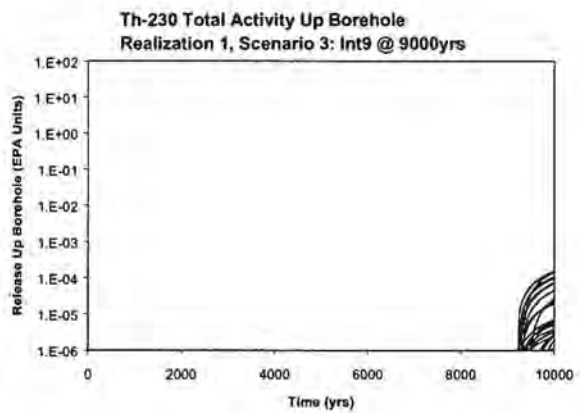
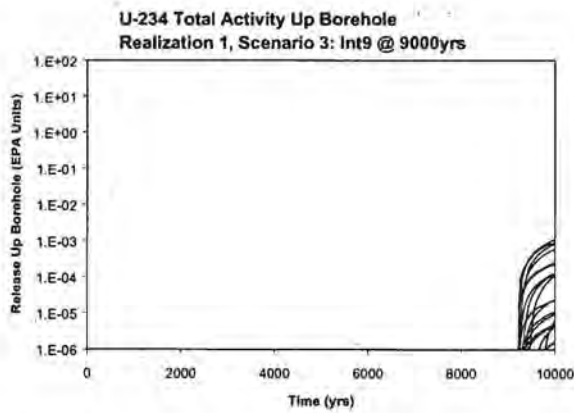
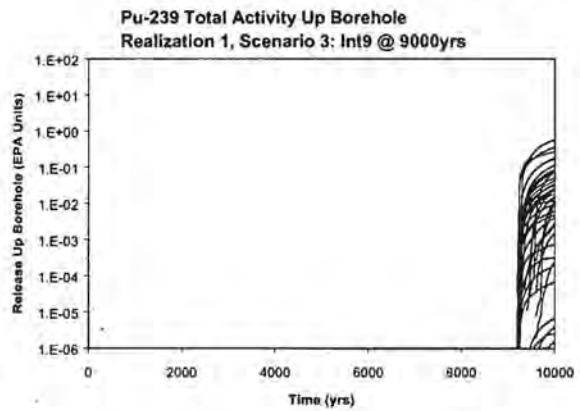
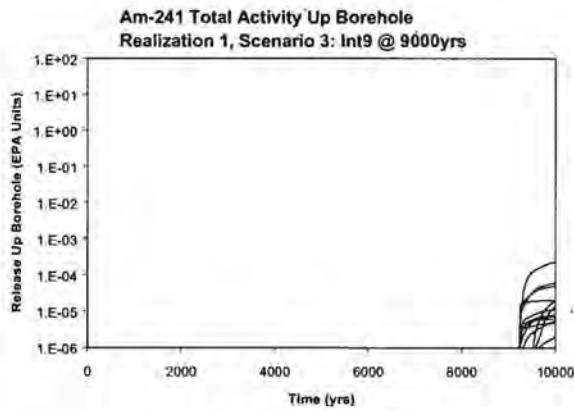


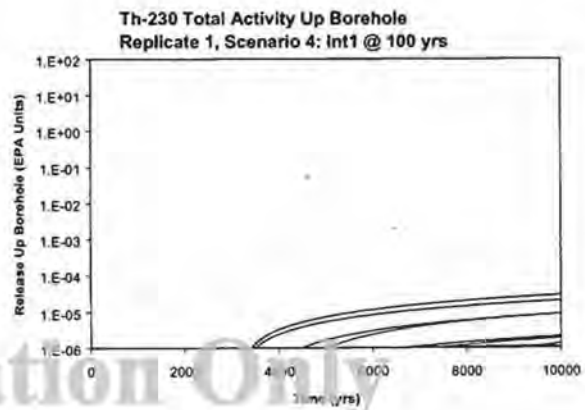
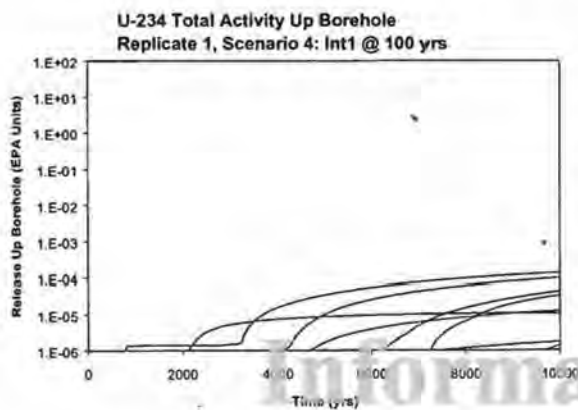
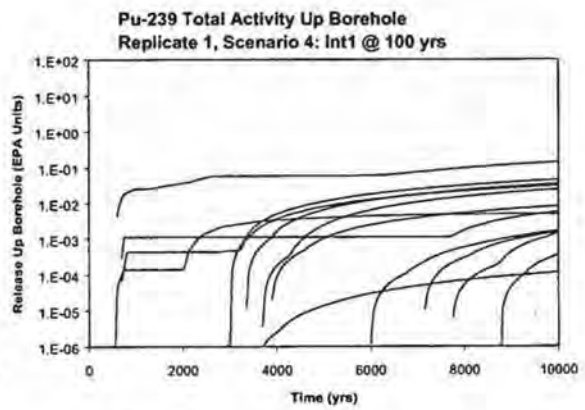
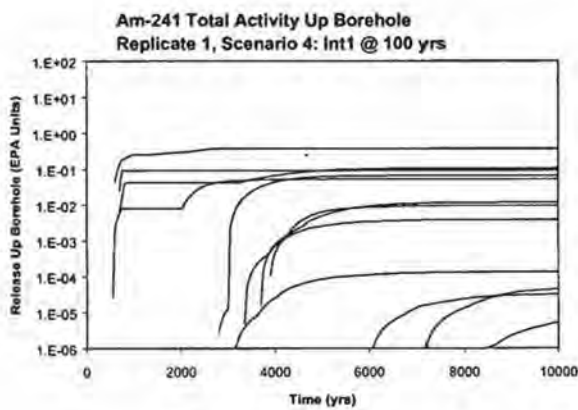
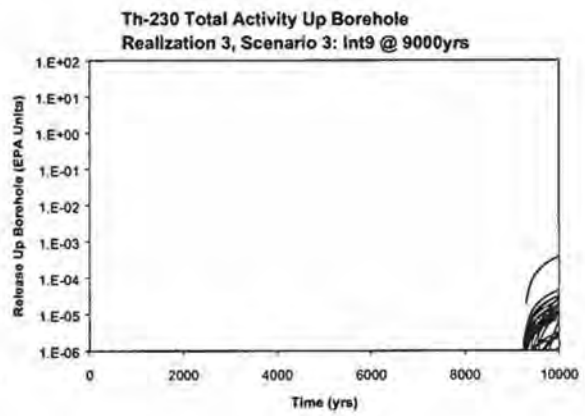
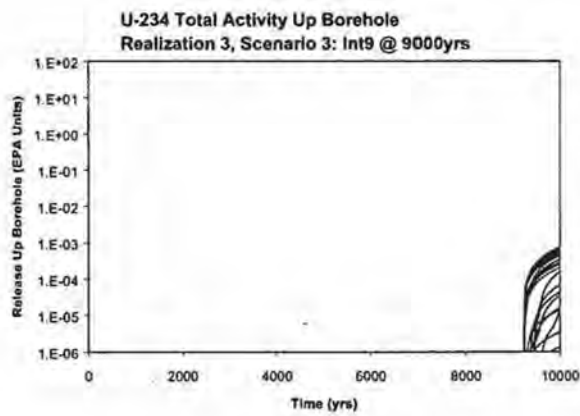
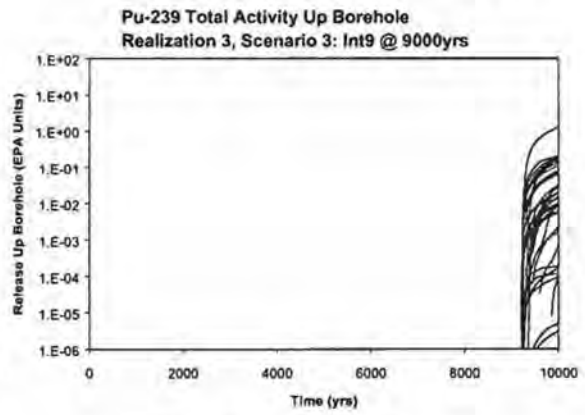
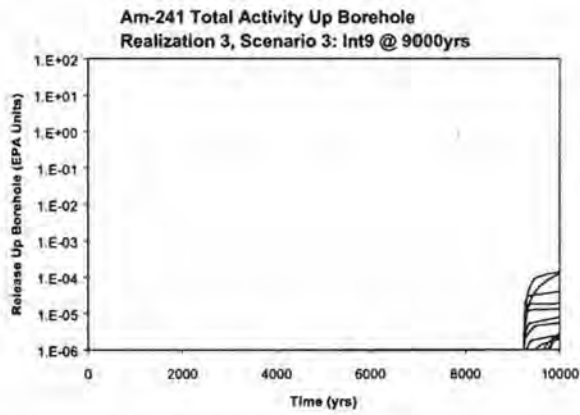


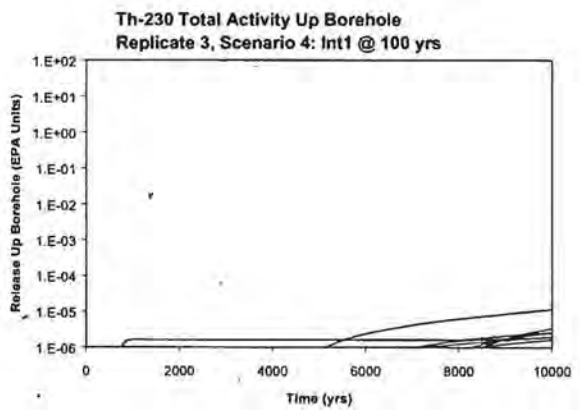
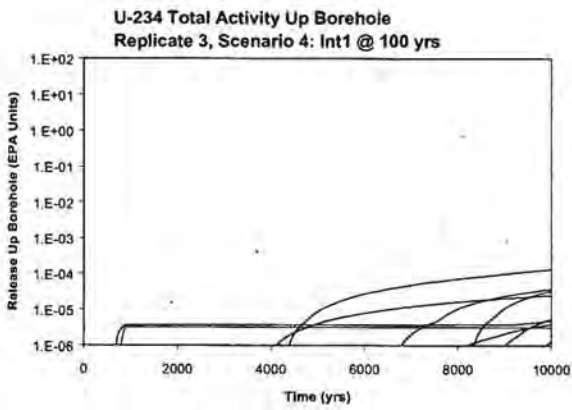
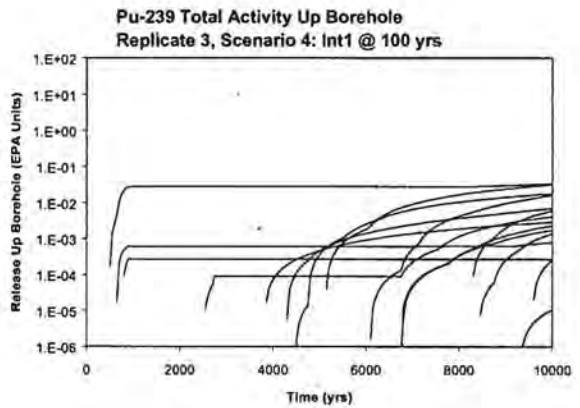
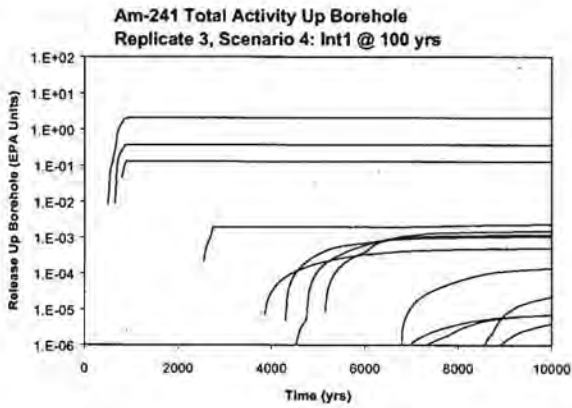
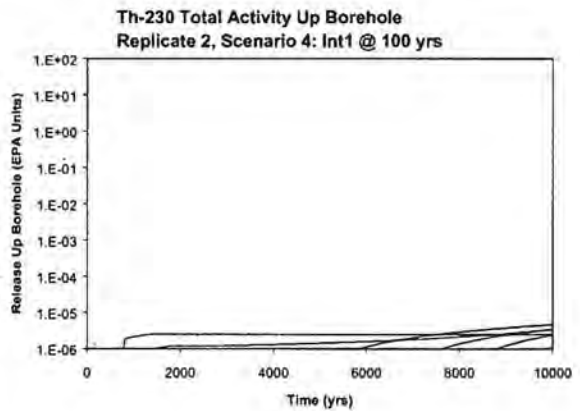
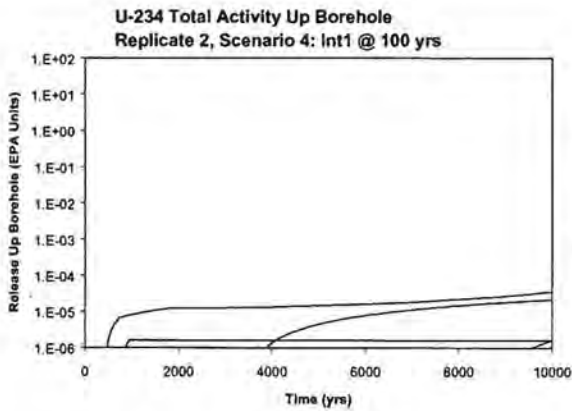
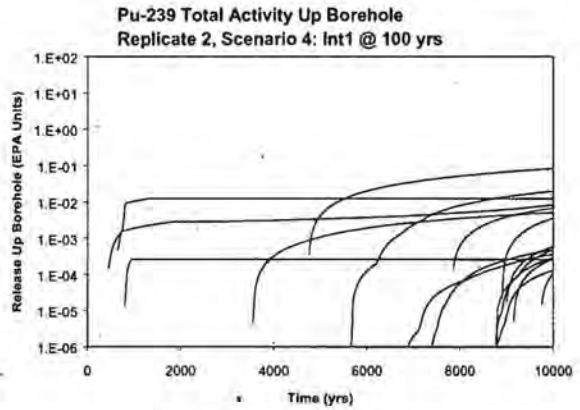
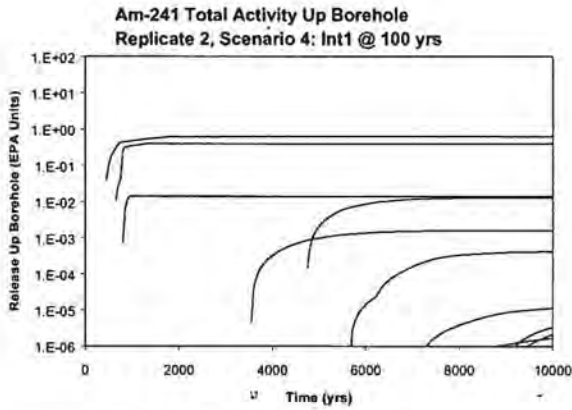


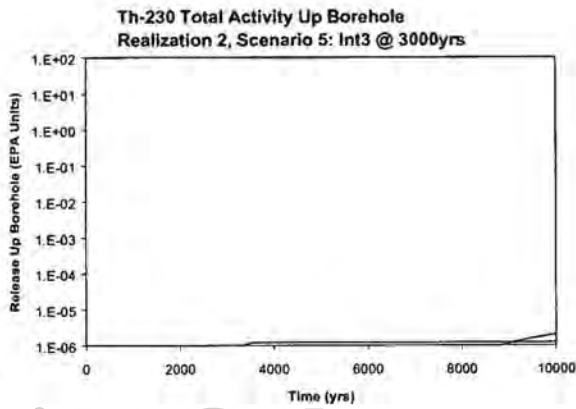
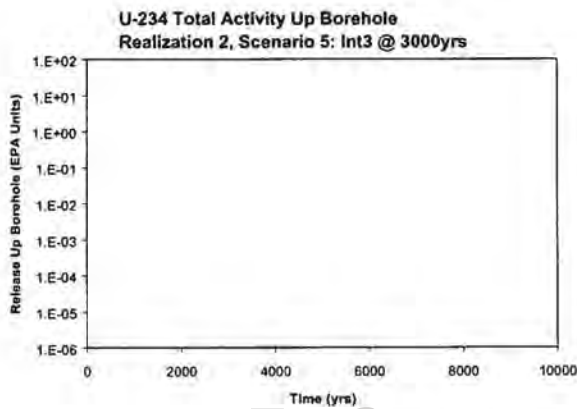
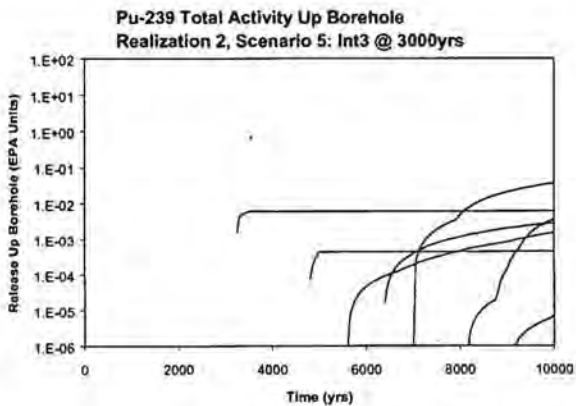
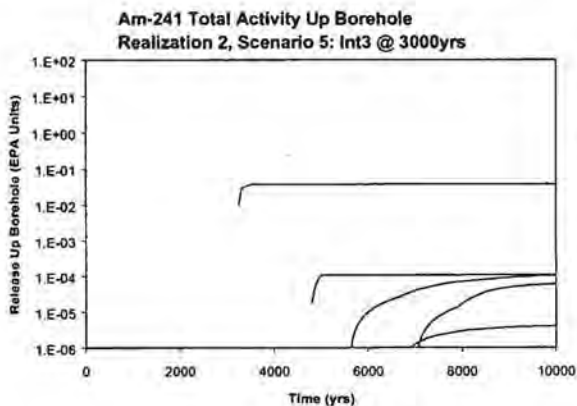
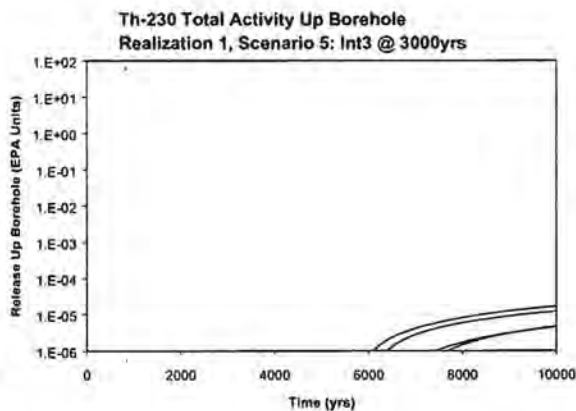
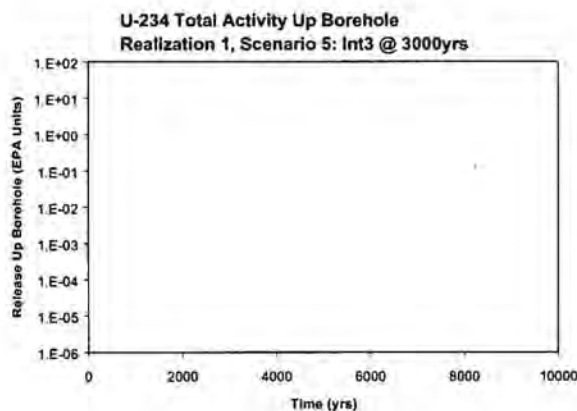
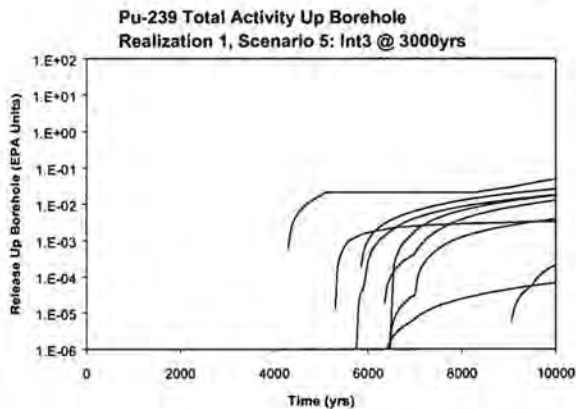
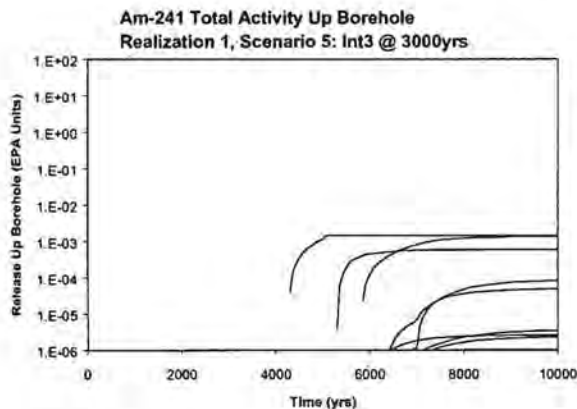


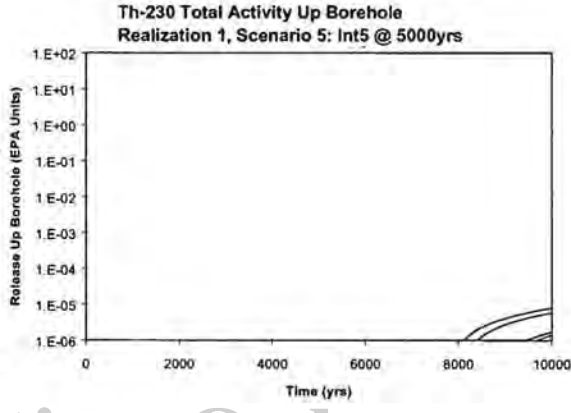
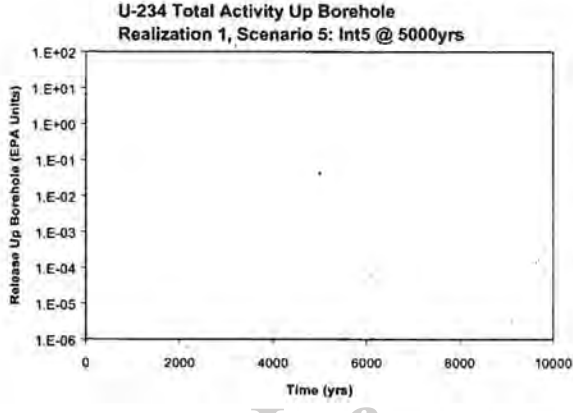
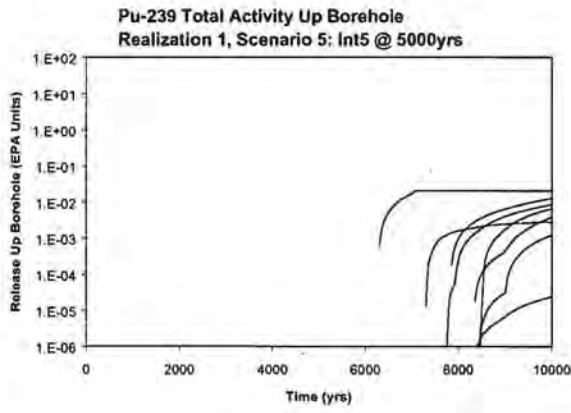
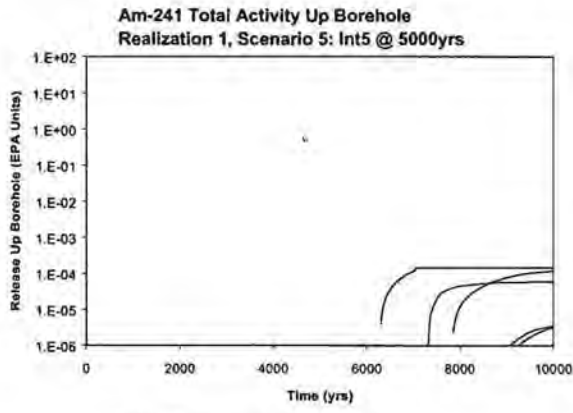
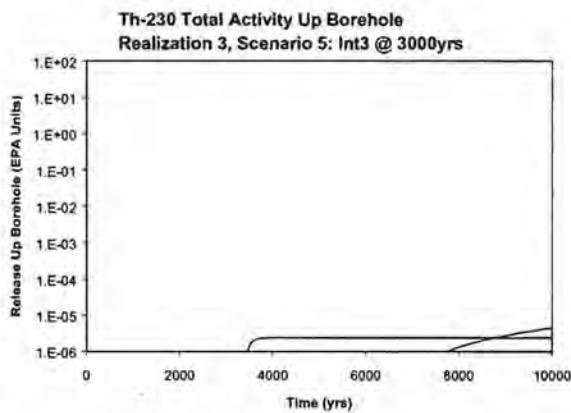
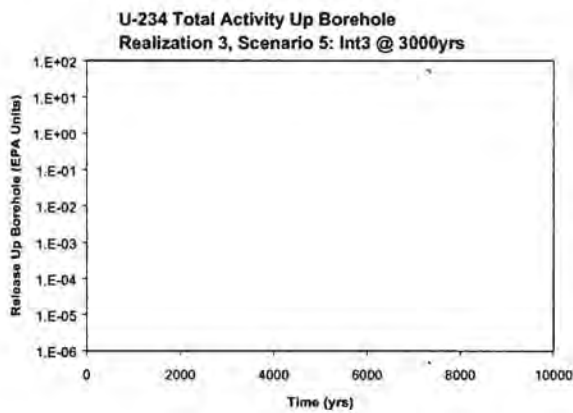
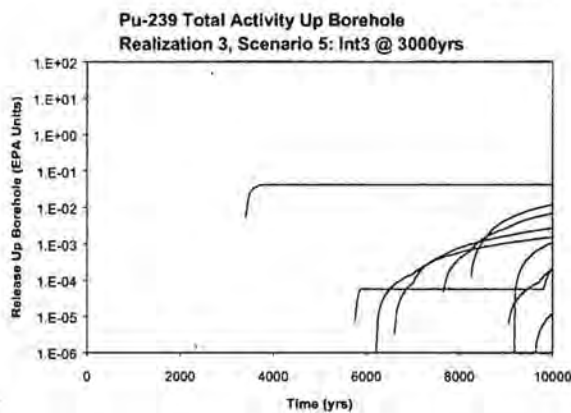
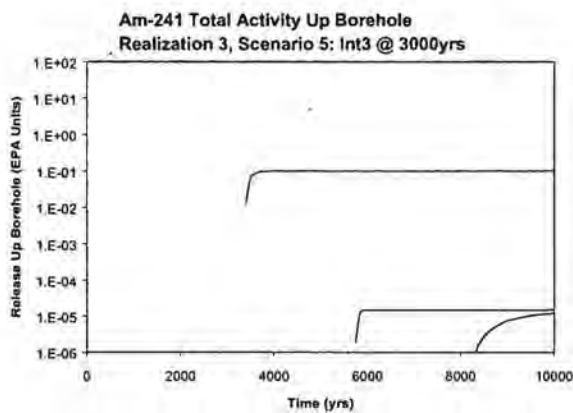




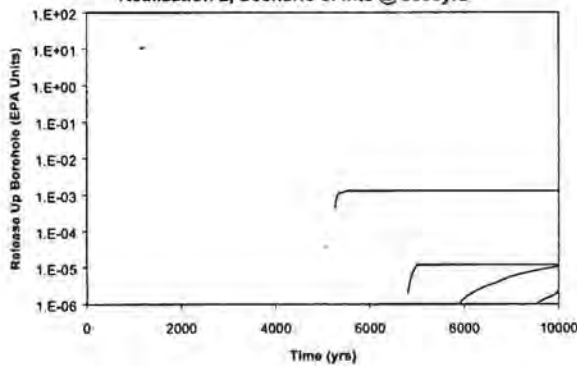




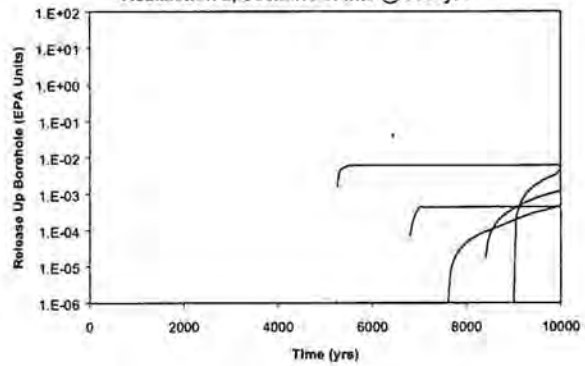




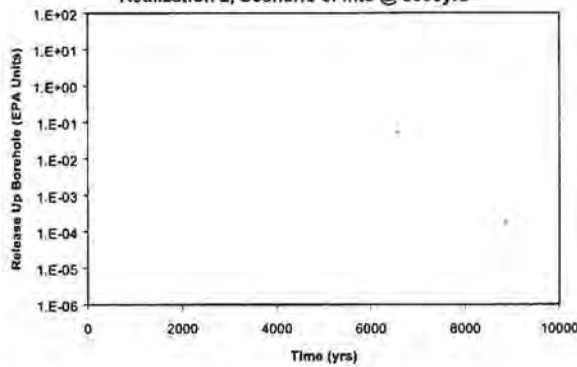
Am-241 Total Activity Up Borehole
Realization 2, Scenario 5: Int5 @ 5000yrs



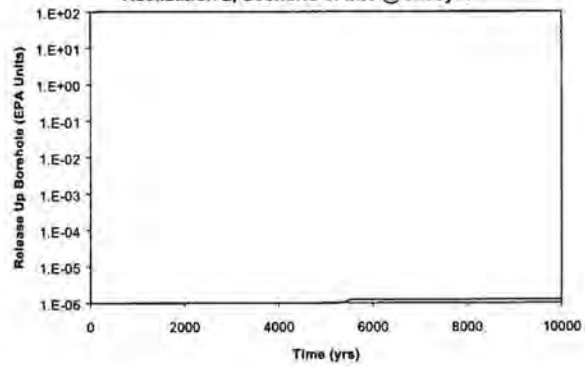
Pu-239 Total Activity Up Borehole
Realization 2, Scenario 5: Int5 @ 5000yrs



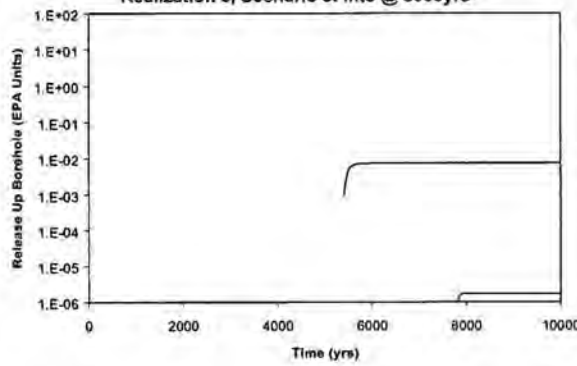
U-234 Total Activity Up Borehole
Realization 2, Scenario 5: Int5 @ 5000yrs



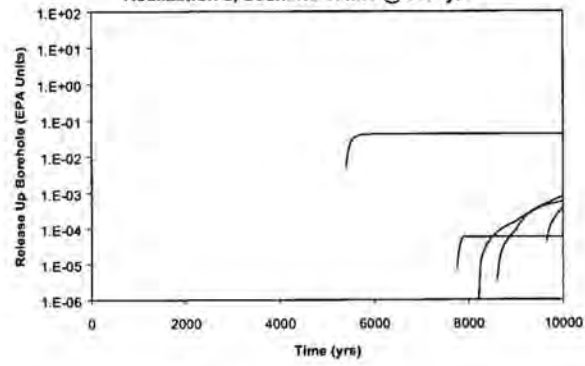
Th-230 Total Activity Up Borehole
Realization 2, Scenario 5: Int5 @ 5000yrs



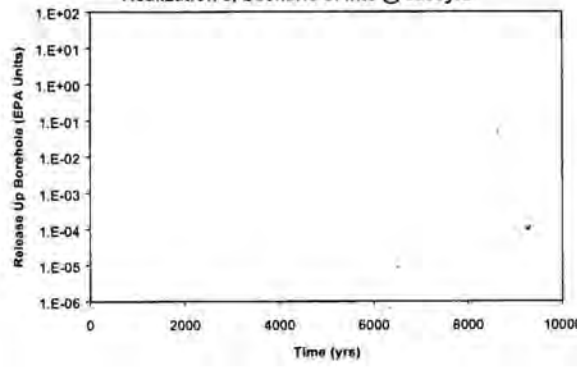
Am-241 Total Activity Up Borehole
Realization 3, Scenario 5: Int5 @ 5000yrs



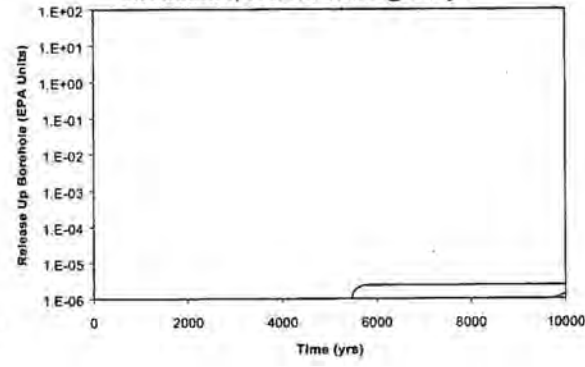
Pu-239 Total Activity Up Borehole
Realization 3, Scenario 5: Int5 @ 5000yrs

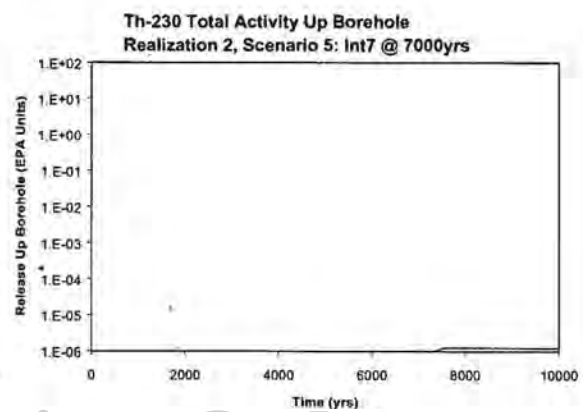
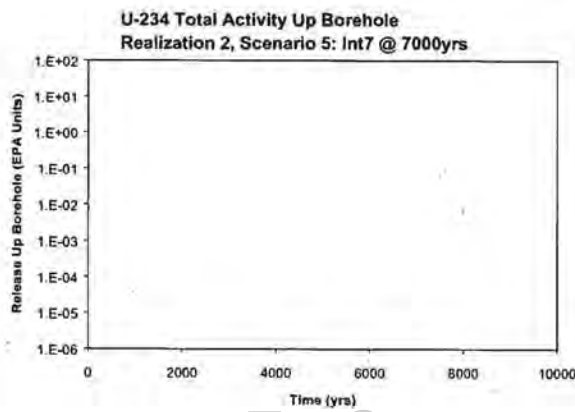
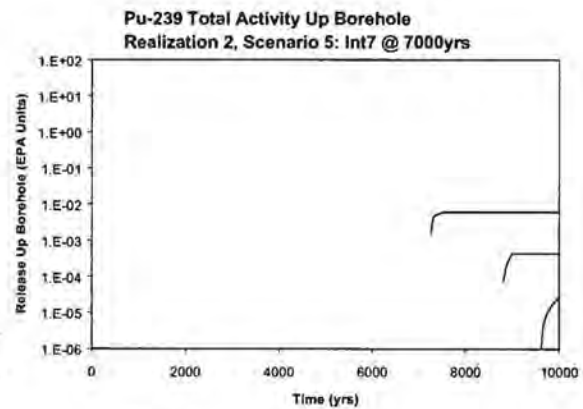
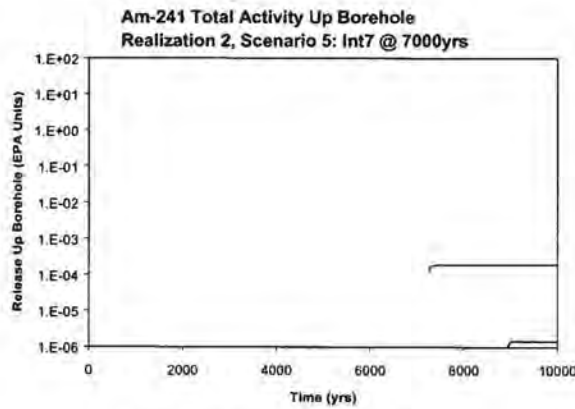
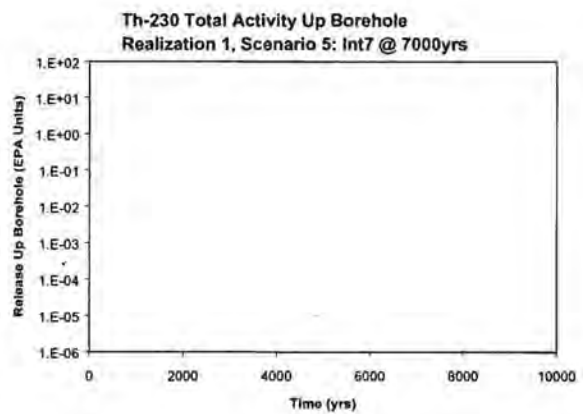
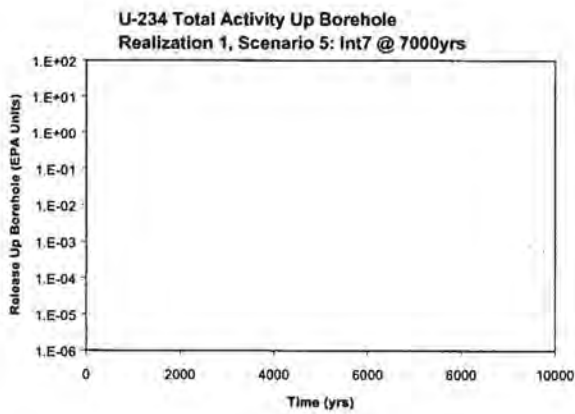
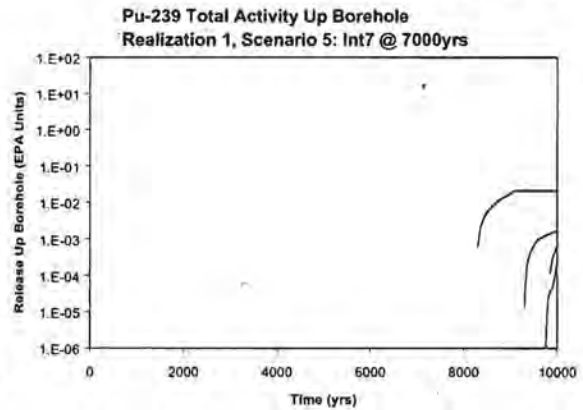
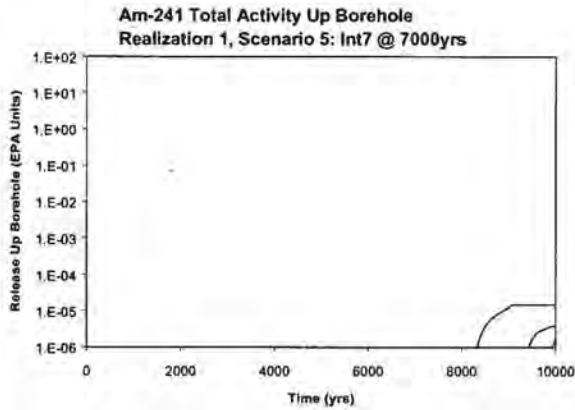


U-234 Total Activity Up Borehole
Realization 3, Scenario 5: Int5 @ 5000yrs

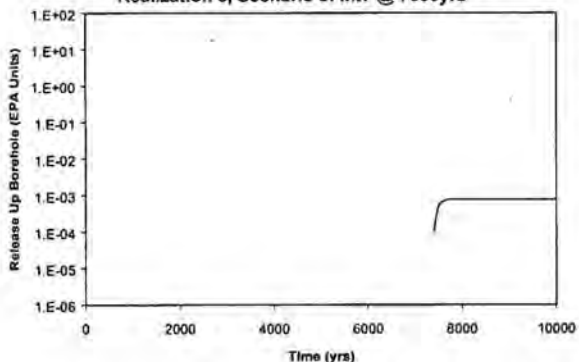


Th-230 Total Activity Up Borehole
Realization 3, Scenario 5: Int5 @ 5000yrs

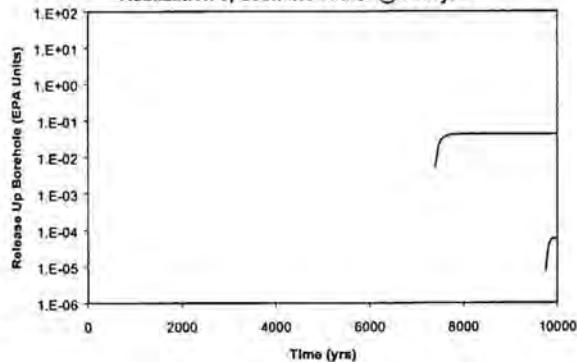




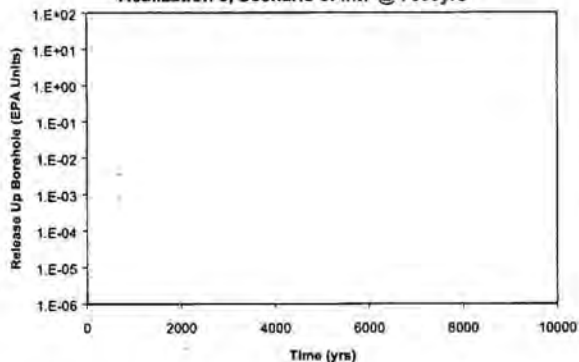
Am-241 Total Activity Up Borehole
Realization 3, Scenario 5: Int7 @ 7000yrs



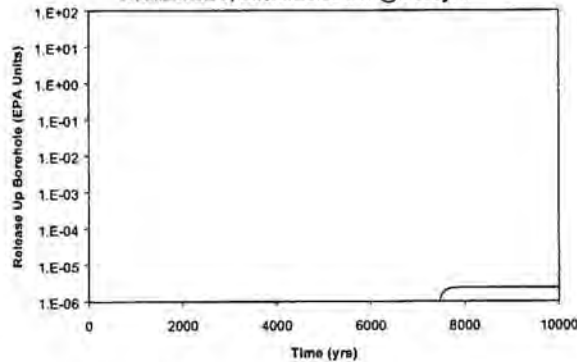
Pu-239 Total Activity Up Borehole
Realization 3, Scenario 5: Int7 @ 7000yrs



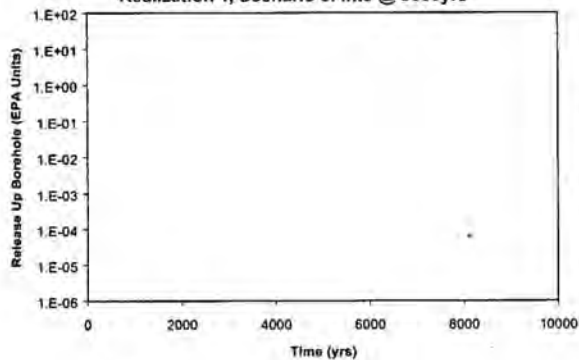
U-234 Total Activity Up Borehole
Realization 3, Scenario 5: Int7 @ 7000yrs



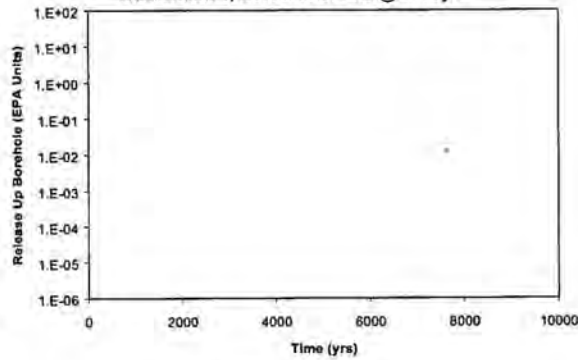
Th-230 Total Activity Up Borehole
Realization 3, Scenario 5: Int7 @ 7000yrs



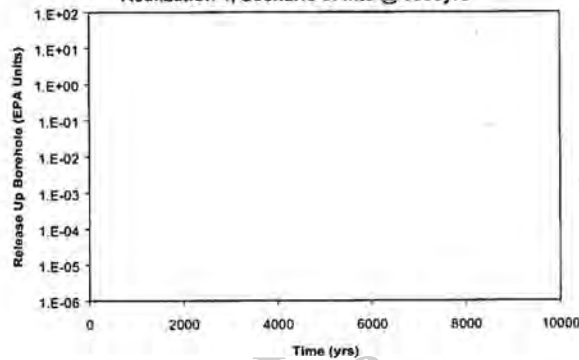
Am-241 Total Activity Up Borehole
Realization 1, Scenario 5: Int9 @ 9000yrs



Pu-239 Total Activity Up Borehole
Realization 1, Scenario 5: Int9 @ 9000yrs



U-234 Total Activity Up Borehole
Realization 1, Scenario 5: Int9 @ 9000yrs



Th-230 Total Activity Up Borehole
Realization 1, Scenario 5: Int9 @ 9000yrs

