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Sandia National Laboratories
Waste Isolation Pilot Plant

Analysis Package for Salado Transport Calculations:
CRA-2004 PA Baseline Calculation
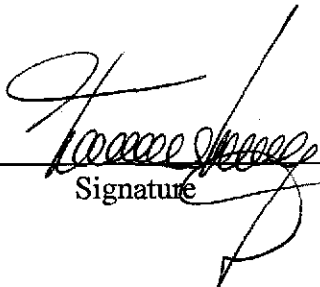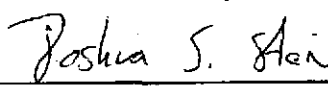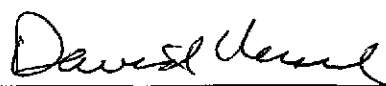## Revison 0

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Author:	Thomas S. Lowry (6115)	*[signature]*	8/30/2005
	Print	Signature	Date
Technical Review:	Joshua S. Stein (6852)	*[signature]*	9/1/2005
	Print	Signature	Date
Management Review:	David Kessel (6821)	*[signature]*	9/23/05
	Print	Signature	Date
QA Review:	Mario Chavez (6820)	*[signature]*	9/23/05
	Print	Signature	Date

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Executive Summary

This analysis package describes the transport calculations that are part of the "Salado Flow and Transport Calculations for the Performance Assessment Baseline Calculations of the Waste Isolation Pilot Plant" as described in Kanney and Leigh (2005). Specifically, it covers the calculations to determine the mobilization and subsequent migration of radioisotopes throughout the repository, the shaft system, the Salado formation, and possible human intrusion boreholes.

Major changes in the CRA-2004 PABC calculations relevant to this Analysis Report can be found in Analysis Plan AP-122 (Kanney and Leigh, 2005)., and Cotsworth (2005) and include:

1. Updated TRU waste inventory
2. Updated actinide solubility values
3. Updated actinide solubility uncertainty ranges
4. Changes to the microbial gas generation model
5. Updated versions of the Latin Hypercube Sampling (LHS) code

The PABC calculations presented here are based on the same performance assessment process as the CRA-2004, but use the updated parameter values listed above.

The screening runs produced 471 '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 release 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.

1. 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. The results of the most recent WIPP PA conducted by Sandia National Laboratories (SNL) have been included in DOE's 2004 WIPP Compliance Recertification Application (CRA-2004) (U.S. DOE 2004), which is currently being reviewed by the EPA.

The EPA has recently sent a letter to DOE regarding a performance assessment baseline calculation (Cotsworth 2005), henceforth referred to as the CRA-2004 PABC. In the letter, the EPA notes that a number of modeling assumptions used in the CRA-2004 have not been sufficiently justified and that alternative modeling assumptions must be used.

Major changes in the CRA-2004 PABC calculations relevant to this Analysis Report can be found in Analysis Plan AP-122 (Kanney and Leigh, 2005)., and Cotsworth (2005) and include:

6. Updated TRU waste inventory
7. Updated actinide solubility values
8. Updated actinide solubility uncertainty ranges
9. Changes to the microbial gas generation model
10. Updated versions of the Latin Hypercube Sampling (LHS) code

The PABC calculations presented here are based on the same performance assessment process as the CRA-2004, but use the updated parameter values listed above.

1.2.   Purpose

This analysis package describes the transport calculations that are part of the "Salado Flow and Transport Calculations for the Performance Assessment Baseline Calculations of the Waste Isolation Pilot Plant" as described in Kanney and Leigh (2005). Specifically, it covers the calculations to determine the mobilization and subsequent migration of radioisotopes throughout the repository, the shaft system, the Salado formation, and possible human intrusion boreholes. Much of the background information for the PABC is based on the CRA-2004. This document presents only the changes and updates in the PABC that differ from the CRA-2004 and thus the reader is advised to review Lowry (2004) 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 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 results. Section 5 provides a summary of the information detailed in Sections 1 to 4. The reader is reminded that this report covers only those items that are different from those used in the CRA-2004 calculations. Where it is appropriate, some detail of the CRA-2004 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 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 and Leigh, 2005). 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 structured Monte Carlo sampling method in which samples are drawn from bins of equal probability and correlations between parameters are minimized. 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.

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 and these results are required prior to running NUTS. NUTS requires as input the BRAGFLO ASCII input file containing the grid specifications, initialization parameters, and material maps as well as the BRAGFLO post-processed binary file (CDB) that describes the flow-field. 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 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, MATLAB v7.0.4.365 is used to plot the breakthrough curves for each replicate/vector/isotope combination.

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 MATLAB and then plotted. The flow chart in Figure 1 illustrates the relationship between the major codes used in this analysis.

Table 1 – List of the major codes used in this analysis for the CRA-2004 PABC.

Code	Version	Code Function
ALGEBRACDB	2.35	Data processor
BRAGFLO	5.00	Brine and gas flow
GENMESH	6.08	Grid generation
ICSET	2.22	Sets initial conditions
LHS	2.42	Latin hypercube sampler
MATSET	9.10	Sets material parameters
NUTS	2.05a	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
SUMMARIZE	2.20	Data interpolation
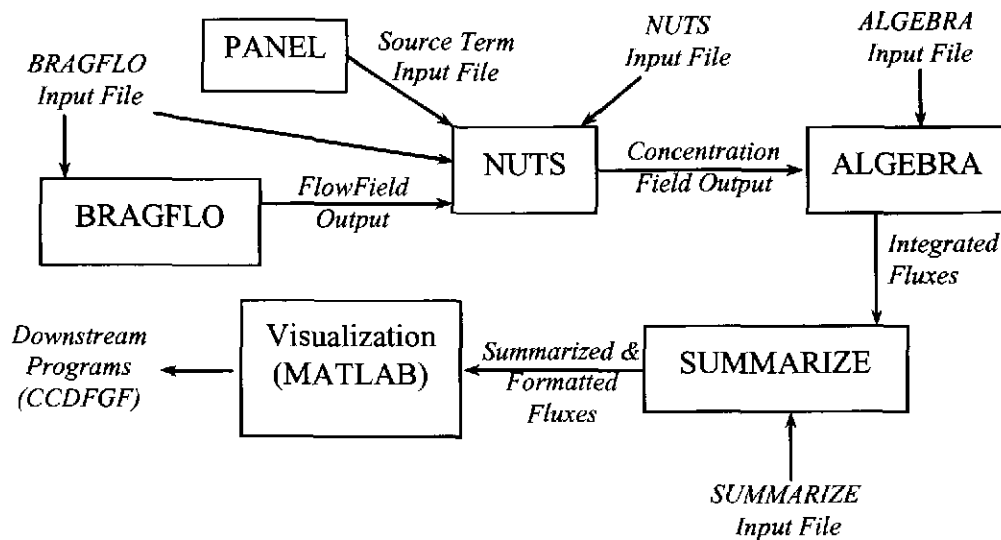
Figure 1 – Relationship and data flow for major codes used in the NUTS analysis.

2.4.   Type of Model Runs

Three types of model runs are performed using NUTS; screening runs (SCN), 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 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" (crosses 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 147, 163, and 161 vectors out of a possible 500 (each), respectively. This is slightly higher than the 134, 146, and 135 vectors screened in for the CRA-2004 calculations. Table 2 lists the screened in vectors for each replicate/scenario combination. For scenario S1, only one vector (vector 53 of R1) was screened in based on the 10^{-7} kg mass flux criteria. The other listed vectors for

S1 (shown in italics) are vectors that were run as an S1 to provide the conditions at the time of intrusion for the ISO and TI runs.

A FORTRAN program called SCREEN.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.FOR and the verfication documentation is reproduced in Appendix A.

Table 2 – Screened-in vectors for each scenario/replicate combination. The vectors shown in italics are vectors that were run as an S1 to provide the conditions at the time of intrusion for the ISO and TI runs. The only vector to be screened-in under S1 was vector 53 (non-italicized).

Replicate	Scenario	Vector Number
R1	S1	*2, 3, 7, 8, 9, 10, 12, 13, 14, 16, 17, 20, 22, 23, 24, 25, 26, 27, 28, 29, 30, 34, 35, 36, 38, 41, 43, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 58, 59, 60, 61, 62, 63, 64, 66, 67, 69, 70, 71, 72, 73, 74, 76, 78, 79, 80, 82, 83, 84, 86, 88, 89, 90, 92, 93, 94, 98*
	S2	2, 3, 7, 8, 9, 10, 12, 13, 14, 16, 17, 20, 22, 23, 24, 25, 26, 27, 28, 29, 30, 34, 35, 36, 38, 41, 43, 45, 46, 47, 48, 49, 50, 51, 52, 54, 55, 58, 59, 60, 61, 62, 63, 64, 66, 67, 69, 70, 71, 72, 73, 74, 76, 78, 79, 80, 82, 83, 84, 86, 88, 89, 90, 92, 93, 94, 98
	S3	2, 3, 7, 8, 9, 10, 12, 13, 14, 16, 17, 20, 22, 23, 25, 27, 28, 29, 30, 34, 35, 36, 41, 43, 45, 46, 47, 49, 50, 54, 55, 58, 59, 60, 61, 62, 63, 66, 67, 70, 71, 76, 78, 79, 80, 82, 83, 84, 86, 89, 90, 92, 93, 94, 98
	S4	7, 9, 12, 16, 17, 27, 36, 45, 50, 55, 76, 78
	S5	7, 9, 12, 16, 17, 27, 36, 45, 50, 55, 76, 78
R2	S1	*2, 3, 4, 6, 8, 9, 10, 11, 12, 14, 16, 17, 18, 19, 20, 21, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 43, 44, 45, 48, 49, 50, 51, 52, 53, 54, 55, 56, 59, 61, 62, 63, 64, 65, 66, 67, 68, 69, 71, 72, 74, 75, 77, 79, 80, 81, 83, 84, 87, 89, 90, 91, 92, 95, 96, 98, 99*
	S2	2, 3, 4, 6, 8, 9, 10, 11, 12, 14, 16, 17, 18, 19, 20, 21, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 43, 44, 45, 48, 49, 50, 51, 52, 53, 54, 55, 56, 59, 61, 62, 63, 64, 65, 66, 67, 68, 69, 71, 72, 74, 75, 77, 79, 80, 81, 83, 84, 87, 89, 90, 91, 92, 95, 96, 98, 99, 100
	S3	3, 4, 6, 8, 9, 12, 14, 16, 17, 18, 20, 21, 24, 25, 26, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 39, 40, 41, 44, 48, 50, 51, 52, 53, 54, 55, 56, 59, 63, 65, 66, 67, 68, 71, 72, 74, 75, 77, 79, 80, 84, 87, 89, 90, 91, 92, 95, 96, 98, 99
	S4	4, 17, 24, 28, 34, 36, 40, 55, 63, 68, 79, 92, 95, 98
	S5	4, 17, 24, 28, 34, 40, 55, 63, 68, 79, 92, 95, 98
R3	S1	*2, 3, 4, 10, 11, 13, 14, 15, 17, 18, 21, 22, 24, 25, 26, 27, 28, 29, 30, 32, 33, 34, 35, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 49, 50, 52, 53, 56, 58, 59, 60, 61, 62, 63, 64, 65, 66, 67, 68, 69, 70, 71, 73, 74, 76, 77, 78, 79, 84, 85, 86, 88, 89, 90, 91, 93, 94, 95, 96, 97, 98, 99*
	S2	2, 3, 4, 10, 11, 13, 14, 15, 17, 18, 21, 22, 24, 25, 26, 27, 28, 29, 30, 32, 33, 34, 35, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 49, 50, 52, 53, 56, 58, 59, 60, 61, 62, 63, 64, 65, 66, 67, 68, 69, 70, 71, 73, 74, 76, 77, 78, 79, 84, 85, 86, 88, 89, 90, 91, 93, 94, 95, 96, 97, 98, 99, 100
	S3	2, 10, 11, 14, 15, 18, 21, 24, 25, 27, 28, 29, 30, 32, 33, 34, 35, 37, 38, 39, 40, 42, 43, 44, 45, 46, 47, 49, 50, 53, 56, 58, 59, 60, 61, 63, 64, 65, 66, 67, 68, 69, 73, 74, 77, 78, 79, 84, 86, 88, 89, 91, 93, 94, 95, 96, 97, 98
	S4	30, 35, 42, 44, 47, 49, 53, 59, 66, 69, 77, 86, 91, 93, 96
	S5	30, 35, 37, 42, 47, 49, 53, 59, 66, 69, 77, 86, 93, 96

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:

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

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 17, below). The final conclusion of the decay chain analysis is that five "lumped" isotopes are modeled based on the following simplified decay chains:

^{241}Am

^{238}Pu $\;\longrightarrow\;$ ^{234}U $\;\longrightarrow\;$ ^{230}Th

^{239}Pu
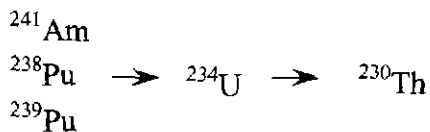
These are the same isotopes modeled for the CRA-2004 and the CCA, justified by the fact that the available isotopes in the waste packages have not changed since that time. A complete justification for the use of these five isotopes can be found in Stockman et al. (1996).

For this analysis, only ^{241}Am, ^{239}Pu, ^{234}U, and ^{230}Th are examined individually in the output since the half-life of ^{238}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}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 3000, 5000, 7000, and 9000 yrs. For times greater then 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 then 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, and/or ES-45, running Open VMS Version 7.3-1 (WIPP PA, 2003a,b). 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, 2003c).

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. A detailed description of the run control procedures used for the CRA-2004 PABC, including the NUTS calculations, is described in Long and Kanney (2005).

There are three sets of input files for all three programs; one each for the SCN, 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 B, C, and D.

CRA-2004 and CRA-2004 PABC BRAGFLO Grid
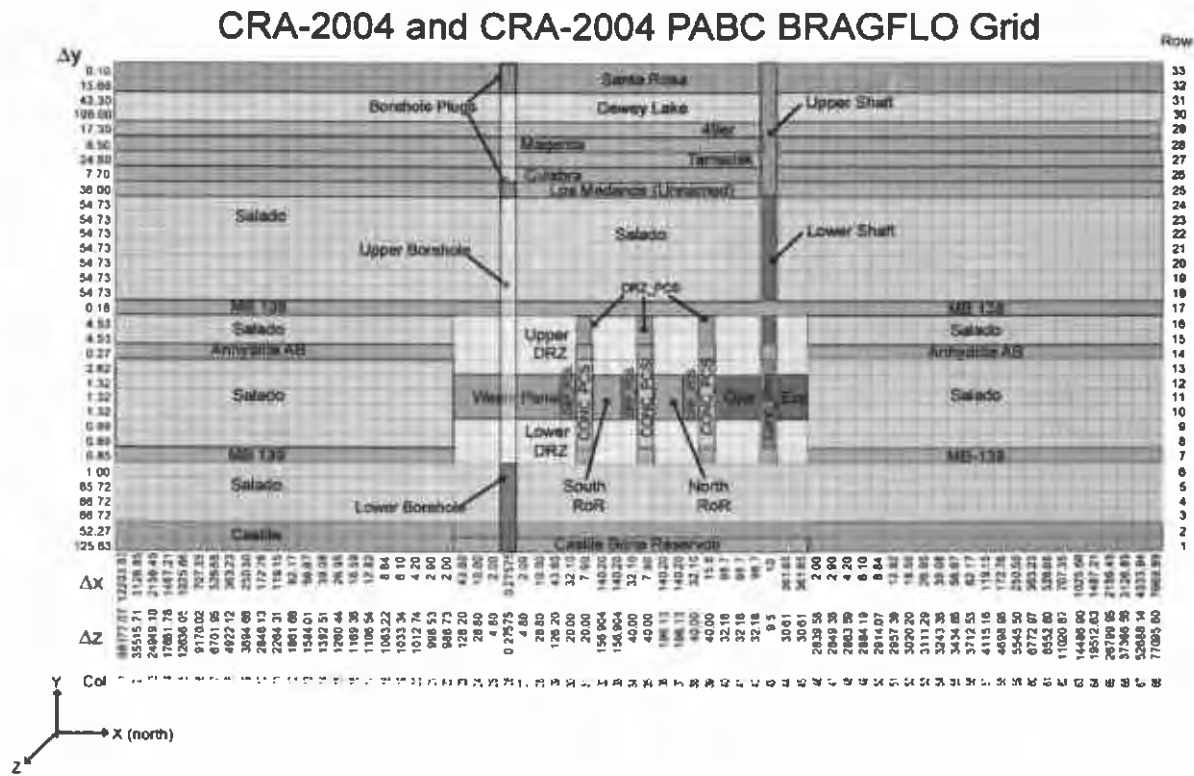
Figure 2 – Computational grid used for the BRAGFLO and NUTS runs for the Salado Flow and transport calculations. MB refers to the marker beds, DRZ is the disturbed rock zone surrounding the repository area, SHFTU is the upper shaft area, SHFTL is the lower shaft area. The green area within the DRZ is 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 PABC 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
LIBCRA1BC_NUT	NUT_SCN_CRA1BC_Ss.INP	NUTS screening runs input
	NUT_ISO_CRA1BC_Ss.INP	NUTS ISO runs input
	NUT_INT_CRA1BC_Ss_Ttttt.INP**	NUTS TI runs input
	ALG_NUT_SCN_CRA1BC.INP	ALGEBRA screening runs input
	ALG_NUT_ISO_CRA1BC_Ss.INP	ALGEBRA ISO runs input
LIBCRA1BC_NUTRxSy	NUT_SCN_CRA1BC_Rr_Ss_Vvvv.CDB	NUTS screening runs binary output
	NUT_ISO_CRA1BC_Rr_Ss_Vvvv.CDB	NUTS ISO runs binary output***
	NUT_INT_CRA1BC_Rr_Ss_Ttttt_Vvvv.CDB**	NUTS TI runs binary output***
	SCREEN_NUT_SCN_CRA1BC_Rr_Ss.OUT	SCREEN.FOR output file
	ALG_NUT_SCN_CRA1BC_Rr_Ss_Vvvv.CDB	ALGEBRA SCN runs binary output
	ALG_NUT_ISO_CRA1BC_Rr_Ss_Vvvv.CDB	ALGEBRA ISO runs binary output***
	ALG_NUT_INT_CRA1BC_Rr_Ss_Ttttt_Vvvv.CDB**	ALGEBRA TI runs binary output***
	SUM_NUT_SCN_CRA1BC_Rr_Ss.INP	SUMMARIZE SCN runs input
	SUM_NUT_SCN_CRA1BC_Rr_Ss.TBL	SUMMARIZE SCN runs output

*File naming convention: Rx refers to the replicate number (r=1, 2, or 3), Ss refers to the scenario number (s=1 to 5), Ttttt refers to the intrusion time ($ttttt$=00100, 03000, 05000, 07000, or 09000), Vvvvv refers to the vector number (vvv = 001, 002, ... , 099, 100)

**TI files are only applicable to scenarios 2 to 5

***These files are generated only for vectors that are 'screened-in'

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 Nemer and Stein (2005).

When brine enters the disposal region, gas is generated by anoxic corrosion of iron and biodegradation of organic materials, resulting in the eventual release of radioisotopes into the brine from the waste. If sufficient quantities of gas are generated, pressures in the disposal region will increase, reducing brine flow into the repository. Brine containing dissolved radioisotopes may be expelled from the repository if pressure in the repository exceeds the brine pressure in the immediately surrounding formation. Brine saturation in the waste 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. 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 and results of the screening runs 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 68, 75, and 73 screened-in runs, respectively. The screenings detected the conservative contaminant at the LWB through the Marker Beds. However, none of the vectors had activities greater than 1.00×10^{-7} EPA Units when modeled for the ISO case. For replicates R1, R2, and R3, the maximum total integrated activity across the LWB was 1.3169×10^{-12}, 1.4880×10^{-25}, and 1.8078×10^{-19} EPA Units, respectively. As explained in Lowry (2004), these values are most likely due to numerical dispersion as a result of the NUTS finite-difference solution method.

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. With the exception of one vector (v053) from R1, all vectors for S2 were screened in due to contaminant movement up the borehole. The v053 vector from the R1 SCN run showed contaminant movement through the Marker Beds. However, for the ISO runs, v053/R1 shows a total integrated activity of 2.379×10^{-12} EPA Units in the Marker Beds at the LWB, which is five orders of magnitude lower than the 1.0×10^{-7} EPA Units threshold. For this reason, the rest of this discussion focuses on the balance of the replicate/vector combinations that showed contaminant movement only up the borehole. Specifically, this 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 7 to Figure 9. 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 R2S2v031, which showed an integrated activity of 43.109 EPA units for ^{239}Pu. For ^{241}Am, vector R3S2v066 showed the maximum with an integrated activity of 36.67 EPA units. Both of these values are higher than the 21.63 EPA Units for ^{241}Am and 5.24 EPA Units for ^{239}Pu from the CRA-2004 calculations (Lowry 2004). ^{234}U and ^{230}Th were comparatively minor with

maximums for each of 0.066813 and 0.14455 EPA units in vectors R3S2v042 and R1S2v017, respectively. On the average, [241]Am and [239]Pu account for 63.6% and 34.8% of the total activity respectively with [234]U and [230]Th comprising 1.2% and 0.4% each. This is similar to the percentages from the CRA-2004, of 68.1%, 31.4% for [241]Am and [239]Pu, and 0.5% for [234]U and [230]Th combined. 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:

$$\frac{\sum_{i=1}^{N_{SI}} \dfrac{EPA_{ISO_i}}{EPA_{T_i}}}{N_{SI}} = \overline{P} \tag{2}$$

where EPA_{ISOi} is the 10,000 year activity for a particular isotope, EPA_{Ti} is the 10,000 year total activity (including [238]Pu), N_{SI} is the number of screened in vectors, $\overline{P}$ 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.

E1 at 350 yrs (R1, R2, R3)

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-in vectors and the maximum activities are slightly less.

The only pathway with any activity for S3 is through the borehole with no activity 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 10 to Figure 12. As can be seen in the figures, and like the S2 scenario, the releases for the S3 take place over a short period of time. The maximum activity for any isotope occurred in R1S3v017, which showed an integrated activity of 16.244 EPA units for ^{241}Am. For ^{239}Pu, vector R2S3v019 showed the maximum with an integrated activity of 30.275 EPA units. ^{234}U and ^{230}Th were comparatively minor with maximums for each of 0.0515 and 0.1346 showing in vector R3S3v042 and R2S3v019, respectively. On the average, ^{241}Am and ^{239}Pu account for 37.9% and 60.0% of the total activity respectively with ^{234}U and ^{230}Th comprising 1.8% and 0.4% each. For the CRA-2004, the percentage contribution for ^{241}Am, ^{239}Pu, ^{234}U and ^{230}Th combined was 48.2%, 50.9%, and 0.9%, respectively. 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 13 to Figure 15 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 18.1% to the total and ^{239}Pu contributes 72.8%. The maximum activities for ^{241}Am, ^{239}Pu, ^{234}U, and ^{230}Th are 1.4906, 2.9345, 0.8047, and 0.0015 EPA units, respectively. The releases in EPA units for each isotope and the total release are shown in Figure 5.
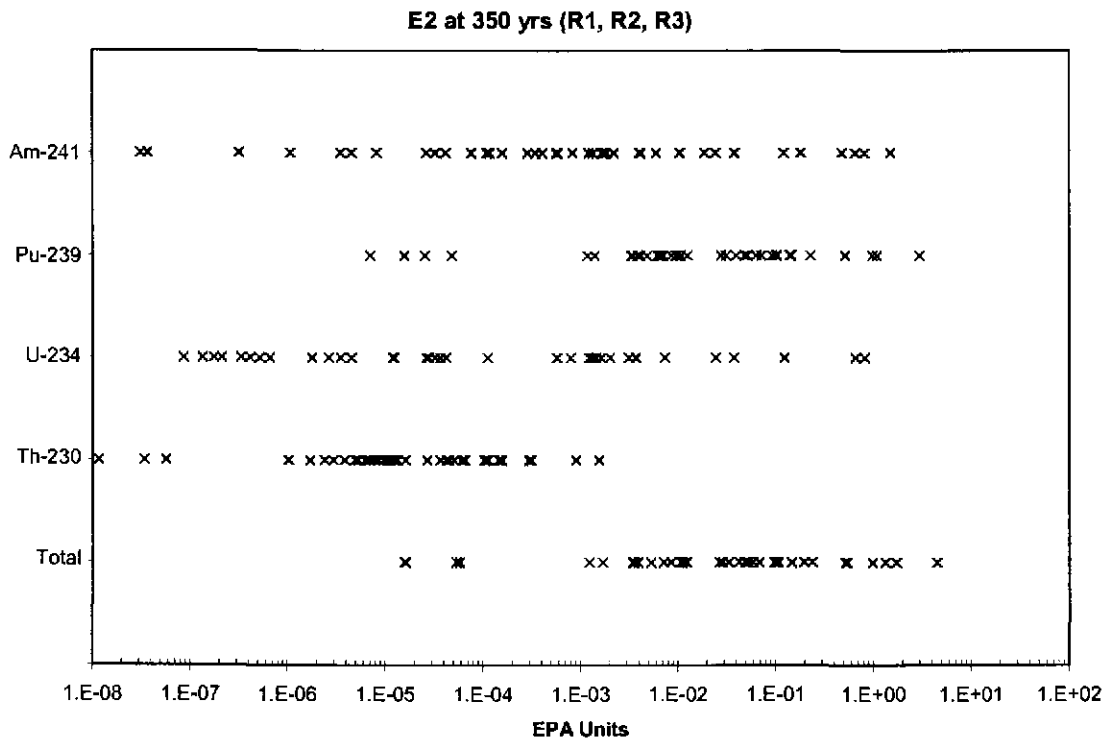
Figure 5 – Normalized Cumulative Release (EPA Units) to the Culebra from the borehole for each isotope and the total for Scenario 4: Borehole intrusion into the repository at 350 years.

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 16 to Figure 18 show the time-series plots for each vector across all replicates. Again, the plots appear more 'disorganized' then the E1 intrusion plots. For S5, ^{241}Am contributes 12.8% to the total and ^{239}Pu contributes 82.2%. 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 0.3204, 1.5313, 0.0072, and 0.0014 EPA units, respectively. The releases in EPA units for each isotope and the total release are shown in Figure 6.
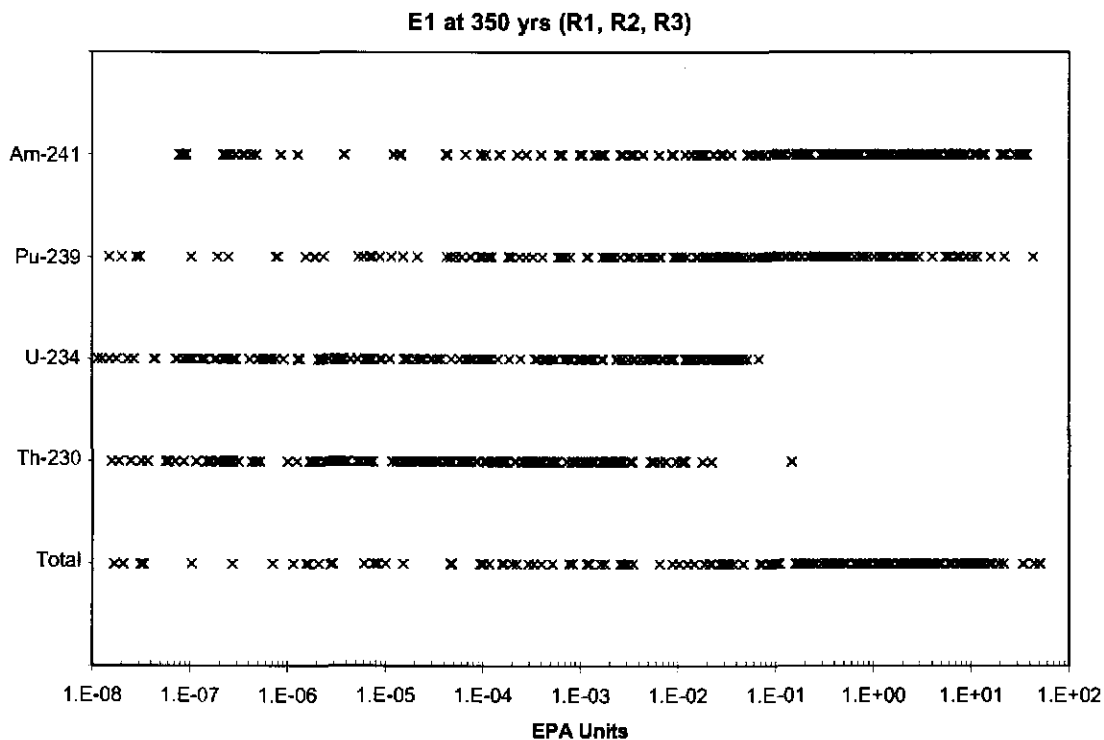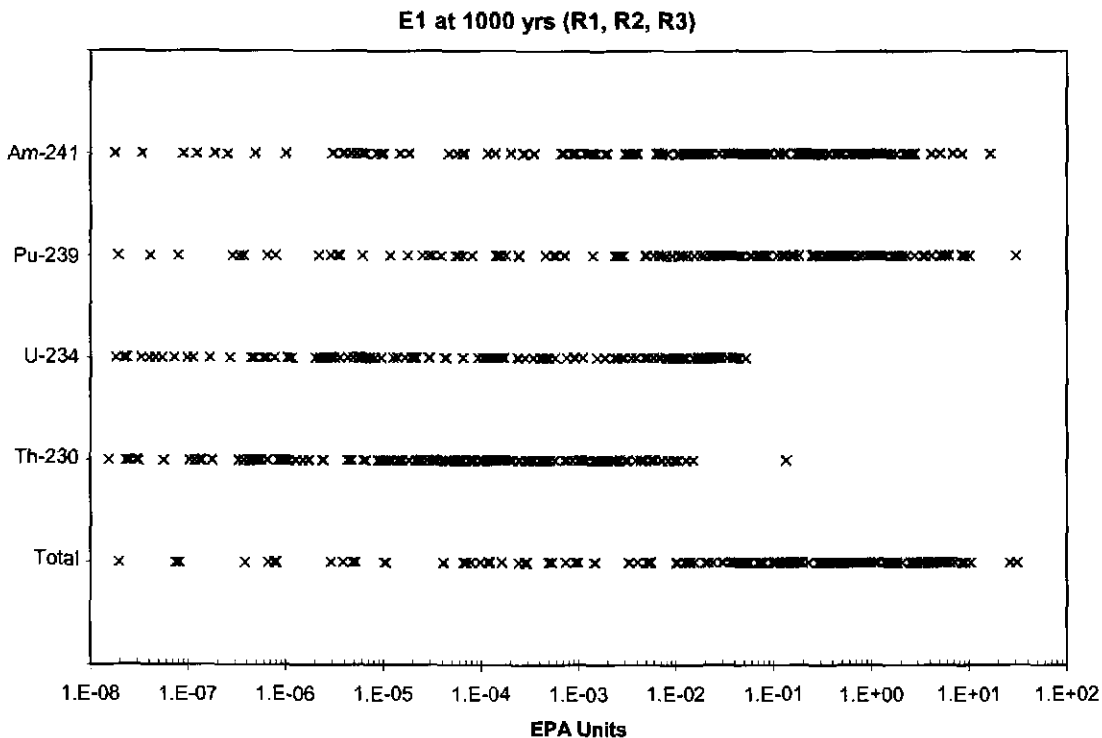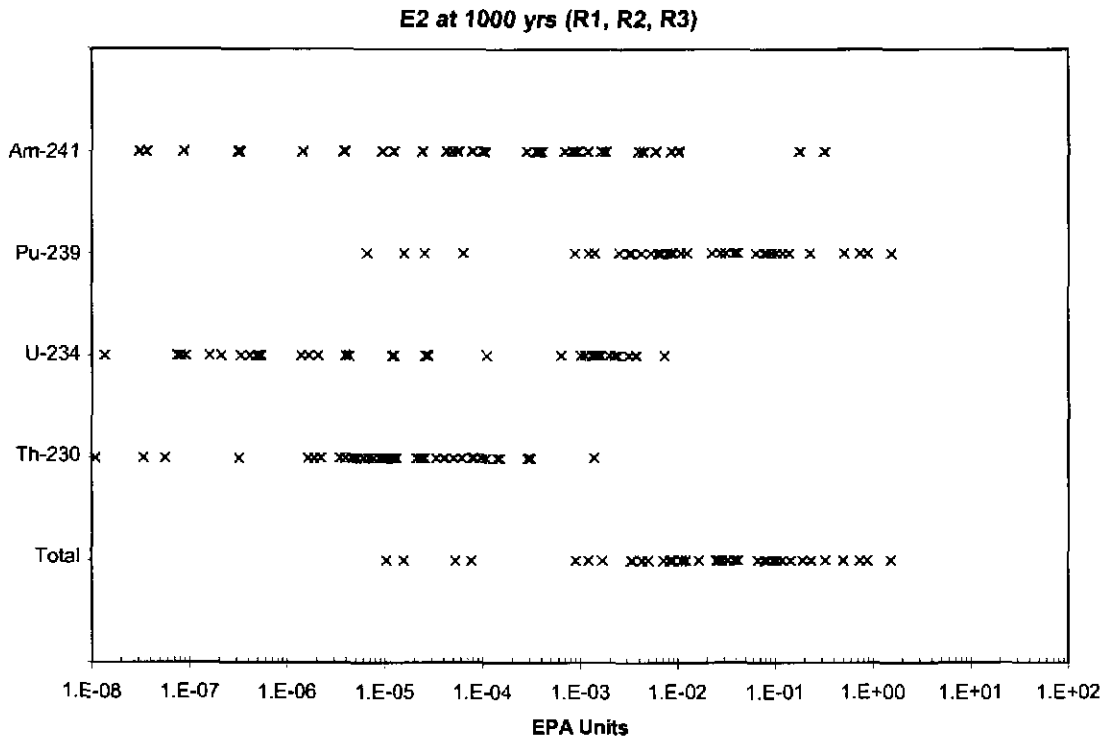

Figure 6 – Normalized Cumulative Release (EPA Units) to the Culebra from the borehole for each isotope and the total for Scenario 5: Borehole intrusion into the repository at 1000 years.

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 4 shows the maximum normalized release in EPA units for each scenario/intrusion time combination. The time series plots for each isotope at each time/vector/replicate combination are presented in Appendix E.

Table 4 – Maximum normalized release (EPA units) of each isotope at the Borehole/Culebra interface at each time interval of intrusion. The 'Total' maximum release is the maximum for a single vector whereas the maximum for each isotope for each scenario may be from different vectors. For this reason, the sum of the maximum for each isotope may not sum to the total maximum.

	Am-241	Pu-239	U-234	Th-230	Total
E1 – 100 yrs	4.24E+01	4.37E+01	6.76E-02	1.46E-01	6.26E+01
3000 yrs	2.14E+01	2.47E+01	5.09E-02	1.16E-01	2.91E+01
5000 yrs	1.55E-01	1.84E+01	3.84E-02	9.59E-02	1.84E+01
7000 yrs	2.08E-02	1.06E+01	3.13E-02	7.48E-02	1.06E+01
9000 yrs	2.80E-03	4.94E+00	1.83E-02	4.09E-02	4.99E+00
E2 – 100 yrs	2.16E+00	3.06E+00	5.67E-03	1.59E-03	5.22E+00
3000 yrs	8.34E-03	3.76E-01	3.89E-03	4.08E-04	3.76E-01
5000 yrs	9.18E-04	2.49E-01	2.27E-03	4.08E-04	2.50E-01
7000 yrs	1.15E-04	6.99E-03	1.53E-03	2.39E-05	7.02E-03
9000 yrs	4.37E-06	6.29E-03	1.25E-03	3.14E-06	6.29E-03

^{239}Pu shows the highest maximum activity (43.7 EPA units) of all the isotopes across all ISO and TI runs for a 100 year, E1 intrusion and is the isotope with the highest release for 113 of the 217 screened in vectors for the 100 year intrusion time across all replicates. For a 350 year intrusion, ^{239}Pu is highest in 63 of the 217 vectors. For intrusion times greater then 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 350 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 5.

Table 5 – Percentage of total activity after 10,000 years for each isotope.

	Am-241	Pu-239	U-234	Th-230
E1-100 yrs	44.79%	52.44%	2.22%	0.54%
350 yrs	63.64%	34.79%	1.21%	0.36%
1000 yrs	37.90%	59.96%	1.76%	0.38%
3000 yrs	16.18%	79.79%	3.46%	0.58%

5000 yrs	1.61%	97.45%	0.73%	0.21%
7000 yrs	0.29%	95.05%	4.02%	0.64%
9000 yrs	0.16%	95.31%	3.90%	0.63%
E2-100 yrs	29.74%	67.30%	2.74%	0.22%
350 yrs	18.12%	72.77%	8.88%	0.23%
1000 yrs	12.78%	82.21%	4.74%	0.26%
3000 yrs	3.08%	91.13%	5.42%	0.37%
5000 yrs	0.58%	93.76%	5.26%	0.40%
7000 yrs	0.20%	93.69%	5.47%	0.64%
9000 yrs	0.14%	83.12%	16.68%	0.06%

5. Summary

This analysis package describes the transport calculations that are part of the "Salado Flow and Transport Calculations for the Performance Assessment Baseline Calculations (PABC) of the Waste Isolation Pilot Plant (WIPP)" as described in Analysis Plan AP-122 (Kanney and Leigh, 2005). 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-2004.

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 and Leigh, 2005) 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 1×10^{-7} 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 BRAGFLO 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 471 '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 release 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.

Figure 7 - Cumulative activity in the borehole at the Culebra in EPA Units for R1S2.
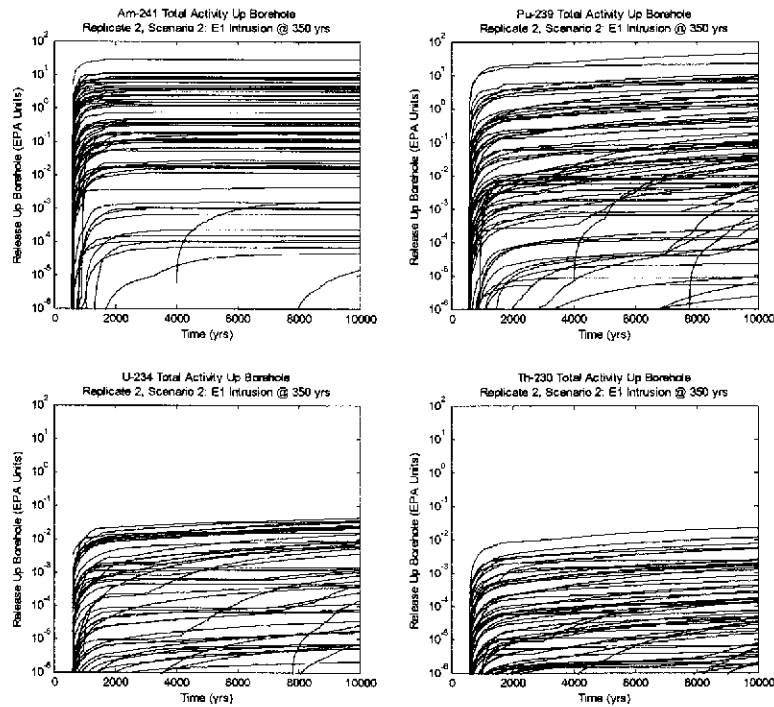
Figure 8 - Cumulative activity in the borehole at the Culebra in EPA Units for R2S2.
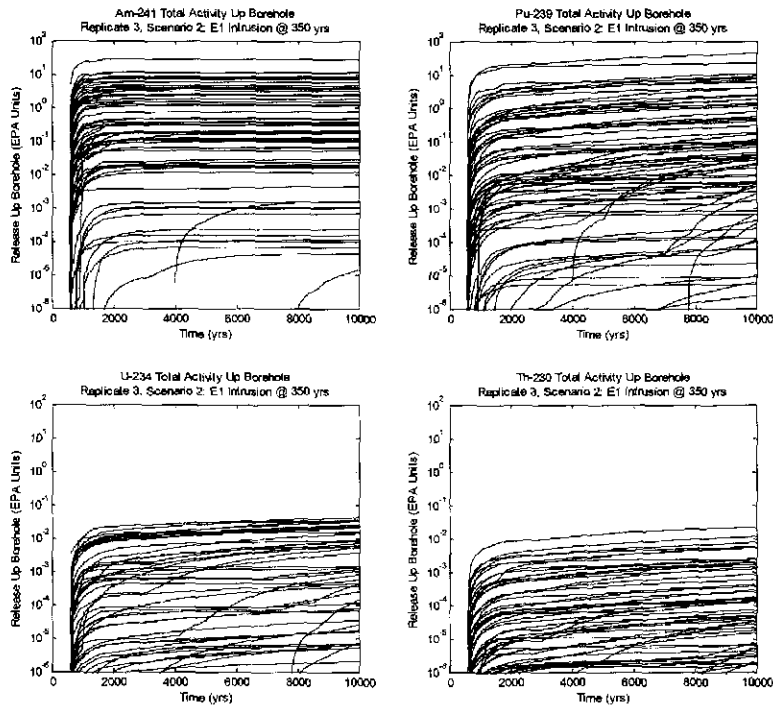
Figure 9 - Cumulative activity in the borehole at the Culebra in EPA Units for R3S2.
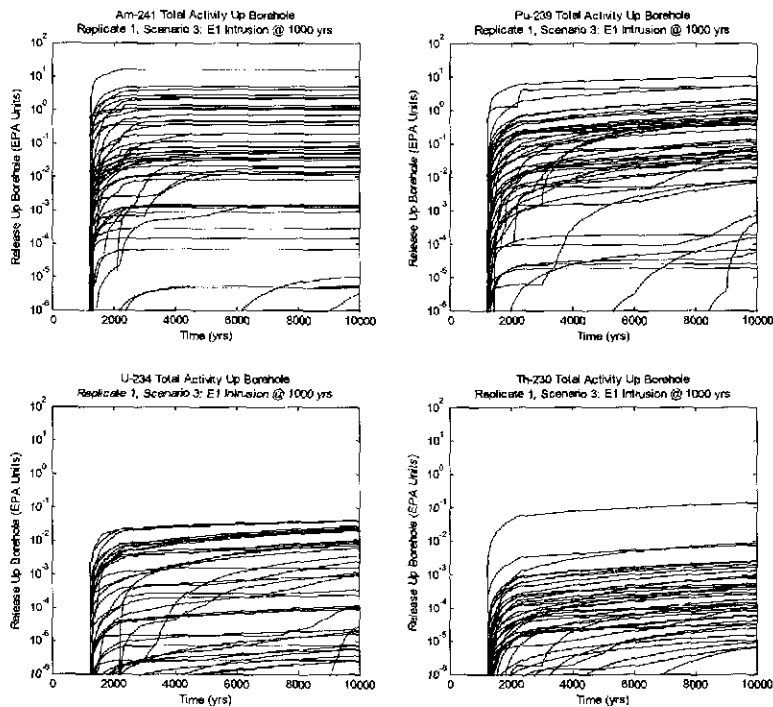
Figure 10 - Cumulative activity in the borehole at the Culebra in EPA Units for R1S3.
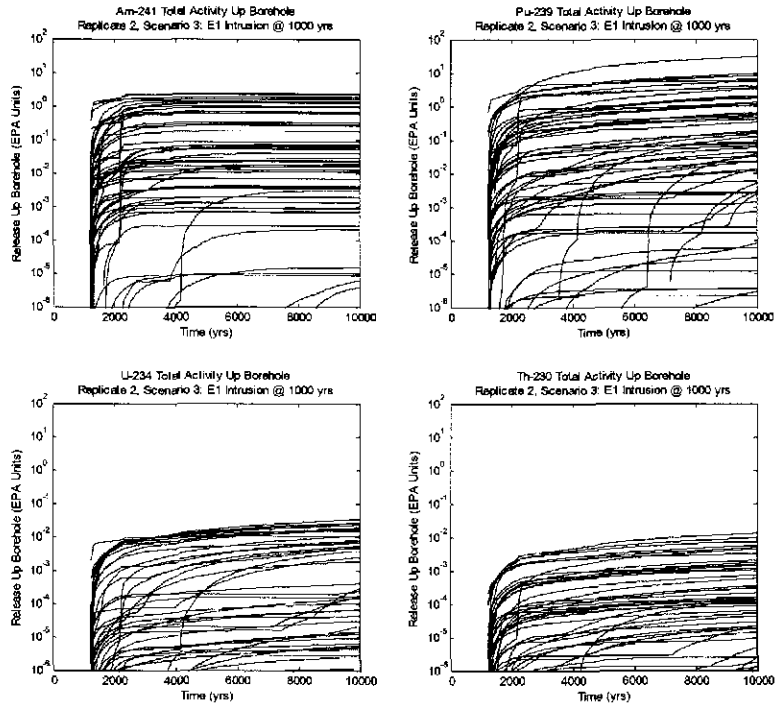
Figure 11 - Cumulative activity in the borehole at the Culebra in EPA Units for R2S3.
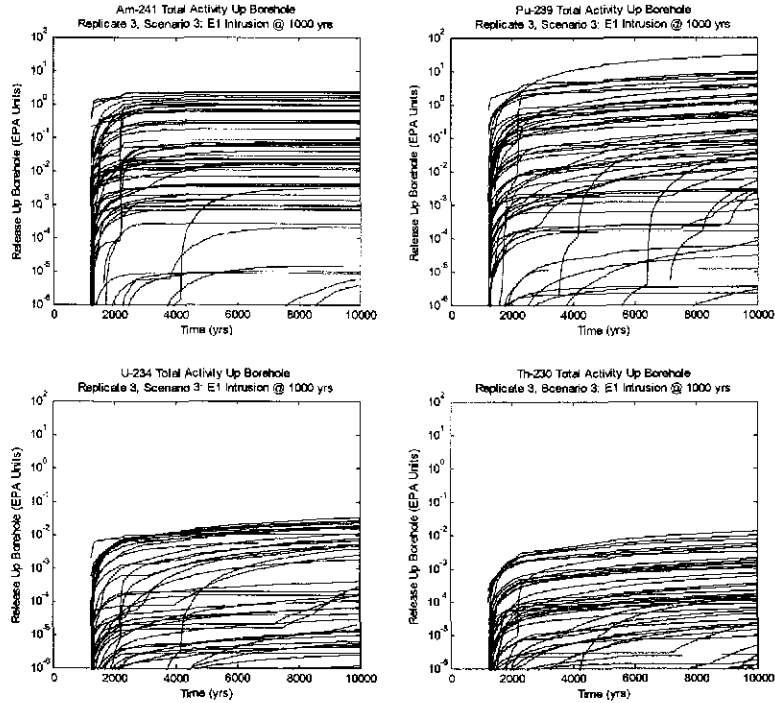
Figure 12 - Cumulative activity in the borehole at the Culebra in EPA Units for R3S3.
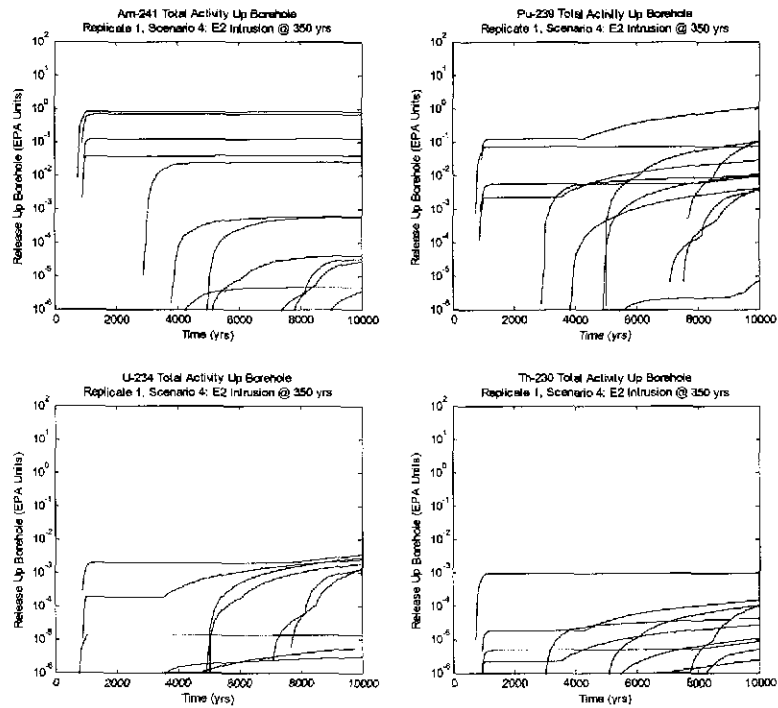
Figure 13 - Cumulative activity in the borehole at the Culebra in EPA Units for R1S4 .
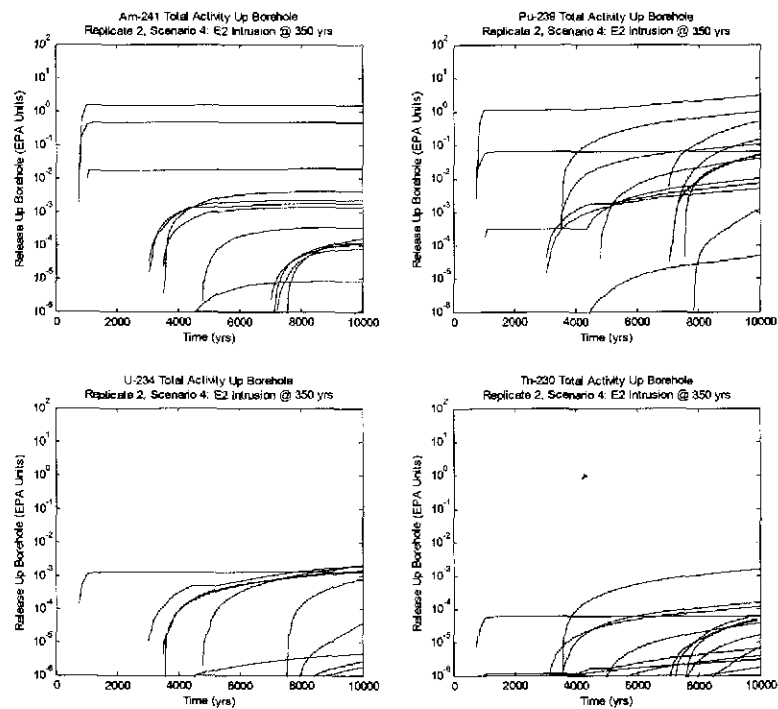
Figure 14 - Cumulative activity in the borehole at the Culebra in EPA Units for R2S4.
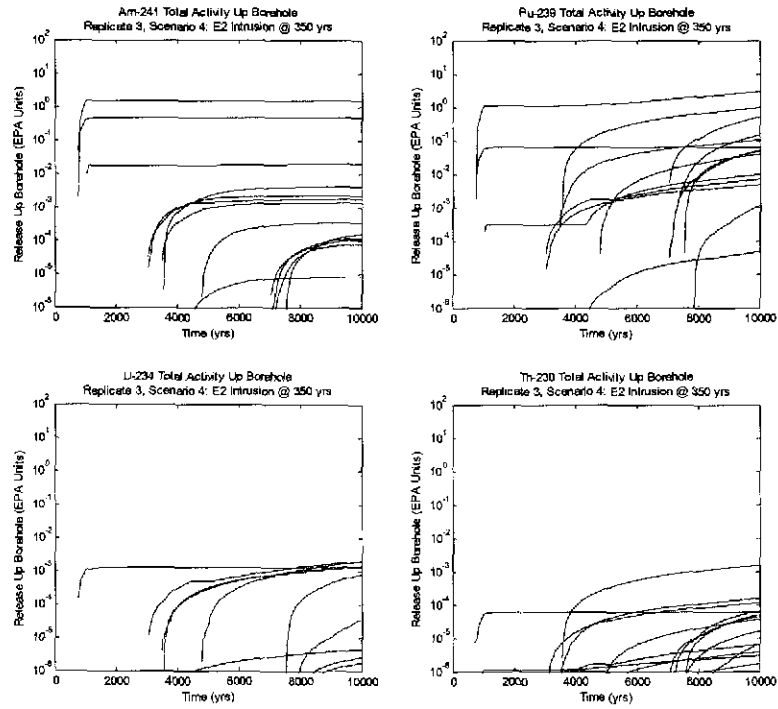
Figure 15 - Cumulative activity in the borehole at the Culebra in EPA Units for R3S4.
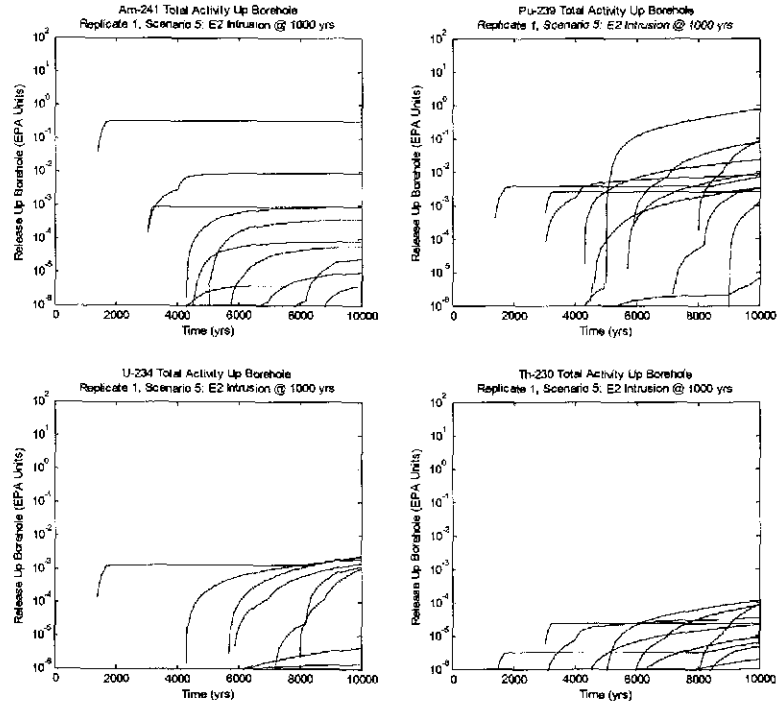
Figure 16 - Cumulative activity in the borehole at the Culebra in EPA Units for R1S5.
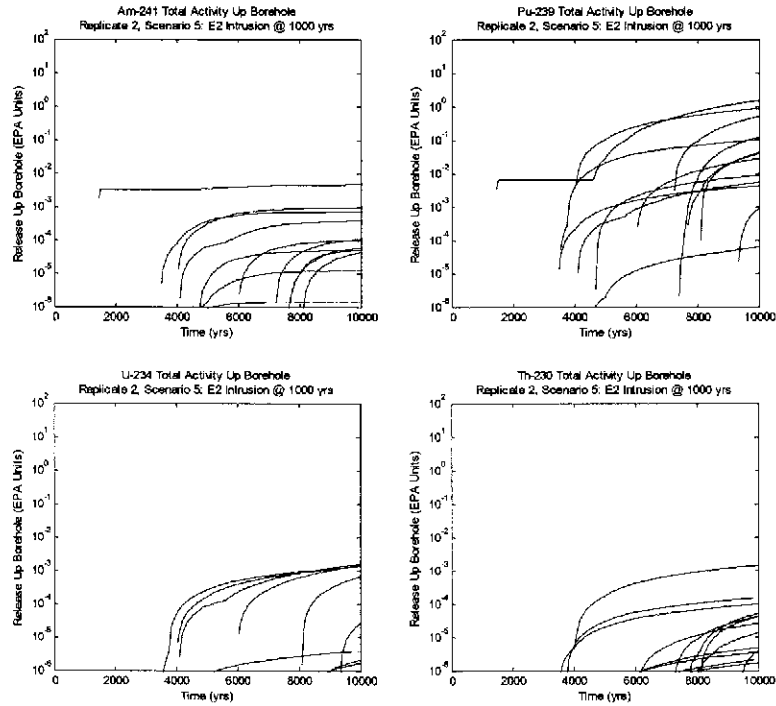
Figure 17 - Cumulative activity in the borehole at the Culebra in EPA Units for R2S5.
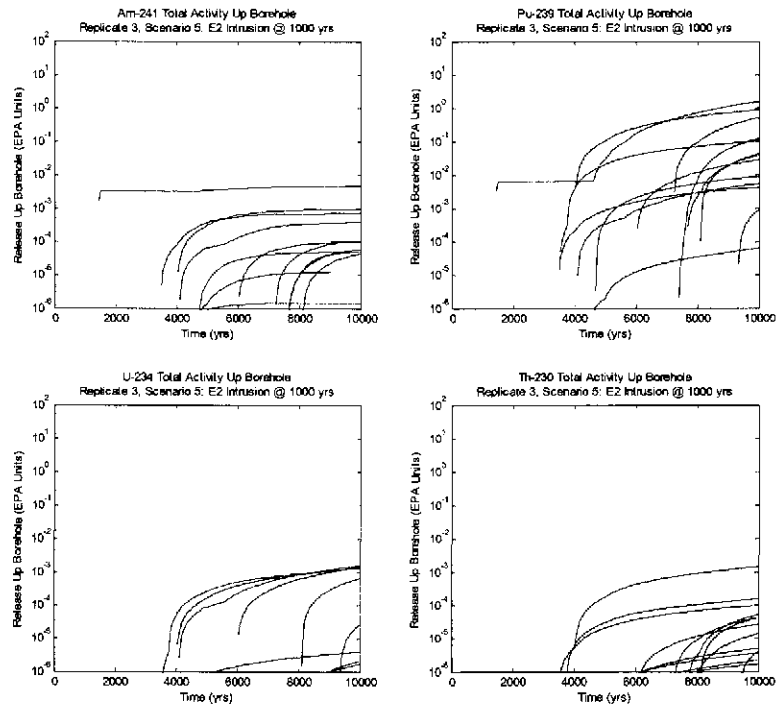
Figure 18 - Cumulative activity in the borehole at the Culebra in EPA Units for R3S5.

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Appendix A: Post-processing code and verification documentation for SCREEN.FOR.

A test case was constructed to demonstrate that SCREEN.FOR performs correctly and to demonstrate its purpose. The executable in CMS was produced by CCA-MASTER using the SCREEN_BUILD.COM script. A log file (SCREEN_BUILD.LOG) was produced and retained in CMS. The test output files in CMS were produced CCA-MASTER using the SCREEN_TEST.COM script. A log file (SCREEN_TEST.LOG) was produced and retained in CMS. The CMS library LIBCRA1BC_NUT, class SCREEN_V1.0, contains the following files from this test:

SCREEN.FOR   - source code

SCREEN_BUILD.COM   - script to build executable

SCREEN.EXE   - executable

SCREEN_BUILD.LOG   - log file from build process

SCREEN_TEST1.INP   - input control file

SCREEN_TEST1_S1.TBL   - input data file from SUMMARIZE for Scenario S1

SCREEN_TEST1_S2.TBL   - input data file from SUMMARIZE for Scenario S2

SCREEN_TEST1_S1.OUT   - output data file from SCREEN.FOR for Scenario S1

SCREEN_TEST1_S2.OUT   - output data file from SCREEN.FOR for Scenario S2

SCREEN_TEST.LOG   - log file for test runs

The above listed files are shown below. The input file SCREEN_TEST1.INP is shown below along with a description in italics. The test input data files constructed for this test each contain twelve vectors. For each vector there is a set of ALGEBRA output variables describing releases to the land withdrawal boundary through the anhydrite markerbeds MB138, MB139, and Anhydrite AB:

SMB38N1C, SMB38S1C, SMBABN1C, SMBABS1C, SMB39N1C, SMB39S1C, and a set of variables that give releases to the Culebra BHUP1C through the borehole and SHUP1C through the shaft. Here N and S denote north or south of the repository.

The test input data files contain various values of the above ALGEGRA output variables. The Fortran code SCREEN.FOR adds up all the markerbed releases into one variable and all releases to the Culebra into another variable. If either of these variables are greater than the tolerance set in the input file, the output file will record this vector with the release size and the type of release (markerbed or borehole). This is contained between the NONUNION_BEGIN and NONUNION_END sections of the output files. One can see by looking at the test input data files and the test output data files that the code correctly sums up the releases.

For Scenario S1, following the NONUNION_BEGIN and NONUNION_END sections of the output file, there is a list of all vectors from all scenarios that contained releases greater than the tolerance. This is contained between the UNION_BEGIN and UNION_END sections of the output file only for Scenario S1. This information is used in the ISO and T1 runs. Looking at the input data files and the output data files it is clear that this section has captured all the vectors that had releases in S1 and S2 from this test problem. Thus the test has shown that the SCREEN.FOR code works correctly.

```
ccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c                                                      c
c   NUTS SCREENING PROGRAM                             c
c   Purpose: Takes output from the NUTS-screening-run- c
c   summarize-output files and determines whether the releases c
c   from these runs are large enough to warrant a      c
c   complete NUTS run with decay and real inventory parameters c
c                                                      c
c    This code was written in June, 2005 by            c
c    Martin Nemer, SNL, 505-234-0005 and               c
c    Jim Garner                                        c
c                                                      c
ccccccccccccccccccccccccccccccccccccccccccccccccccccccc


        program screen
        implicit none

        integer mxfile
        PARAMETER (mxfile = 10)
        integer mxscen
        PARAMETER (mxscen = 10)
        integer mxvect
        PARAMETER (mxvect = 1000)
        integer mxunion
        PARAMETER (mxunion = 10*mxvect)

        integer nfiles,nfiler,i,icount,scenario,
      & replicate,
      & totscen,scen(mxscen),indicator,union(mxunion),
      & ucount,j,utot,totvect

        double precision TIME,SWASTE1C,SMB39S1C,SMBABS1C,
      & SMB38N1C,SMB38S1C,SMB39N1C,SMBABN1C,SCULBR1C,
      & SHUP1C,SURFSH1C,SSHM1C,BHUP1C,SURFBH1C,SBHM1C,
      & SSALAD1C,critical,SUMMB,IVECTOR1,SUMBH

        CHARACTER*120 filenm(mxfile)
        CHARACTER*120 sumfile(mxscen),outfile(mxscen),
      & inpfile,analysis
        CHARACTER*80 filine

        CHARACTER *10,CHAR1,CHAR2,DUMMY

        nfiles = 1
        nfiler = 0
        write(*,*) nfiles,nfiler
        CALL filcmdlin(nfiles,nfiler,filenm)

        IF ( nfiler .GT. nfiles ) THEN
           CALL QAABORT('Too many command line arguments')
        ELSE
           IF ( nfiler .LT. nfiles-1 ) THEN
              CALL QAABORT('Too few command line arguments')
           ENDIF
        ENDIF

c       sumfile, then outfile, then scenario, then tolerance
```

```
        inpfile = filenm(1)
        write(*,*) filenm(1)
        if(filenm(1) .ne. '') then
         open(10,file=inpfile,err=300,status='old',blank='null')
        else
         write(*,*) 'error no input file name specified'
        endif
        indicator = 0
5       read(10,'(a80)',end=20) filine

        write(*,*) filine

        if((filine(1:5) .eq. '!Anal') .or.
     &  (filine(1:6) .eq. '! Anal')) then
         read(10,*,end=20) analysis
         write(*,*) 'analysis: ',analysis(1:30)
         indicator = indicator + 1
        endif

        if((filine(1:5) .eq. '!Repl') .or.
     &  (filine(1:6) .eq. '! Repl')) then
         read(10,*,end=20) replicate
         write(*,*) 'replicate: ',replicate
         indicator = indicator + 1
        endif

        if((filine(1:5) .eq. '!Numb') .or.
     &  (filine(1:6) .eq. '! Numb')) then
         read(10,*,end=20) totscen
         write(*,*) 'number of scenarios: ',totscen
         indicator = indicator + 1
        endif

        if((filine(1:5) .eq. '!Vect') .or.
     &  (filine(1:6) .eq. '! Vect')) then
         read(10,*,end=20) totvect
         write(*,*) 'number of vectors: ',totvect
         indicator = indicator + 1
        endif

        if((filine(1:5) .eq. '!Scen') .or.
     &  (filine(1:6) .eq. '! Scen')) then
         read(10,*,end=20) (scen(i),i=1,totscen)
         write(*,*) 'scenarios: ',(scen(i),i=1,totscen)
         indicator = indicator + 1
        endif

        if((filine(1:5) .eq. '!Tole') .or.
     &  (filine(1:6) .eq. '! Tole')) then
         read(10,*,end=20) critical
         write(*,*) 'tolerance: ',critical
         indicator = indicator + 1
        endif

        if((filine(1:5) .eq. '!Inpu') .or.
     &  (filine(1:6) .eq. '! Inpu')) then
```

```
        do i = 1,totscen
         read(10,*,end=20) sumfile(i)
         write(*,*) 'sumarize file for scenario ',i,'
:',sumfile(i)(1:50)
        enddo
        indicator = indicator + 1
       endif

       if((filine(1:5) .eq. '!Outp') .or.
      & (filine(1:6) .eq. '! Outp')) then
        do i = 1,totscen
         read(10,*,end=20) outfile(i)
         write(*,*) 'output file for scenario ',i,' :',outfile(i)(1:50)
        enddo
        indicator = indicator + 1
       endif

       goto 5

20     if(indicator .ne. 8) then
        write(*,*) 'input file not correct, something isnt defined'
        goto 500
       endif
       close(10)

       ucount = 0
       do j = totscen,1,-1
        scenario = scen(j)

       write(*,*) sumfile(j)(1:30),' ',outfile(j)(1:40),' ',
      & scenario,critical

       OPEN (10,FILE=sumfile(j),err=300,STATUS='OLD',
      &      BLANK='NULL')



       OPEN (20,FILE=outfile(j),STATUS='NEW',recl=1024)

       CHAR1 = 'Borehole'
       CHAR2 = 'Markerbeds'

         write(20,*) 'analysis: ',analysis(1:40)
         write(20,*) 'replicate: ',replicate
         write(20,*) 'data source: ',sumfile(j)(1:40)
         write(20,*) 'scenario: ',scenario
         write(20,*) 'nuts tolerance: ',critical
         write(20,*) 'NONUNION_BEGIN'

         READ(10,*)
         READ(10,*)
         READ(10,*)

         ICOUNT = 0
         DO 100 I = 1,totvect

c simple check to make sure correct things are being read in
```

Information Only

```
       IVECTOR1 = 1.d9
       TIME = 1.d9
       SMB39S1C = 1.d9
       SMB39N1C = 1.d9
       SMBABS1C = 1.d9
       SMB38N1C = 1.d9
       SMB38S1C = 1.d9
       SMBABN1C = 1.d9
       SHUP1C = 1.d9
       BHUP1C = 1.d9


       READ(10,*) IVECTOR1,TIME,SMB38N1C,SMB38S1C,
     & SMBABN1C,SMBABS1C,SMB39N1C,SMB39S1C,BHUP1C,SHUP1C
       READ(10,*)


       SUMMB = SMB38N1C+SMB38S1C+SMB39N1C+SMB39S1C+SMBABN1C+SMBABS1C
       SUMBH = SHUP1C+BHUP1C


       if((summb .ge. 1.d9) .or. (sumbh .gt. 1.d9)) then
        goto 400
       endif


       IF((SUMMB .gt. critical) .and. (SUMBH .gt. critical))
     & then
       ICOUNT = ICOUNT + 1
         ucount = ucount + 1
         union(ucount) = INT(IVECTOR1)
         WRITE (20,'(i4,a1,a12,a12,2e25.15)') INT(IVECTOR1),' ',
     & CHAR1,CHAR2,SUMBH,SUMMB
        ELSEIF (SUMMB .gt. critical) THEN
            ICOUNT = ICOUNT + 1
            ucount = ucount + 1
            union(ucount) = INT(IVECTOR1)
            WRITE (20,'(i4,a1,a12,1e25.15)') INT(IVECTOR1),' ',CHAR2,
     & SUMMB
          ELSEIF (SUMBH .gt. critical) THEN
            ICOUNT = ICOUNT + 1
            ucount = ucount + 1
            union(ucount) = INT(IVECTOR1)
            WRITE (20,'(i4,a1,a12,1e25.15)') INT(IVECTOR1),' ',CHAR1,
     & SUMBH
          ENDIF
100      CONTINUE
         write(20,*) 'NONUNION_END'
         WRITE (20,*) 'NONUNION_TOTAL ',ICOUNT
         if(scenario .ne. 1) then
          WRITE (20,*) 'GRAND_TOTAL ',ICOUNT
          close(20)
         endif
         close(10)
       enddo

       if((scenario .eq. 1) .and. (ucount .gt. 0)) then
        call sort(union,ucount)
        write(20,*) 'UNION_BEGIN'
        WRITE (20,'(i4)') union(1)
```

```
         utot = 1
         ICOUNT = ICOUNT + 1
         do i = 2,ucount
          if(union(i) .ne. union(i-1)) then
           WRITE (20,'(i4)') union(i)
           ICOUNT = ICOUNT + 1
           utot = utot + 1
          endif
         enddo
         write (20,*) 'UNION_END'
         write (20,*) 'UNION_TOTAL ',utot
         WRITE (20,*) 'GRAND_TOTAL ',ICOUNT
         close(20)
        endif


        goto 500

300    write(*,*) 'SCREEN_BL: error opening file'
        GOTO 500
400    write(*,*) 'error reading SUM file'
500      END



        subroutine sort (a,length)

        implicit none

        integer a(*),length,i,j,key

        do j = 2,length
         key = a(j)
         i = j-1
         do while((i .gt. 0) .and. (a(i) .gt. key))
          a(i+1) = a(i)
          i = i - 1
          a(i+1) = key
         enddo
        enddo

        end
```

`*****************************************************************************`

SCREEN_TEST1.INP

```
!---------------------------------------
! Some lines of header info
!---------------------------------------
!
!Analysis ID                              Gives the analysis name to be
CRA1BC                                    printed in the output files
!
```

```
!Replicate                              Gives the replicate number to
1                                       be printed in the output files
!
!Number of Scenarios                    Number of scenarios to be
2                                       processed in input data files
!
! Scenario list                         Which scenarios are to be
1,2                                     processed in input data files
!
!Vectors (number of)                    Number of vectors in each
12                                      input data file
!
!Tolerance                              Minimum release to be output
1E-10                                   to the output files
!
!Input summarize tables, put scenario 1 first
SCREEN_TEST1_S1.TBL                      Names/locations of
SCREEN_TEST1_S2.TBL                      input data files
!
!Output screened-in vector data files
SCREEN_TEST1_S1.OUT                      Names/location of
SCREEN_TEST1_S2.OUT                      output data files
!-------------------
! End of input
!-------------------
***********************************************************************
```

SCREEN_TEST1_S1.TBL

```
vector,time,SMB38N1C,SMB38S1C,SMBABN1C,SMBABS1C,SMB39N1C,SMB39S1C,BHUP1
C  ,SHUP1C
,,[G],[G],[G],[G],[G],[G],[G],[G]
,,,,,,,,,
 100.0000E-02, 100.0000E+02, 1.000000E+00, 0.000000E+00, 0.000000E+00,
0.000000E+00, 0.000000E+00, 0.000000E+00, 0.000000E+00, 0.000000E+00,
*break
 200.0000E-02, 100.0000E+02, 0.000000E+00, 2.000000E+00, 0.000000E+00,
0.000000E+00, 0.000000E+00, 0.000000E+00, 0.000000E+00, 0.000000E+00,
*break
 300.0000E-02, 100.0000E+02, 0.000000E+00, 0.000000E+00, 3.000000E+00,
0.000000E+00, 0.000000E+00, 0.000000E+00, 0.000000E+00, 0.000000E+00,
*break
 400.0000E-02, 100.0000E+02, 0.000000E+00, 0.000000E+00, 0.000000E+00,
4.000000E+00, 0.000000E+00, 0.000000E+00, 0.000000E+00, 0.000000E+00,
*break
```

```
 500.0000E-02, 100.0000E+02, 0.000000E+00, 0.000000E+00, 0.000000E+00,
0.000000E+00, 5.000000E+00, 0.000000E+00, 0.000000E+00, 0.000000E+00,
*break
 600.0000E-02, 100.0000E+02, 1.000000E+00, 1.000000E+00, 1.000000E+00,
1.000000E+00, 1.000000E+00, 1.000000E+00, 0.000000E+00, 0.000000E+00,
*break
 700.0000E-02, 100.0000E+02, 0.000000E+00, 0.000000E+00, 0.000000E+00,
0.000000E+00, 0.000000E+00, 0.000000E+00, 1.000000E+00, 0.000000E+00,
*break
 800.0000E-02, 100.0000E+02, 0.000000E+00, 0.000000E+00, 0.000000E+00,
0.000000E+00, 0.000000E+00, 0.000000E+00, 0.000000E+00, 1.000000E+00,
*break
 900.0000E-02, 100.0000E+02, 0.000000E+00, 0.000000E+00, 0.000000E+00,
0.000000E+00, 0.000000E+00, 0.000000E+00, 1.000000E+00, 1.000000E+00,
*break
 100.0000E-01, 100.0000E+02, 0.000000E+00, 0.000000E+00, 0.000000E+00,
1.000000E-11, 0.000000E+00, 0.000000E+00, 0.000000E+00, 0.000000E+00,
*break
 110.0000E-01, 100.0000E+02, 0.000000E+00, 0.000000E+00, 0.000000E+00,
0.000000E+00, 0.000000E+00, 0.000000E+00, 0.000000E+00, 1.000000E-11,
*break
 120.0000E-01, 100.0000E+02, 0.000000E+00, 0.000000E+00, 0.000000E+00,
0.000000E+00, 0.000000E+00, 0.000000E+00, 0.000000E+00, 0.000000E+00,
*break
****************************************************************************
```

SCREEN_TEST1_S2.TBL

```
vector,time,SMB38N1C,SMB38S1C,SMBABN1C,SMBABS1C,SMB39N1C,SMB39S1C,BHUP1
C  ,SHUP1C
,,[G],[G],[G],[G],[G],[G],[G],[G]
,,,,,,,,,
 100.0000E-02, 100.0000E+02, 1.000000E+00, 0.000000E+00, 0.000000E+00,
0.000000E+00, 0.000000E+00, 0.000000E+00, 0.000000E+00, 0.000000E+00,
*break
 200.0000E-02, 100.0000E+02, 0.000000E+00, 2.000000E+00, 0.000000E+00,
0.000000E+00, 0.000000E+00, 0.000000E+00, 0.000000E+00, 0.000000E+00,
*break
 300.0000E-02, 100.0000E+02, 0.000000E+00, 0.000000E+00, 3.000000E+00,
0.000000E+00, 0.000000E+00, 0.000000E+00, 0.000000E+00, 0.000000E+00,
*break
 400.0000E-02, 100.0000E+02, 0.000000E+00, 0.000000E+00, 0.000000E+00,
4.000000E+00, 0.000000E+00, 0.000000E+00, 0.000000E+00, 0.000000E+00,
*break
 500.0000E-02, 100.0000E+02, 0.000000E+00, 0.000000E+00, 0.000000E+00,
0.000000E+00, 5.000000E+00, 0.000000E+00, 0.000000E+00, 0.000000E+00,
```

```
*break
  600.0000E-02, 100.0000E+02, 1.000000E+00, 1.000000E+00, 1.000000E+00,
1.000000E+00, 1.000000E+00, 1.000000E+00, 0.000000E+00, 0.000000E+00,
*break
  700.0000E-02, 100.0000E+02, 0.000000E+00, 0.000000E+00, 0.000000E+00,
0.000000E+00, 0.000000E+00, 0.000000E+00, 1.000000E+00, 0.000000E+00,
*break
  800.0000E-02, 100.0000E+02, 0.000000E+00, 0.000000E+00, 0.000000E+00,
0.000000E+00, 0.000000E+00, 0.000000E+00, 0.000000E+00, 1.000000E+00,
*break
  900.0000E-02, 100.0000E+02, 0.000000E+00, 0.000000E+00, 0.000000E+00,
0.000000E+00, 0.000000E+00, 0.000000E+00, 1.000000E+00, 1.000000E+00,
*break
  100.0000E-01, 100.0000E+02, 0.000000E+00, 0.000000E+00, 0.000000E+00,
1.000000E-11, 0.000000E+00, 0.000000E+00, 0.000000E+00, 0.000000E+00,
*break
  110.0000E-01, 100.0000E+02, 0.000000E+00, 0.000000E+00, 0.000000E+00,
0.000000E+00, 0.000000E+00, 0.000000E+00, 0.000000E+00, 1.000000E-11,
*break
  120.0000E-01, 100.0000E+02, 1.000000E+00, 0.000000E+00, 0.000000E+00,
0.000000E+00, 0.000000E+00, 0.000000E+00, 0.000000E+00, 0.000000E+00,
*break
*******************************************************************************
```

SCREEN_TEST1_S1.OUT

```
analysis: CRA1BC
 replicate:            1
 data source: SCREEN_TEST1_S1.TBL
 scenario:             1
 nuts tolerance:    1.000000000000000E-010
 NONUNION_BEGIN
    1    Markerbeds    0.100000000000000E+01
    2    Markerbeds    0.200000000000000E+01
    3    Markerbeds    0.300000000000000E+01
    4    Markerbeds    0.400000000000000E+01
    5    Markerbeds    0.500000000000000E+01
    6    Markerbeds    0.600000000000000E+01
    7    Borehole      0.100000000000000E+01
    8    Borehole      0.100000000000000E+01
    9    Borehole      0.200000000000000E+01
 NONUNION_END
 NONUNION_TOTAL            9
 UNION_BEGIN
    1
    2
```

```
     3
     4
     5
     6
     7
     8
     9
    12
 UNION_END
 UNION_TOTAL              10
 GRAND_TOTAL              19
```
****

SCREEN_TEST1_S2.OUT

```
analysis: CRA1BC
 replicate:              1
 data source: SCREEN_TEST1_S2.TBL
 scenario:               2
 nuts tolerance:    1.000000000000000E-010
 NONUNION_BEGIN
    1     Markerbeds      0.100000000000000E+01
    2     Markerbeds      0.200000000000000E+01
    3     Markerbeds      0.300000000000000E+01
    4     Markerbeds      0.400000000000000E+01
    5     Markerbeds      0.500000000000000E+01
    6     Markerbeds      0.600000000000000E+01
    7     Borehole        0.100000000000000E+01
    8     Borehole        0.100000000000000E+01
    9     Borehole        0.200000000000000E+01
   12     Markerbeds      0.100000000000000E+01
 NONUNION_END
 NONUNION_TOTAL              10
 GRAND_TOTAL                 10
```

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

```
** Thomas Lowry, SNL Dept 6115, 13 May 2005 **
'CRA-2004 PA Baseline Calculation, AP-122, SCN_CRA1BC_S1, Screening
Run'
** 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
** 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
** TIME DEPENDENT SOURCE IN THE MATRIX **
** MATRIX CONCENTRATION INITIALIZATION **
** COLLOID TRANSPORT VELOCITY SCALING FACTORS IN THE MATRIX **
```

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

```
!----------------------------------------------------------------
!Author          : Thomas S. Lowry
!Organization    : Sandia National Laboratories (Dept. 6115)
!Date            :13 May 2005
!----------------------------------------------------------------
!Analysis        :CRA-2004 PA Baseline Calculations (PABC) AP-122
!Analysis ID     :CRA1BC
!Remark          :Screening runs, scenario 1
!----------------------------------------------------------------
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
!
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.)
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.)
!

!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.)
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 D: Sample SUMMARIZE screening input file for replicate 1, scenario 1.

```
!
!**-EVAL->> *****************************************************
!**-EVAL->> Time Stamp : 2005-07-08 13:25:25.51
!**-EVAL->> *****************************************************
!**-EVAL->> User : CCA_MASTER
!**-EVAL->> *****************************************************
!**-EVAL->> Script Name    : EVAL_NUT_STEP2
!**-EVAL->> Script Version : 1.00
!**-EVAL->> Release Date   : 2005-07-07
!**-EVAL->> *****************************************************
!**-EVAL->> Template File  : SUM_NUT_SCN_CRA1BC.TMPL
!**-EVAL->> *****************************************************
!
*INPUT FILES
        template=ALG_NUT_SCN_CRA1BC_R1_S1_V###
        TYPE       = CDB

*VECTORS
        id=#
        vector=1 to 100

*TIMES
        READ    = SECONDS
        INPUT   = YEARS
        OUTPUT  = YEARS
        TIMES   = 10000

*ITEM
        TYPE    = GLOBAL
        NAME    = SMB38N1C, SMB38S1C, &
                  SMBABN1C, SMBABS1C, &
                  SMB39N1C, SMB39S1C, &
                  BHUP1C,   SHUP1C

*OUTPUT
        DRIVER = EXCEL
        WRITE  = TIME VS ITEM
          name=SUM_NUT_SCN_CRA1BC_R1_S1.TBL
*END
```

Appendix E: TI Time Series Plots

Am-241 Total Activity Up Borehole
Replicate 3, Scenario 2: Intrusion @ 100 yrs

Pu-239 Total Activity Up Borehole
Replicate 3, Scenario 2: Intrusion @ 100 yrs

U-234 Total Activity Up Borehole
Replicate 3, Scenario 2: Intrusion @ 100 yrs

Th-230 Total Activity Up Borehole
Replicate 3, Scenario 2: Intrusion @ 100 yrs

Am-241 Total Activity Up Borehole
Replicate 1, Scenario 3: Intrusion @ 3000 yrs

Pu-239 Total Activity Up Borehole
Replicate 1, Scenario 3: Intrusion @ 3000 yrs

U-234 Total Activity Up Borehole
Replicate 1, Scenario 3: Intrusion @ 3000 yrs

Th-230 Total Activity Up Borehole
Replicate 1, Scenario 3: Intrusion @ 3000 yrs

Am-241 Total Activity Up Borehole
Replicate 2, Scenario 3: Intrusion @ 7000 yrs

Pu-239 Total Activity Up Borehole
Replicate 2, Scenario 3: Intrusion @ 7000 yrs

U-234 Total Activity Up Borehole
Replicate 2, Scenario 3: Intrusion @ 7000 yrs

Th-230 Total Activity Up Borehole
Replicate 2, Scenario 3: Intrusion @ 7000 yrs

Am-241 Total Activity Up Borehole
Replicate 3, Scenario 3: Intrusion @ 7000 yrs

Pu-239 Total Activity Up Borehole
Replicate 3, Scenario 3: Intrusion @ 7000 yrs

U-234 Total Activity Up Borehole
Replicate 3, Scenario 3: Intrusion @ 7000 yrs

Th-230 Total Activity Up Borehole
Replicate 3, Scenario 3: Intrusion @ 7000 yrs

Am-241 Total Activity Up Borehole
Replicate 1, Scenario 3: Intrusion @ 9000 yrs

Pu-239 Total Activity Up Borehole
Replicate 1, Scenario 3: Intrusion @ 9000 yrs

U-234 Total Activity Up Borehole
Replicate 1, Scenario 3: Intrusion @ 9000 yrs

Th-230 Total Activity Up Borehole
Replicate 1, Scenario 3: Intrusion @ 9000 yrs

Am-241 Total Activity Up Borehole
Replicate 2, Scenario 3: Intrusion @ 9000 yrs

Pu-239 Total Activity Up Borehole
Replicate 2, Scenario 3: Intrusion @ 9000 yrs

U-234 Total Activity Up Borehole
Replicate 2, Scenario 3: Intrusion @ 9000 yrs

Th-230 Total Activity Up Borehole
Replicate 2, Scenario 3: Intrusion @ 9000 yrs

Am-241 Total Activity Up Borehole
Replicate 3, Scenario 3: Intrusion @ 9000 yrs

Pu-239 Total Activity Up Borehole
Replicate 3, Scenario 3: Intrusion @ 9000 yrs

U-234 Total Activity Up Borehole
Replicate 3, Scenario 3: Intrusion @ 9000 yrs

Th-230 Total Activity Up Borehole
Replicate 3, Scenario 3: Intrusion @ 9000 yrs

Am-241 Total Activity Up Borehole
Replicate 1, Scenario 4: Intrusion @ 100 yrs

Pu-239 Total Activity Up Borehole
Replicate 1, Scenario 4: Intrusion @ 100 yrs

U-234 Total Activity Up Borehole
Replicate 1, Scenario 4: Intrusion @ 100 yrs

Th-230 Total Activity Up Borehole
Replicate 1, Scenario 4: Intrusion @ 100 yrs

Am-241 Total Activity Up Borehole
Replicate 2, Scenario 4: Intrusion @ 100 yrs

Pu-239 Total Activity Up Borehole
Replicate 2, Scenario 4: Intrusion @ 100 yrs

U-234 Total Activity Up Borehole
Replicate 2, Scenario 4: Intrusion @ 100 yrs

Th-230 Total Activity Up Borehole
Replicate 2, Scenario 4: Intrusion @ 100 yrs

Am-241 Total Activity Up Borehole
Replicate 3, Scenario 4: Intrusion @ 100 yrs

Pu-239 Total Activity Up Borehole
Replicate 3, Scenario 4: Intrusion @ 100 yrs

U-234 Total Activity Up Borehole
Replicate 3, Scenario 4: Intrusion @ 100 yrs

Th-230 Total Activity Up Borehole
Replicate 3, Scenario 4: Intrusion @ 100 yrs

Am-241 Total Activity Up Borehole
Replicate 1, Scenario 5: Intrusion @ 7000 yrs

Pu-239 Total Activity Up Borehole
Replicate 1, Scenario 5: Intrusion @ 7000 yrs

U-234 Total Activity Up Borehole
Replicate 1, Scenario 5: Intrusion @ 7000 yrs

Th-230 Total Activity Up Borehole
Replicate 1, Scenario 5: Intrusion @ 7000 yrs

Am-241 Total Activity Up Borehole
Replicate 2, Scenario 5: Intrusion @ 7000 yrs

Pu-239 Total Activity Up Borehole
Replicate 2, Scenario 5: Intrusion @ 7000 yrs

U-234 Total Activity Up Borehole
Replicate 2, Scenario 5: Intrusion @ 7000 yrs

Th-230 Total Activity Up Borehole
Replicate 2, Scenario 5: Intrusion @ 7000 yrs

Am-241 Total Activity Up Borehole
Replicate 3, Scenario 5: Intrusion @ 7000 yrs

Pu-239 Total Activity Up Borehole
Replicate 3, Scenario 5: Intrusion @ 7000 yrs

U-234 Total Activity Up Borehole
Replicate 3, Scenario 5: Intrusion @ 7000 yrs

Th-230 Total Activity Up Borehole
Replicate 3, Scenario 5: Intrusion @ 7000 yrs

Am-241 Total Activity Up Borehole
Replicate 1, Scenario 5: Intrusion @ 9000 yrs

Pu-239 Total Activity Up Borehole
Replicate 1, Scenario 5: Intrusion @ 9000 yrs

U-234 Total Activity Up Borehole
Replicate 1, Scenario 5: Intrusion @ 9000 yrs

Th-230 Total Activity Up Borehole
Replicate 1, Scenario 5: Intrusion @ 9000 yrs

Am-241 Total Activity Up Borehole
Replicate 2, Scenario 5: Intrusion @ 9000 yrs

Pu-238 Total Activity Up Borehole
Replicate 2, Scenario 5: Intrusion @ 9000 yrs

U-234 Total Activity Up Borehole
Replicate 2, Scenario 5: Intrusion @ 9000 yrs

Th-230 Total Activity Up Borehole
Replicate 2, Scenario 5: Intrusion @ 9000 yrs

Am-241 Total Activity Up Borehole
Replicate 3, Scenario 5: Intrusion @ 9000 yrs

Pu-239 Total Activity Up Borehole
Replicate 3, Scenario 5: Intrusion @ 9000 yrs

U-234 Total Activity Up Borehole
Replicate 3, Scenario 5: Intrusion @ 9000 yrs

Th-230 Total Activity Up Borehole
Replicate 3, Scenario 5: Intrusion @ 9000 yrs