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Sandia National Laboratories
Waste Isolation Pilot Plant

Analysis Package for Salado Transport Calculations: CRA-2014 Performance Assessment

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1 Introduction

The Waste Isolation Pilot Plant (WIPP), located in southeastern New Mexico, 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), Part 191. The DOE demonstrates compliance with the containment requirements according to the Certification Criteria in Title 40 CFR Part 194 by means of performance assessment (PA) calculations performed by Sandia National Laboratories (SNL). WIPP PA calculations estimate the probability and consequence of potential radionuclide releases from the repository to the accessible environment for a regulatory period of 10,000 years after facility closure. The models used in PA are maintained and updated with new information as part of an ongoing process. Improved information regarding important WIPP features, events, and processes typically results in refinements and modifications to PA models and the parameters used in them. Planned changes to the repository and/or the components therein also result in updates to WIPP PA models. WIPP PA models are used to support the repository recertification process that occurs at five-year intervals following the receipt of the first waste shipment at the site in 1999.

PA calculations were included in the 1996 Compliance Certification Application (CCA) (US DOE, 1996), and in a subsequent Performance Assessment Verification Test (PAVT) (MacKinnon and Freeze, 1997a, b, c). Based in part on the CCA and PAVT PA calculations, the EPA certified that the WIPP met the regulatory containment criteria. The facility was approved for disposal of transuranic waste in May 1998 (US EPA, 1998). PA calculations were an integral part of the 2004 Compliance Recertification Application (CRA-2004) (US DOE, 2004). During their review of the CRA-2004, the EPA requested an additional PA calculation, referred to as the CRA-2004 Performance Assessment Baseline Calculation (PABC) (Leigh et al., 2005), be conducted with modified assumptions and parameter values (Cotsworth, 2005). Following review of the CRA-2004 and the CRA-2004 PABC, the EPA recertified the WIPP in March 2006 (US EPA, 2006).

PA calculations were completed for the second WIPP recertification and documented in the 2009 Compliance Recertification Application (CRA-2009). The CRA-2009 PA resulted from continued review of the CRA-2004 PABC, including a number of technical changes and corrections, as well as updates to parameters and improvements to the PA computer codes (Clayton et al., 2008). To incorporate additional information which was received after the CRA-2009 PA was completed, but before the submittal of the CRA-2009, the EPA requested an additional PA calculation, referred to as the 2009 Compliance Recertification Application Performance Assessment Baseline Calculation (PABC-2009) (Clayton et al., 2010), be undertaken which included updated information (Cotsworth, 2009). Following the completion and submission of the PABC-2009, the WIPP was recertified in 2010 (US EPA, 2010).

The Land Withdrawal Act (US Congress, 1992) requires that the DOE apply for WIPP recertification every five years following the initial 1999 waste shipment. The 2014 Compliance Recertification Application (CRA-2014) is the third WIPP recertification application submitted by the DOE for EPA approval. The PA executed by SNL in support of the CRA-2014 is detailed in AP-164 (Camphouse, 2013b). As a part of the CRA-2014, the CRA-2014 BL compares the impact of a baseline set (BL) of changes relative to the CRA-2009 PABC. The CRA-2014 BL consists of a single replicate (Replicate 1) consisting of 100 vectors. The CRA-2014 PA includes a number of technical changes and parameter refinements in addition to the CRA-2014 BL. Results found in the CRA-2014 BL and CRA-2014 PA are compared to those obtained in the PABC-2009 in order to assess repository performance in terms of the current regulatory baseline. This analysis package documents the Salado transport of radionuclides for the CRA-2014 BL and CRA-2014 PA.

2 Methodology

2.1 Modeling Scenarios

For transport of radionuclides within the Salado Formation, the presence of brine is required. There are two main sources of brine available within the repository. First, a limited quantity of brine is contained in inclusions in the rock surrounding the WIPP repository. WIPP PA assumes that all of the brine in the Disturbed Rock Zone (DRZ) will be available for reaction with the waste in the repository. Additionally, in the case of an intrusion into and below the repository that penetrates a brine pocket in the Castile Formation underneath the repository, substantial quantities of brine may flow into a panel. However, because the location of brine pockets underneath the repository is unknown, it is not guaranteed that an intrusion through the repository will intersect a brine pocket.

There are two primary mechanisms by which radionuclide-contaminated brine can reach the WIPP boundary. Brine in the repository can flow through the marker beds towards the Land Withdrawal Boundary (LWB). In addition, following an intrusion, brine can flow up the resulting borehole until it comes into contact with the Culebra Dolomite member of the Rustler Formation. The brine is then assumed to be added to the Culebra, where it again begins to be transported towards the LWB.

To represent possible future states of the repository and to predict possible releases through the Salado and to the Culebra, WIPP PA considers six different modeling scenarios, as defined in Table 1. The scenarios are differentiated by the number of intrusions, the time at which intrusions occur, and whether or not the intrusion encounters a brine pocket. Scenario S1-BF assumes that the repository remains undisturbed throughout the 10,000-year horizon of WIPP PA. Four of the scenarios assume that a single drilling intrusion into the repository occurs. Scenarios S2-BF and S3-BF model an E1 intrusion, which assumes that a brine pocket in the Castile Formation is encountered while drilling. Two other scenarios (Scenarios S4-BF and S5-BF) model an E2 intrusion, in which a Castile brine pocket is not encountered. The remaining scenario, Scenario S6-BF, describes a two-intrusion process consisting of an E2 intrusion after 1000 years followed by an E1 intrusion after 2000 years.

The first five scenarios are modeled using NUTS, while the sixth scenario is modeled using PANEL. Scenario S6-BF cannot be modeled in NUTS because the model for the two-intrusion scenario assumes that the two boreholes are drilled in different locations; this assumption cannot be explicitly handled in NUTS unless it is first modeled in BRAGFLO or another fluid transport code, as NUTS does not compute its own flow fields.

Table 1 Intrusion Scenarios Considered in WIPP PA as modeled by NUTS and PANEL

Scenario	Number of Drilling Intrusions	Intrusion Time(s) (Years)	Castile Brine Pocket Encountered (Intrusion type)	Code Used for Salado Transport Analysis	Other Intrusion Times Analyzed
S1-BF	0	N/A	N/A	NUTS	N/A
S2-BF	1	350	Yes (E1)	NUTS	100
S3-BF	1	1000	Yes (E1)	NUTS	3000, 5000, 7000, 9000
S4-BF	1	350	No (E2)	NUTS	100
S5-BF	1	1000	No (E2)	NUTS	3000, 5000, 7000, 9000
S6-BF	2	1000 and 2000	Only for intrusion at 2000 years (E2-E1)	PANEL	100, 350, 4000, 6000, 9000

2.2 Summary of Potential Release Processes

We present below a brief overview of the physical processes leading to releases from the Salado formation; Camphouse (Camphouse, 2013a) gives a complete analysis of the Salado flow results.
When brine enters the disposal region, gas is generated by anoxic corrosion of iron and biodegradation of organic materials. Corrosion of the metal containers, along with structural deformation caused by the viscoelastic response of the mined salt, leads to container failure and the eventual release of radioisotopes into the brine from the waste. If sufficient quantities of gas are generated, pressures in the disposal region will increase, reducing brine flow into the repository. Brine containing dissolved radioisotopes may be expelled from the repository if pressure in the repository exceeds the brine pressure in the immediately surrounding formation. Brine saturation in the waste must exceed residual brine saturation in order for brine to be expelled from the repository.

Three potential pathways for migration of radioisotopes in dissolved brine are considered in this analysis. The first and most important pathway is a human intrusion 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 using a different code, and are not considered in this report. In the second pathway, brine may migrate through or around the panel seals through the 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 interbeds (Marker Beds 138 and 139 in Figure 1).

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

2.3 Uncertainty

To address uncertainty in many of the input parameters used in PA calculations, sets of Latin hypercube-sampled parameters are defined; each unique parameter set is called a vector. Latin Hypercube Sampling (LHS) is a structured Monte Carlo sampling method in which samples are drawn from bins of equal probability with correlations between parameters minimized. Each group of 100 vectors is called a replicate. Three replicates (Replicates 1, 2, and 3) are run in a full PA calculation.

While six scenarios are considered for Salado transport in WIPP PA, the total number of simulations that must be run for each replicate is larger than 600 (six scenarios times 100 vectors). As shown in Table 1, each scenario except for the undisturbed scenario (S1-BF) includes between one and five additional calculations representing intrusions at times other than the default times for the scenario. As a result, it may be necessary to perform as many as 21 runs per vector in each replicate. To reduce the number of runs that are performed, a series of screening calculations is performed prior to the start of the NUTS calculations to determine which vectors must be sampled.

2.4 Modeling Grid

The grid used for BRAGFLO calculations, which is stored in the WIPP CMS system in library **LIBCRA14_BF**, file **gm_bf_cra14.cdb**, is also used for NUTS calculations. The grid is shown in Figure 1. This grid is modified from the grid used for the PCS-2012 PA, which incorporates additional mined volume in the repository experimental region. Width of columns 44 and 45 was increased from 30.61 and 30.61 to 51.67 and 51.68, respectively. The extent of the modeling domain is 46,630 m in the horizontal direction by 940 m in the vertical direction. The domain is discretized into a non-uniform 68 × 33 grid with higher resolution in the repository area and lower resolution towards the edges of the modeling domain.

Unlike NUTS, which uses the grid provided by BRAGFLO, PANEL uses a one-cell grid that encompasses the intruded panel.

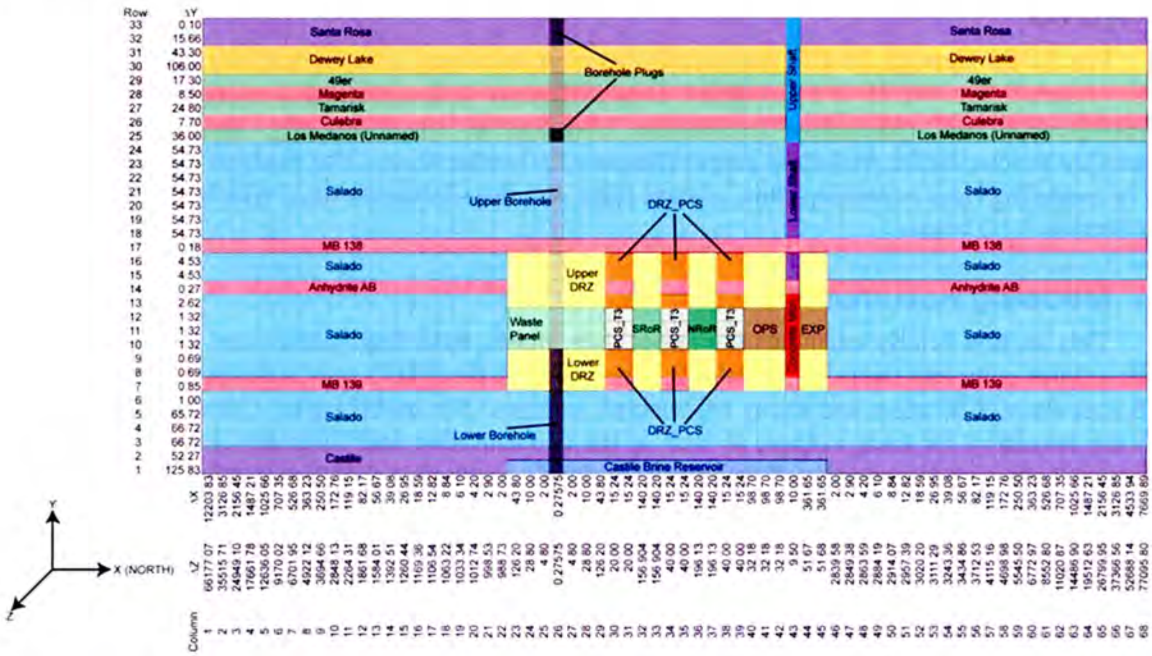


Figure 1 Computational grid used for Salado Flow and transport calculations.

DRZ represents the Disturbed Rock Zone surrounding the repository area and MB refers to the marker beds. The light green area between the upper and lower DRZ's represents the waste area of the repository, while the light brown areas represent the operations (Ops) and experimental (Exp) areas of the repository. The grayed cells extending from the Castile to the surface in column 26 show the borehole location. Concrete_MON represents a concrete monolith, PCS_T3 is ROM salt (generated from mining operation at the WIPP) that is healed fractures for 200 to 10,000 years, DRZ_PCS is the disturbed rock zone directly above the concrete portion of the panel closure system, and RoR is the rest of the repository. The *x*-axis corresponds to north, the *y*-axis to depth, and the *z*-axis to east; all distances are given in meters. Figure is not drawn to scale.

2.5 Other Codes

BRAGFLO, POSTBRAG, and PREBRAG must be run prior to NUTS and PANEL because the former codes provide input files necessary for the execution of the latter. Uncertainty in the input parameters is included through the use of LHS. For NUTS calculations, MATSET has been used to add selected material properties and parameters to the NUTS output files for use in downstream processing. ALGEBRACDB calculates the integrated fluxes up the borehole, up the shafts, or out through the marker beds. SUMMARIZE is then used to provide a summary of the fluxes, which is used as input to a plotting program to visualize the results. For the present analysis, the *matplotlib* module in Python has been used to produce the cumulative release plots for each replicate/vector/isotope combination.

3 An Overview of NUTS and PANEL

3.1 NUTS

For S1-BF through S5-BF, the overall transport and decay of radionuclides are calculated using NUTS, version 2.05c. NUTS is a five-point finite-difference code designed to model multi-dimensional, multi-component, and radioactive-contaminant transport in single-porosity, dual-porosity, or dual-permeability porous media, including parent/daughter first-order decay. The analysis is composed of three types of modeling runs: screening runs, isotope runs, and time-intrusion runs, which are discussed in detail in Section 3.1.3 below.

3.1.1 Modeling Assumptions

This section briefly examines the major data inputs, modeling factors, and assumptions used in NUTS; a more complete overview of NUTS is provided in the NUTS user's manual (Treadway, 1997). NUTS models mobilization and decay of selected isotopes. For mobilization calculations, the code requires the inventory for each isotope, as well as the concentration and solubility limit for each element. The isotope inventory is apportioned among the various computational cells according to their volume or areal fractions of the repository; this approach is equivalent to assuming a homogeneous waste inventory.

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

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

3.1.2 Data Flow

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

The NUTS binary output file is used by ALGEBRACDB, which in turn produces output used by SUMMARIZE. The output from SUMMARIZE is imported into a graphics package such as *matplotlib* or Microsoft Excel and then plotted. Figure 2 shows the relationship between the major codes used in the NUTS analysis.

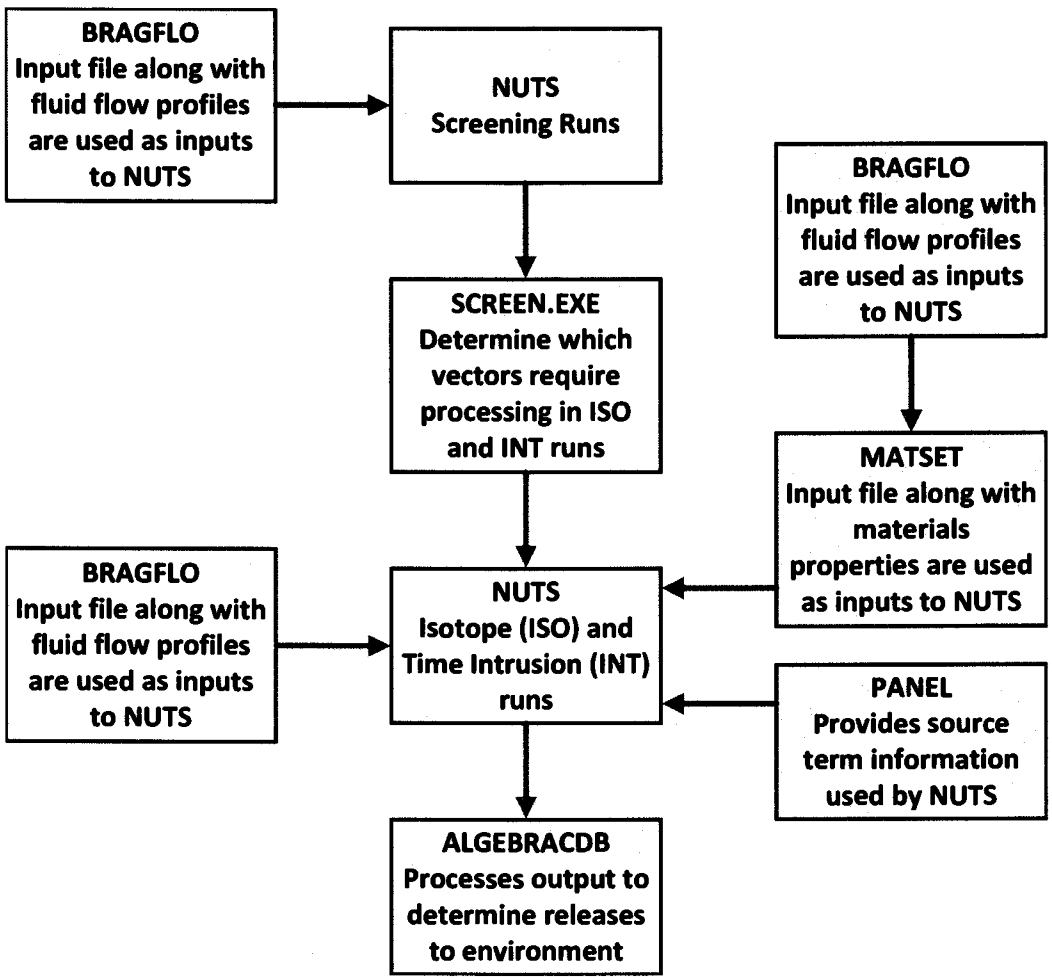


Figure 2 Run sequence showing major steps for NUTS in the CRA-2014 PA.

3.1.3 Type of Model Runs

In WIPP PA, three different types of runs are performed with NUTS: screening, which identifies those vectors which must be analyzed in greater detail; isotope, which determine the amount of radionuclides transported throughout the repository; and time-intrusion, which repeats the isotope calculations with different starting times. The following sections describe each type of run.

3.1.3.1 Screening Runs

Because the transport calculations performed by NUTS are computationally intensive, preliminary screening runs reduce the overall running time required by filtering out vectors that have no potential to release significant quantities of radionuclides either to the Culebra or across the land withdrawal boundary (LWB). Screening runs calculate the transport of a temporally continuous tracer with an initial concentration of 1 kg/m^3 in all waste disposal areas over 10,000 years. A vector is included for further analysis if the cumulative tracer concentration that reaches the accessible environment, either by crossing the LWB or by entering the Culebra via the borehole or shaft, exceeds 10^{-7} kg/m^3 (Ismail, 2008; Ismail and Nemer, 2008; Kim and Camphouse, 2013; US DOE, 2009). The magnitude of the initial tracer and screening cutoff concentrations are considered conservative; as discussed in Stockman *et al.*(Stockman et al., 1996), the tracer concentration was chosen to be greater than the maximum observed concentration of any radionuclide in the repository, while the cumulative limits underestimate the minimum amount of mass required for a release. Vectors not "screened in" are excluded from isotope and time-intrusion calculations, where specific isotopes and more complicated chemistry are modeled.

SCREEN.FOR, a Fortran 90 program, post-processes output from the screening runs and lists which vectors satisfy the screening criteria and where the breach occurs (borehole, markerbeds, or shaft). It also totals the number of included vectors for each scenario. Details of the verification process are provided in Appendix B.2; see Long (Long, 2013) for information on the run control used for SCREEN.FOR.

The potential computational savings from eliminating a vector from further consideration is substantial. A total of five isotope runs and ten time intrusion runs are performed for each included vector; thus, fifteen different simulations are avoided for each vector that does not lead to significant releases during the screening runs.

3.1.3.2 Isotope Runs

The isotope runs consist of modeling each isotope for each vector included for further analysis during the previous step and calculating the time-integrated flux for each isotope across the LWB or up to the Culebra. The NUTS isotope runs consist of the undisturbed scenario (S1-BF) as well as the 350- and 1000-year intrusion scenarios (S2-BF through S5-BF) listed in Table 1.

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

(1) ^{241}Am
(2) ^{239}Pu
(3) $^{238}\text{Pu} \rightarrow {}^{234}\text{U} \rightarrow {}^{230}\text{Th}$

A more recent analysis(Kicker and Zeitler, 2013), based on updated inventory information, yielded the same set of lumped isotopes in the same decay chains. Consequently, no changes to the code or analysis scripts were required. Note that while ^{241}Am and ^{239}Pu have parent and daughter isotopes, those other isotopes are not explicitly considered. Moreover, since the half-life of ^{238}Pu is 87.7 years, most of the ^{238}Pu initially present in the repository will have decayed in the time frames of interest. Therefore ^{238}Pu is not considered individually in the remainder of this analysis, although total releases presented below do include contributions from ^{238}Pu.

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

$$\boldsymbol{R_n} = \sum \frac{Q_i}{L_i}\left(\frac{10^6\text{Ci}}{C}\right) \quad \textbf{(1)}$$

where Q_i is the 10,000-year cumulative release of radionuclide i, L_i is the release limit for radionuclide i (as specified by 40.CFR 194), and C is the total transuranic inventory in the WIPP, and all measurements are in curies (Ci).

3.1.3.3 Time Intrusion Runs

NUTS time intrusion runs simulate intrusions that occur at times other than the 350- and 1000-year intrusions modeled in the isotope runs. The flow fields for these simulations are obtained by shifting the time index for the corresponding BRAGFLO flow fields. For instance, the flow field for an intrusion at 100 years is obtained by shifting the 350-year intrusion simulation backwards by 250 years. (The flow is assumed to be steady-state for the last 250 years of the 100-year intrusion simulation.)

Transport calculations are also done with intrusion times of 3000, 5000, 7000, and 9000 yrs. For these cases, the repository is assumed to remain undisturbed until the time of intrusion, at which point the 1000-year intrusion flow-field is used. This approach is justified since previous BRAGFLO simulations have shown that the undisturbed scenario reaches steady state conditions in less than 3000 years. In addition, repository performance is most sensitive to gas-pressure relief and brine inflow from the high-pressure brine pocket or marker beds that occur at or soon after intrusion, but is insensitive to changes that occur prior to intrusion, such as fracturing (Nemer, 2010; Stockman et al., 1996). Thus, the flow field after intrusion depends much more on an intrusion event occurring than on the conditions before intrusion.

3.1.4 Computational Procedure

This section outlines the simulation method used to analyze Salado Transport. A detailed description of the run control procedures used for the CRA-2014 BL and CRA-2014 PA, including the NUTS calculations, and the input, log, script, and output files for each step are described in Long (Long, 2013).

3.1.4.1 Step 1: NUTS Screening Runs

Step 1 invokes NUTS in "screening" mode to compute the transport of a conservative tracer for the flow fields calculated by BRAGFLO for every vector in each of the three replicates. The screening calculations are performed for each scenario and time combination considered in S1-BF through S5-BF.

3.1.4.2 Step 2: SUMMARIZE and SCREEN

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

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

3.1.4.3 Step 3: NUTS Isotope Runs

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

3.1.4.4 Step 4: NUTS Time Intrusion Runs

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

3.2 PANEL

PANEL is unique in the WIPP PA framework in that it produces information for several of the downstream WIPP PA codes: NUTS (for Salado transport), CCDFGF (for Culebra releases), and CCDFGF (for DBR releases). The calculated outputs in each case are different. NUTS needs information for the "lumped" radionuclides ^{241}Am, ^{238}Pu, ^{239}Pu, ^{234}U, and ^{230}Th. CCDFGF (for DBR releases) needs the mobilized radionuclide concentrations in brine (Salado and/or Castile brine), while CCDFGF (for Culebra releases in S6-BF) needs the EPA units of the "lumped" radionuclides ^{241}Am, ^{238}Pu, ^{239}Pu, ^{234}U, and ^{230}Th up the borehole to the Culebra. In addition to providing inputs used by other PA codes, PANEL is frequently used in a stand-alone mode to calculate radionuclide decay. For S6-BF, PANEL was run in STANDARD mode, which computes the amount of radionuclides transported up the borehole to the Culebra. Because a new inventory was implemented for the CRA-2014 PA (Kicker and Zeitler, 2013), DECAY and CONCENTRATION runs were also performed as part of the CRA-2014 PA (Long, 2013); an analysis of the results is provided elsewhere (Kim, 2013).

A detailed description of the run control procedures used for the PANEL calculations, as well as the names and locations of the input, log, script, and output files for each step, are described in Long (Long, 2013).

3.2.1 BRAGFLO Output to PANEL

As mentioned above, PANEL requires BRAGFLO. The required PANEL input for S6-BF is generated by BRAGFLO and written to the files **ALG2_BF_CRA14_R*r*_S6_V*vvv*.CDB** and **ALG2_BF_CRA14BL_R*r*_S6_V*vvv*.CDB** (*r* = 1, 2, 3; *vvv* = 001, 002, ... 100) stored in CMS library **LIBCRA14_BFR*r*S6**.

3.2.2 SUMMARIZE

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

4 Results

This section presents the results from NUTS and PANEL simulations for transport of the major lumped radioisotopes within the Salado formation for S1-BF through S6-BF as discussed above. As mentioned, while NUTS models five isotopes, ^{238}Pu is a small fraction of the inventory within the repository and has a relatively short half-life (87.7 years). In the CRA-2009 PABC, activity of CH TRU ^{238}Pu was 1.47×10^6 Ci (47.4% of total activity 3.10×10^6 Ci) (Fox et al., 2009). In the CRA-2014 PA, activity of CH TRU ^{238}Pu is 5.95×10^5 Ci (22.0% of total activity 2.70×10^6 Ci) (Kicker and Zeitler, 2013). ^{238}Pu is no longer the most dominant radionuclide in the CRA-2014 PA, while it was the most dominant in the CRA-2009 PABC. Therefore ^{238}Pu is excluded from further consideration. PANEL was performed with five different brine volumes (BV), and BV*k* was added to analysis name CRA14, where the number *k* means 1 ×, 2 ×, 3 ×, 4 ×, and 5 × 17,400 m³ (Brush et al., 2012). For Salado transport, the PANEL BV1 output files were used for NUTS calculations for the CRA-2014 PA. Only one set of PANEL output files were used to keep the overall NUTS calculations at a feasible level. The PANEL BV1 output files were chosen as the calculated concentrations would be conservatively highest due to the small brine volume. This is confirmed by Kim (Kim, 2013), in which total mobilization potentials for a radionuclide (Am and Pu) in both Salado and Castile brines decrease as the brine volume increases.

4.1 NUTS

4.1.1 Screening Runs

Screening runs reduce the total number of simulations necessary by eliminating vectors that cannot transport sufficient quantities of radionuclides beyond the LWB. Screening runs model a conservative tracer with a concentration of 1 kg/m^3. The cumulative mass of tracer is monitored at the intersection of the borehole and the Culebra, at the intersection of the shaft and the Culebra, and at the LWB in the marker beds. Vectors with a cumulative tracer release of 10^{-7} kg/m^3 or more (Ismail, 2008; Ismail and Nemer, 2008; Kim and Camphouse, 2013; US DOE, 2009) at any of these key points are included for further analysis and passed through to the full radionuclide transport simulations. The results of the screening runs are presented in Table 2.

Examining Table 2, it is clear that most of the vectors that are screened in are found in S2-BF and S3-BF; there are roughly four times as many vectors screened in for these scenarios as for S4-BF and S5-BF in both the CRA-2009 PABC, CRA-2014 BL and CRA-2014 PA. The greater number of screened-in vectors in S2-BF and S3-BF is the result of the E1 intrusion penetrating a brine pocket, thereby having a greater effect on the flow field within the repository compared to the E2 scenarios.

In comparing the results from the CRA-2014 PA to those from the CRA-2009 PABC, we see that there is an increase in the number of vectors in the E1 intrusion scenarios; in the E2 intrusion scenarios, there are a few additional vectors that satisfy the screening criteria. On the other hands, for the CRA-2014 BL, there are comparable number of vectors in the E1 intrusion scenarios compared to those for the CRA-2009 PABC; in the E2 intrusion scenarios, there are a few additional vectors that the satisfy the screening criteria. It should be noted that Table 2 indicates the potential pathways through which releases can occur. In the actual release scenarios considered, the lower concentration of nuclides may significantly reduce the amount of radionuclides that can reach the Land Withdrawal Boundary or the Culebra.

For this analysis, Replicates 1, 2, and 3 screened in 202, 213, and 209 vectors out of a possible 500 each in the CRA-2014 PA, compared to 162, 171, and 171 vectors, respectively, in the CRA-2009 PABC. In the CRA-2014 BL, Replicate 1 screened in 168 vectors. These vectors are listed in Table 2, sorted by replicate and scenario. In addition to these vectors, it was also necessary to screen in 87 vectors from Replicate 1, 88 vectors from Replicate 2, and 92 vectors from Replicate 3 in the CRA-2014 PA, and 72 vectors from Replicate 1 for S1-BF to provide the flow conditions needed for the time-intrusion calculations. Like the CRA-2009 PABC calculations, vector 53 in the CRA-2014 BL showed potential release to markerbeds in the undisturbed scenario. Unlike the CRA-2009 PABC calculations, in the CRA-2014 PA we find that there is no vector that showed potential releases in the undisturbed scenario. In addition, no vector in this analysis showed releases at the shaft-Culebra interface. Vectors from S1-BF listed in Table 3 are analyzed only to provide the fluid flow profiles needed for the intrusion scenarios.

Table 2 Vectors included for further analysis in the CRA-2009 PABC, CRA-2014 BL and CRA-2014 PA

Rep.	Scen.	CRA-2009 PABC		CRA-2014 BL		CRA-2014 PA	
		Vectors[a]	Count	Vectors[a]	Count	Vectors[a]	Count
1	S1-BF	53M	1	53M	1	None	0
	S2-BF	2, 3, 5, 6, 7, 8, 9, 10, 12, 13, 14, 16, 17, 19, 20, 22, 23, 24, 25, 26, 27, 28, 29, 30, 34, 35, 36, 38, 41, 43, 45, 46, 47, 48, 49, 50, 51, 52, 53M, 54, 55, 58, 59, 60, 61, 62, 63, 64, 66, 67, 69, 70, 71, 72, 73, 74, 76, 78, 79, 80, 82, 83, 84, 86, 88, 89, 90, 92, 93, 94, 98	71	2, 3, 5, 6, 7, 8, 9, 10, 12, 13, 14, 16, 17, 19, 20, 22, 23, 24, 25, 26, 27, 28, 29, 30, 34, 35, 36, 38, 39, 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, 74, 76, 78, 79, 80, 82, 83, 84, 86, 88, 89, 90, 91, 92, 93, 94, 98	71	1, 2, 3, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 16, 17, 19, 20, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 33, 34, 35, 36, 37, 38, 39, 41, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 58, 59, 60, 61, 62, 63, 64, 66, 67, 68, 69, 70, 71, 72, 74, 75, 76, 77, 78, 79, 80, 82, 83, 84, 85, 86, 87, 88, 89, 90, 91, 92, 93, 94, 95, 96, 97, 98, 100	87
	S3-BF	2, 3, 7, 8, 9, 10, 12, 13, 14, 16, 17, 20, 22, 23, 24, 25, 27, 28, 29, 30, 34, 35, 36, 41, 43, 45, 46, 47, 49, 50, 52, 54, 55, 58, 59, 60, 61, 62, 63, 66, 67, 70, 71, 76, 78, 79, 80, 82, 83, 84, 86, 89, 90, 93, 94, 98	56	2, 3, 7, 8, 9, 10, 12, 13, 14, 16, 17, 20, 22, 23, 24, 25, 27, 28, 29, 30, 34, 35, 36, 38, 41, 43, 45, 46, 47, 49, 50, 51, 52, 54, 55, 58, 59, 60, 61, 62, 63, 66, 67, 69, 70, 72, 76, 78, 79, 80, 82, 83, 86, 89, 90, 93, 98	57	1, 2, 3, 5, 6, 7, 8, 9, 11, 12, 13, 14, 16, 17, 19, 20, 22, 23, 24, 25, 26, 27, 28, 29, 30, 34, 35, 36, 37, 38, 39, 41, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 54, 55, 58, 59, 60, 61, 62, 63, 64, 66, 67, 69, 70, 71, 72, 74, 75, 76, 77, 78, 79, 80, 82, 83, 84, 86, 88, 89, 90, 92, 93, 94, 95, 96, 97, 98, 100	79
	S4-BF	7, 9, 16, 17, 27, 30, 36, 45, 50, 53M, 55, 67, 76, 78, 82, 83, 98	17	2, 7, 9, 12, 16, 17, 27, 28, 30, 36, 45, 50, 55, 67, 76, 78, 79, 83, 93, 98	20	2, 7, 9, 12, 16, 17, 20, 27, 28, 30, 36, 45, 50, 63, 66, 67, 76, 78, 98	19
	S5-BF	7, 9, 16, 17, 27, 30, 36, 45, 50, 53M, 55, 67, 76, 78, 82, 83, 98	17	2, 7, 9, 12, 16, 17, 27, 28, 30, 36, 45, 50, 55, 67, 76, 78, 79, 83, 93, 98	20	7, 9, 12, 16, 17, 27, 28, 30, 36, 45, 50, 63, 66, 67, 76, 78, 98	17
2	S1-BF	None	0			None	0
	S2-BF	2, 3, 4, 6, 8, 9, 10, 11, 12, 14, 16, 17, 18, 19, 20, 21, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 43, 44, 45, 48, 49, 50, 51, 52, 53, 54, 55, 56, 59, 61, 62, 63, 64, 65, 66, 67, 68, 69, 71, 72, 74, 75, 77, 79, 80, 81, 83, 84, 87, 89, 90, 91, 92, 95, 96, 98, 99, 100	76			1, 2, 3, 4, 6, 7, 8, 9, 10, 11, 12, 13, 14, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 59, 61, 62, 63, 65, 66, 67, 68, 69, 70, 71, 72, 73, 74, 75, 77, 79, 80, 81, 82, 83, 84, 86, 87, 88, 89, 90, 92, 93, 94, 95, 96, 98, 99, 100	88

Rep.	Scen.	CRA-2009 PABC		CRA-2014 BL		CRA-2014 PA	
		Vectors[a]	Count	Vectors[a]	Count	Vectors[a]	Count
	S3-BF	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, 38, 39, 40, 41, 44, 48, 50, 51, 52, 53, 54, 55, 59, 63, 64, 65, 66, 67, 68, 71, 72, 74, 75, 77, 79, 80, 84, 87, 89, 90, 92, 95, 96, 98, 99	60			1, 2, 3, 4, 6, 8, 9, 10, 11, 12, 13, 14, 16, 17, 18, 19, 20, 21, 22, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 59, 61, 62, 63, 65, 66, 67, 68, 70, 71, 72, 74, 75, 77, 79, 80, 81, 83, 84, 86, 87, 89, 90, 92, 94, 95, 96, 98, 99, 100	81
	S4-BF	4, 17, 21, 24, 28, 30, 34, 36, 40, 53, 55, 63, 68, 79, 90, 92, 95, 98	18			4, 17, 21, 24, 25, 28, 30, 34, 36, 40, 53, 55, 59, 63, 67, 68, 79, 90, 92, 95, 96, 98	22
	S5-BF	4, 17, 21, 24, 28, 30, 34, 40, 53, 55, 63, 68, 79, 90, 92, 95, 98	17			4, 17, 21, 24, 25, 28, 30, 34, 36, 40, 53, 55, 59, 63, 67, 68, 79, 90, 92, 95, 96, 98	22
3	S1-BF	None	0			None	0
	S2-BF	2, 3, 4, 7, 10, 11, 13, 14, 15, 17, 18, 19, 21, 22, 24, 25, 26, 27, 28, 29, 30, 32, 33, 34, 35, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 49, 50, 52, 53, 56, 57, 58, 59, 60, 61, 62, 63, 64, 65, 66, 67, 68, 69, 70, 71, 73, 74, 76, 77, 78, 79, 84, 85, 86, 88, 89, 90, 91, 93, 94, 95, 96, 97, 98, 99, 100	77			2, 3, 5, 6, 7, 8, 9, 10, 11, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 55, 56, 57, 58, 59, 60, 61, 62, 63, 64, 65, 66, 67, 68, 69, 70, 71, 72, 73, 74, 75, 77, 78, 79, 81, 83, 84, 85, 86, 87, 88, 89, 90, 91, 92, 93, 94, 95, 96, 97, 98, 99, 100	92
	S3-BF	2, 10, 11, 14, 15, 18, 21, 24, 25, 26, 27, 28, 29, 30, 32, 33, 34, 35, 37, 38, 39, 40, 42, 43, 44, 45, 46, 47, 49, 50, 53, 56, 58, 59, 60, 61, 63, 64, 65, 66, 67, 68, 69, 73, 74, 77, 78, 79, 84, 85, 86, 88, 89, 91, 93, 94, 95, 96, 97, 98, 99	61			2, 3, 5, 7, 8, 10, 11, 13, 14, 15, 17, 18, 20, 21, 22, 24, 25, 26, 27, 28, 29, 30, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 49, 50, 51, 52, 53, 56, 57, 58, 59, 60, 61, 62, 63, 64, 65, 66, 67, 68, 69, 70, 71, 73, 74, 75, 77, 78, 79, 81, 84, 85, 86, 88, 89, 90, 91, 93, 94, 95, 96, 97, 98, 99, 100	81
	S4-BF	30, 35, 37, 42, 44, 47, 49, 53, 59, 66, 69, 77, 79, 86, 91, 93, 96	17			30, 35, 37, 40, 42, 44, 47, 49, 53, 59, 61, 63, 66, 69, 77, 86, 91, 93, 96, 97	20
	S5-BF	30, 35, 37, 42, 44, 47, 49, 53, 59, 66, 69, 77, 86, 91, 93, 96	16			30, 35, 40, 42, 44, 47, 49, 53, 59, 63, 66, 69, 77, 86, 93, 96	16

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

Table 3 Undisturbed vectors run to provide conditions for intrusion scenarios for the CRA-2009 PABC, CRA-2014 BL and CRA-2014 PA

Rep.	CRA-2009 PABC		CRA-2014 BL		CRA-2014 PA	
	Vectors	Count	Vectors	Count	Vectors	Count
1	2, 3, 5, 6, 7, 8, 9, 10, 12, 13, 14, 16, 17, 19, 20, 22, 23, 24, 25, 26, 27, 28, 29, 30, 34, 35, 36, 38, 41, 43, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 58, 59, 60, 61, 62, 63, 64, 66, 67, 69, 70, 71, 72, 73, 74, 76, 78, 79, 80, 82, 83, 84, 86, 88, 89, 90, 92, 93, 94, 98	71	2, 3, 5, 6, 7, 8, 9, 10, 12, 13, 14, 16, 17, 19, 20, 22, 23, 24, 25, 26, 27, 28, 29, 30, 34, 35, 36, 38, 39, 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, 74, 76, 78, 79, 80, 82, 83, 84, 86, 88, 89, 90, 91, 92, 93, 94, 98	72	1, 2, 3, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 16, 17, 19, 20, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 33, 34, 35, 36, 37, 38, 39, 41, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 58, 59, 60, 61, 62, 63, 64, 66, 67, 68, 69, 70, 71, 72, 74, 75, 76, 77, 78, 79, 80, 82, 83, 84, 85, 86, 87, 88, 89, 90, 91, 92, 93, 94, 95, 96, 97, 98, 100	87
2	2, 3, 4, 6, 8, 9, 10, 11, 12, 14, 16, 17, 18, 19, 20, 21, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 43, 44, 45, 48, 49, 50, 51, 52, 53, 54, 55, 56, 59, 61, 62, 63, 64, 65, 66, 67, 68, 69, 71, 72, 74, 75, 77, 79, 80, 81, 83, 84, 87, 89, 90, 91, 92, 95, 96, 98, 99, 100	76			1, 2, 3, 4, 6, 7, 8, 9, 10, 11, 12, 13, 14, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 59, 61, 62, 63, 65, 66, 67, 68, 69, 70, 71, 72, 73, 74, 75, 77, 79, 80, 81, 82, 83, 84, 86, 87, 88, 89, 90, 92, 93, 94, 95, 96, 98, 99, 100	88
3	2, 3, 4, 7, 10, 11, 13, 14, 15, 17, 18, 19, 21, 22, 24, 25, 26, 27, 28, 29, 30, 32, 33, 34, 35, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 49, 50, 52, 53, 56, 57, 58, 59, 60, 61, 62, 63, 64, 65, 66, 67, 68, 69, 70, 71, 73, 74, 76, 77, 78, 79, 84, 85, 86, 88, 89, 90, 91, 93, 94, 95, 96, 97, 98, 99, 100	77			2, 3, 5, 6, 7, 8, 9, 10, 11, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 55, 56, 57, 58, 59, 60, 61, 62, 63, 64, 65, 66, 67, 68, 69, 70, 71, 72, 73, 74, 75, 77, 78, 79, 81, 83, 84, 85, 86, 87, 88, 89, 90, 91, 92, 93, 94, 95, 96, 97, 98, 99, 100	92

4.1.2 Isotope Runs

Isotope runs represent the undisturbed case (S1-BF), as well as 350- and 1000-year E1 intrusions (S2-BF and S3-BF) and of type E2 (S4-BF and S5-BF). The maximum releases for each species in the various isotope cases analyzed are summarized in Table 4.

Table 4 Maximum radionuclide and total releases at the Borehole/Culebra interface in NUTS isotope calculations

Analysis	Intrusion	Scenario	Time (yr)	Maximum Releases (EPA units)				
				^{241}Am	^{239}Pu	^{234}U	^{230}Th	Total
CRA-2009 PABC	None	S1-BF	N/A	0.0	0.0	0.0	0.0	0.0
	E1	S2-BF	350	3.47E+01	4.25E+01	2.47E-01	2.61E-01	6.45E+01
		S3-BF	1000	1.31E+01	2.74E+01	2.09E-01	2.41E-01	4.08E+01
	E2	S4-BF	350	2.95E+00	8.05E+00	4.34E-02	1.97E-02	1.10E+01
		S5-BF	1000	1.39E-01	4.24E+00	3.88E-02	1.54E-02	4.32E+00
CRA-2014 PA BL (Replicate 1)	None	S1-BF	N/A	0.0	0.0	0.0	0.0	0.0
	E1	S2-BF	350	6.96E+01	8.94E+01	3.75E-02	1.40E-01	1.49E+02
		S3-BF	1000	2.72E+01	7.28E+01	3.38E-02	1.58E-01	1.00E+02
	E2	S4-BF	350	4.97E+00	9.19E+00	4.42E-03	2.22E-03	9.41E+00
		S5-BF	1000	8.32E-02	8.18E+00	3.52E-03	2.55E-04	8.18E+00
CRA-2014 PA	None	S1-BF	N/A	0.0	0.0	0.0	0.0	0.0
	E1	S2-BF	350	4.98E+01	1.51E+02	5.53E-02	1.52E-01	2.01E+02
		S3-BF	1000	1.17E+01	1.09E+02	4.59E-02	1.49E-01	1.20E+02
	E2	S4-BF	350	1.07E+01	3.23E+01	1.03E-02	2.20E-03	4.29E+01
		S5-BF	1000	1.59E+00	2.06E+01	8.26E-03	6.75E-04	2.07E+01

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

In addition to the maximum releases for each radionuclide and the maximum overall releases shown in Table 4, the average release for each scenario plus the percentage contribution of each of the lumped isotopes to the scenario average has been calculated in Table 5. The average release, reported in EPA units, is determined by taking the average of all of the cumulative releases across the three replicates. The percentage assigned to each isotope is the average release for the given isotope divided by the average cumulative release.

Examining Table 5, we notice significant differences in the distribution of isotopes between the E1 and E2 intrusion types, and between the 350-yr and 1000-yr intrusion times in both analyses. The differences between the 350-yr and 1000-yr intrusions are the result of the difference in the half-lives of the two isotopes (430 years for ^{241}Am versus 24,000 years for ^{239}Pu). Comparing the intrusion types, we can see by comparing the average total release to the maximum total release that a handful of vectors dominate the releases in each scenario. Differences in the brine volumes between the two scenarios, combined with speciation-dependent variations in the solubility, are largely responsible for the difference in compositions between the E1 and E2 releases. The relative magnitude of the E1 and E2 releases is a result of the smaller brine volumes available in the E2 scenarios.

Table 5 Percentage of lumped isotopes relative to average release at the Borehole/Culebra interface for isotope scenarios

Analysis	Intrusion	Scenario	Time (years)	Percentage of Isotope in Average Release (%)				Average Release (EPA units)
				^{241}Am	^{239}Pu	^{234}U	^{230}Th	
CRA-2009 PABC	None	S1-BF	N/A	0.0	0.0	0.0	0.0	0.0
	E1	S2-BF	350	6.31E+01	3.65E+01	3.51E-01	8.07E-02	2.53E+00
		S3-BF	1000	3.26E+01	6.67E+01	5.69E-01	1.74E-01	9.19E-01
	E2	S4-BF	350	3.43E+01	6.49E+01	7.10E-01	1.13E-01	8.92E-02
		S5-BF	1000	3.05E+00	9.56E+01	1.20E+00	1.83E-01	4.02E-02
CRA-2014 PA BL (Replicate 1)	None	S1-BF	N/A	0.0	0.0	0.0	0.0	0.0
	E1	S2-BF	350	4.60E+01	5.39E+01	4.89E-02	4.29E-02	5.17E+00
		S3-BF	1000	2.21E+01	7.77E+01	7.68E-02	9.82E-02	2.21E+00
	E2	S4-BF	350	3.02E+01	6.97E+01	1.03E-01	2.14E-02	1.88E-01
		S5-BF	1000	1.55E+00	9.83E+01	1.42E-01	1.52E-02	1.02E-01
CRA-2014 PA	None	S1-BF	N/A	0.0	0.0	0.0	0.0	0.0
	E1	S2-BF	350	4.80E+01	5.19E+01	6.21E-02	2.42E-02	5.14E+00
		S3-BF	1000	1.81E+01	8.17E+01	8.09E-02	4.43E-02	2.24E+00
	E2	S4-BF	350	2.65E+01	7.34E+01	7.44E-02	1.11E-02	3.16E-01
		S5-BF	1000	5.83E+00	9.41E+01	1.00E-01	1.25E-02	1.62E-01

Comparing the CRA-2014 BL and CRA-2014 PA with the CRA-2009 PABC results presented in Table 4 and Table 5, we see that the maximum releases of ^{239}Pu for both the CRA-2014 BL and CRA-2014 PA are uniformly larger than the corresponding maximum releases in the CRA-2009 PABC, while the maximum releases of ^{234}U and ^{230}Th are uniformly smaller. The composition data in Table 5 suggest that the isotopes ^{241}Am, ^{234}U, and ^{230}Th make up a smaller portion of the average release compared to their proportions in the CRA-2009 PABC, while the corresponding percentage of ^{239}Pu has increased. However, for S5-BF (E2 intrusion) in the CRA-2014 PA, two isotopes change their proportions of the average release in an opposite way: ^{239}Pu decreases a portion of the average release, and ^{241}Am increases a portion of the average release compared to their portions in the CRA-2009 PABC. The increase in the releases, as well as the radionuclide distribution, can be attributed to the change in solubilities of the +III and +IV actinides (Brush, 2013; Brush and Domski, 2013; Kim, 2013).

In all the runs discussed in this section, releases to the markerbed do not exceed 1×10^{-7} kg/m^3 in any scenario in the CRA-2014 PA compared to the CRA-2009 PABC. In the CRA-2014 BL and CRA-2009 PABC, vector 53 of Replicate 1 in the undisturbed scenario exceeded this limit. For the CRA-2009 PABC, vector 53 of replicate 1 for an E1 intrusion at 350 years has additionally exceeded this limit. Changes included in the CRA-2014 PA result in an overall reduction in the cumulative volume of brine reaching the LWB through the markerbeds for undisturbed repository conditions (Figure 1 in Kim and Camphouse (Kim and Camphouse, 2013)).

4.1.2.1 Scenario S1-BF: Undisturbed Scenario

S1-BF represents the undisturbed state of the repository. In the CRA-2014 PA, there were 87, 88, and 92 vectors included for further analysis in Replicate 1, 2, and 3, respectively; in the CRA-2014 BL there were 72 vectors in Replicate 1. The vectors for each replicate that satisfied the screening criteria are listed in Table 3. These vectors were analyzed because their flow and transport profiles were needed for the isotope or time intrusion runs. For the disturbed scenarios, all the vectors that met the screening criteria for S1-BF showed movement of the tracer up the borehole. As seen in Table 3, no vector of any replicate in the CRA-2014 PA showed tracer releases to the markerbeds but vector 53 in Replicate 1 for the CRA-2014 BL did.

The statutory requirements of 40 CFR 194.55 require that DOE determine the maximum total radioactivity level for ^{226}Ra and ^{228}Ra in any underground source of drinking water for 10,000 years after decommissioning (Ismail 2008b). Although the CRA-2014 BL calculation results showed tracer component releases to markerbeds, the CRA-2014 PA calculations including all changes and modifications showed that no vector results in a tracer component release exceeding the NUTS screening limit 1.0×10^{-7} kg/m^3. Consequently, any calculated value would be below numerical precision and is effectively zero in the CRA-2014 PA (Kim and Camphouse, 2013; US DOE, 2009).

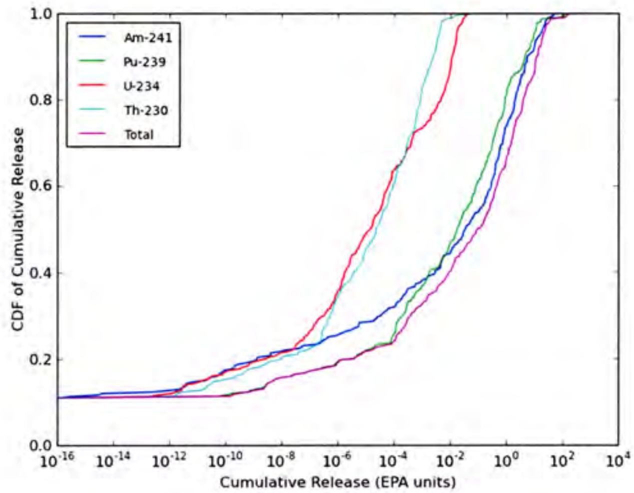
4.1.2.2 Scenario S2-BF: E1 Intrusion at 350 Years

S2-BF models an E1 intrusion, which penetrates the repository and a brine pocket in the lower Castile formation 350 years after closure. S2-BF is highly influenced by 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-BF has both the greatest number of screened-in vectors and the largest outward fluxes of brine and radioisotopes for the CRA-2014 PA. The only pathway with any cumulative releases in S2-BF is through the borehole. No releases occur through the markerbeds or the shaft for any of the vectors.

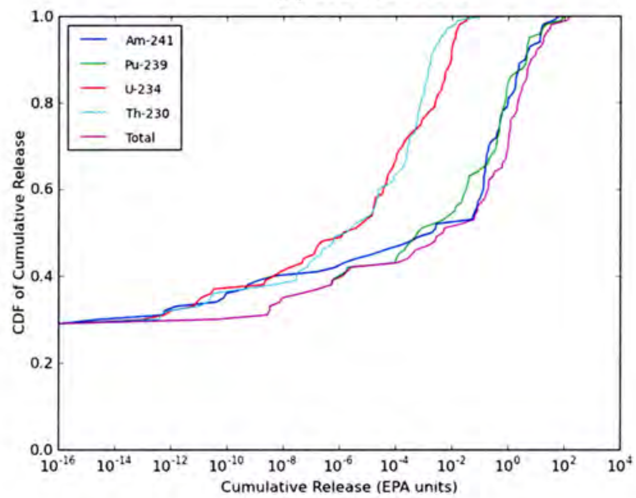
The distribution of releases in EPA units for each isotope and the total release are shown in Figure 3. Figure 3 indicates that, because of limited brine flow, more than a tenth of the vectors in each analysis had cumulative releases at the borehole of less than 10^{-16} EPA units. In addition, it can be seen that for small total releases (less than about 10^{-2} EPA units (CRA-2014 PA) or 10^{-3} EPA units (CRA-2014 BL and CRA-2009 PABC)), the largest contributions come from ^{239}Pu. For larger total releases, ^{241}Am is the dominant contributor for the CRA-2014 PA and CRA-2009 PABC; for the CRA-2014 BL, ^{241}Am and ^{239}Pu are the dominant contributor.

Appendix A shows the cumulative releases as a function of time for all vectors that exhibit releases of 10^{-6} EPA units or larger. Examining the graphs relevant for this scenario (shown in Figure 13), we see that a few hundred years after the release event, the magnitude of the release in most vectors is nearly equal to its final value after 10,000 years. Further increases then occur at either a much slower rate or stop altogether. Although some vectors do not follow this pattern, the corresponding releases from those vectors are much smaller, rarely exceeding 0.001 EPA units.

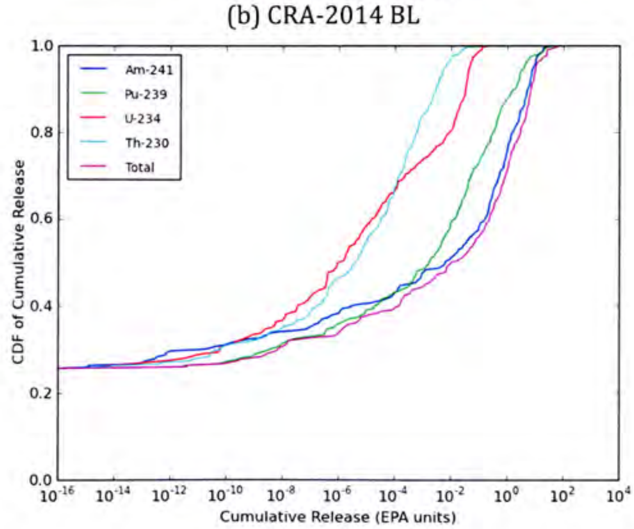
In the CRA-2014 PA the maximum activity for any individual isotope occurred in Replicate 2, vector 68, which had an integrated activity of 151.3 EPA units for ^{239}Pu. For ^{241}Am, Replicate 1, vector 7 had the maximum integrated activity, 49.8 EPA units. The total activities of ^{234}U and ^{230}Th are negligible in comparison: the maxima for those isotopes were 0.055 and 0.152 EPA units in vectors Replicate 3, vector 42 and Replicate 1, vector 17, respectively. The largest total magnitude for a single vector in the CRA-2014 PA, 200.6 EPA units, was found in vector 68 of Replicate 2.



(a) CRA-2014 PA



(b) CRA-2014 BL



(c) CRA-2009 PABC

Figure 3 Normalized cumulative release (EPA units) to the Culebra from the borehole for each isotope and the total for an E1 intrusion at 350 years: (a) CRA-2014 PA, (b) CRA-2014 BL, and (c) CRA-2009 PABC.

In the CRA-2014 BL the maximum activity for any individual isotope occurred in Replicate 1, vector 7, which had an integrated activity of 89.4 EPA units for ^{239}Pu. For ^{241}Am, Replicate 1, vector 17 had the maximum integrated activity, 69.6 EPA units. The total activities of ^{234}U and ^{230}Th are negligible in comparison: the maxima for those isotopes were 0.038 and 0.140 EPA units in vectors Replicate 1, vector 12 and Replicate 1, vector 17, respectively. The largest total magnitude for a single vector in the CRA-2014 BL, 148.8 EPA units, was found in vector 17 of Replicate 1.

4.1.2.3 Scenario S3-BF: E1 Intrusion at 1000 Years

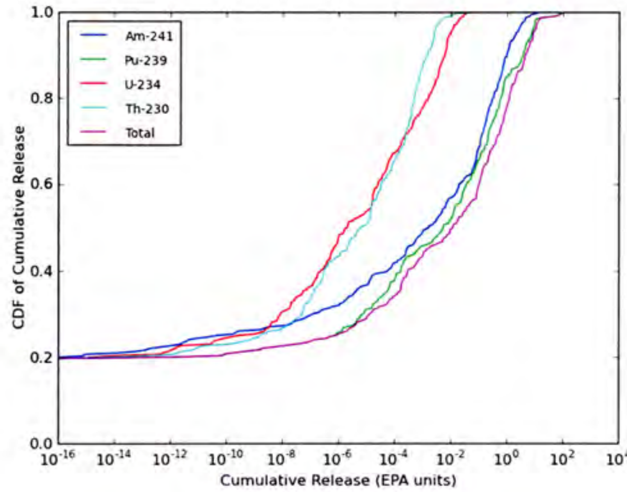
The difference in intrusion times for S2-BF and S3-BF allows more time for chemical and biological activity in S3-BF to either consume brine or produce gas, both of which reduce the amount of brine in the repository at the time of intrusion. This in turn reduces the capacity for nuclide transport. However, like S2-BF, the results of S3-BF are highly influenced by the conditions in the pressurized Castile brine pocket and thus we see that S3-BF has similar characteristics to S2-BF, although the number of screened-in vectors is slightly smaller and the maximum activities are lower.

Like S2-BF, the only pathway with any cumulative releases in S3-BF is through the borehole. No releases occur through the markerbeds or the shaft for any of the vectors. The releases in EPA units for each isotope and the total release are shown in Figure 14. As in S2-BF, releases are dominated by ^{241}Am and ^{239}Pu, with the releases of ^{234}U and ^{230}Th nearly two orders of magnitude smaller than for americium and plutonium. Like S2-BF, the releases for S3-BF primarily take place over a short period of time, as shown.

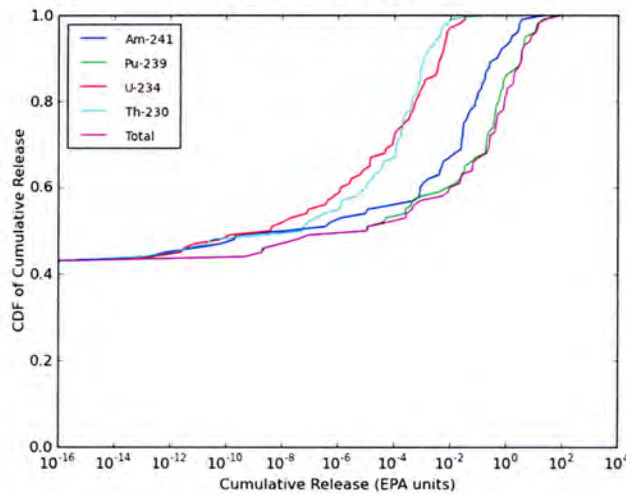
In the CRA-2014 PA the maximum activity for any isotope occurred in Replicate 2, vector 68, which had an integrated activity of 108.7 EPA units for ^{239}Pu. Replicate 1, vector 17 also had the maximum activity of ^{241}Am, 11.7 EPA units. The releases of ^{234}U and ^{230}Th were significantly smaller, with maxima of 0.046 and 0.149 EPA units found in Replicate 3, vector 42 and Replicate 1, vector 17, respectively. The largest total magnitude for a single vector in the CRA-2014 PA, 120.1 EPA units, was found in vector 68 of replicate 2.

In the CRA-2014 BL the maximum activity for any isotope occurred in Replicate 1, vector 17, which had an integrated activity of 72.8 EPA units for ^{239}Pu. Replicate 1, vector 17 also had the maximum activity of ^{241}Am, 27.2 EPA units. The releases of ^{234}U and ^{230}Th were significantly smaller, with maxima of 0.034 and 0.158 EPA units found in Replicate 1, vector 98 and Replicate 1, vector 17, respectively. The largest total magnitude for a single vector in the CRA-2014 BL, 100.2 EPA units, was found in vector 17 of Replicate 1.

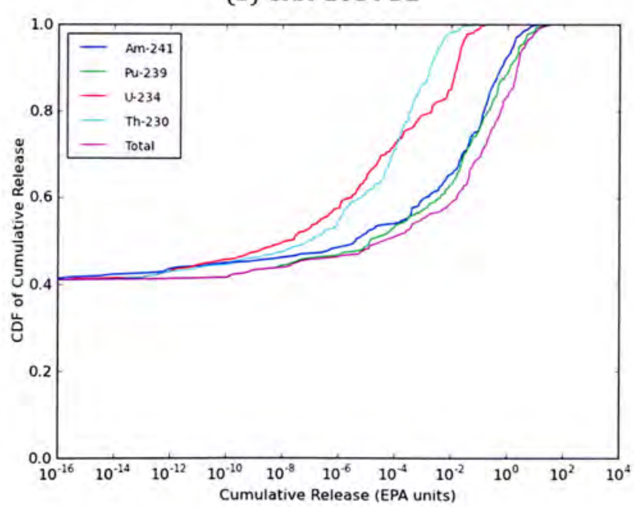
The difference in the distribution of releases between S2-BF and S3-BF can be attributed to the time lag for the intrusion and the most dominant release isotope in S3-BF. For most releases, releases will be dominated by ^{239}Pu, with an additional contribution from ^{241}Am. With increasing time, ^{241}Am is lost due to decay, and the release is continuously dominated by ^{239}Pu due to its longer half-life.



(a) CRA-2014 PA



(b) CRA-2014 BL

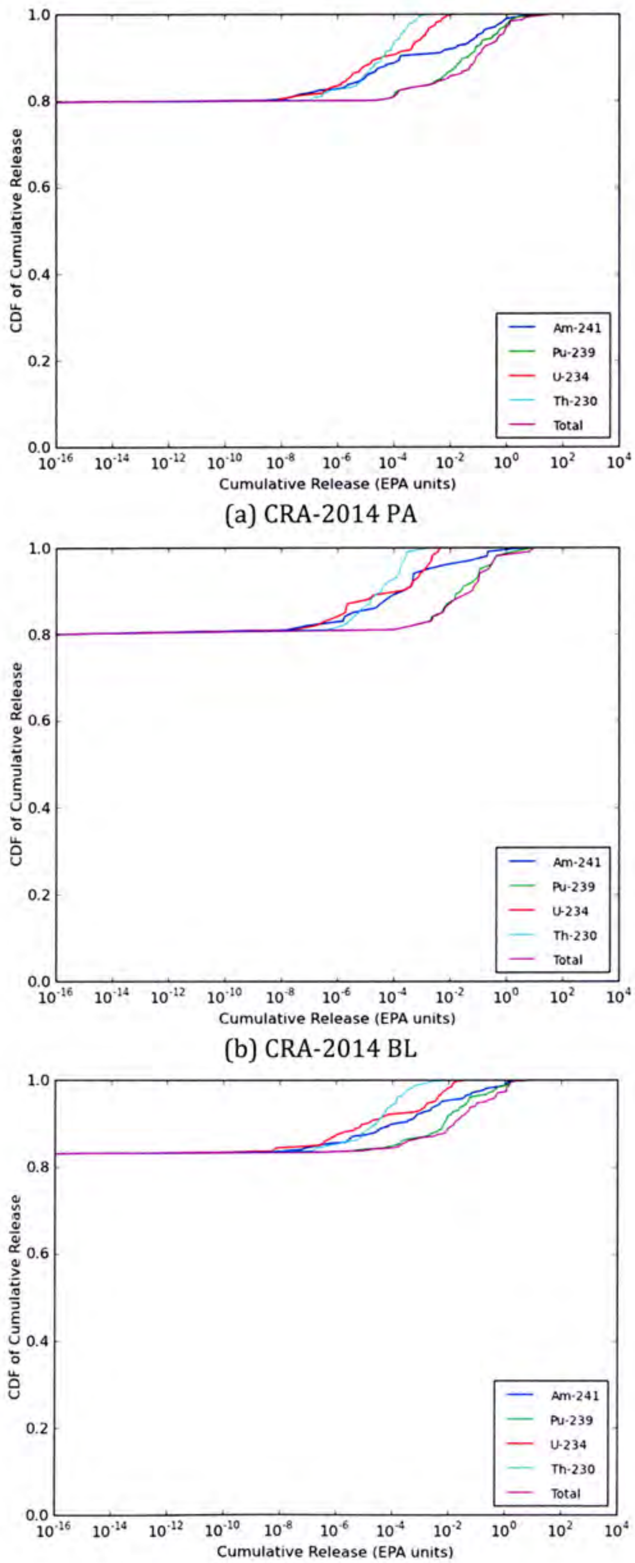


(c) CRA-2009 PABC

Figure 4 Normalized cumulative release (EPA units) to the Culebra from the borehole for each isotope and the total for an E1 intrusion at 1000 years; (a) CRA-2014 PA, (b) CRA-2014 BL, and (c) CRA-2009 PABC.

4.1.2.4 Scenario S4-BF: E2 Intrusion at 350 Years

For most vectors associated with an E2 intrusion, BRAGFLO predicts no or very little brine flow from the repository to the Culebra, as can be seen from Figure 5, less than a fifth of all vectors demonstrate the possibility of a significant release. Time-series plots for each vector across all replicates are shown in Figure 20. Unlike the brine pocket pressure release associated with an E1 intrusion, physical processes do not dominate E2 releases; greater variation therefore exists in the distribution of times at which releases first occur. This also creates a difference in the distribution of total activities, with the activities nearly an order of magnitude smaller than the comparable releases in S2-BF. The maximum activities for ^{241}Am, ^{239}Pu, ^{234}U, and ^{230}Th are 10.6, 32.3, 0.0103, and 0.0022 EPA units for the CRA-2014 PA, and 4.9, 9.2, 0.0044, and 0.0022 EPA units for the CRA-2014 BL. For releases 1.0 EPA units or smaller in Figure 5, ^{239}Pu is the largest contributor; larger releases may be dominated by either ^{239}Pu or ^{241}Am.



(a) CRA-2014 PA

(b) CRA-2014 BL

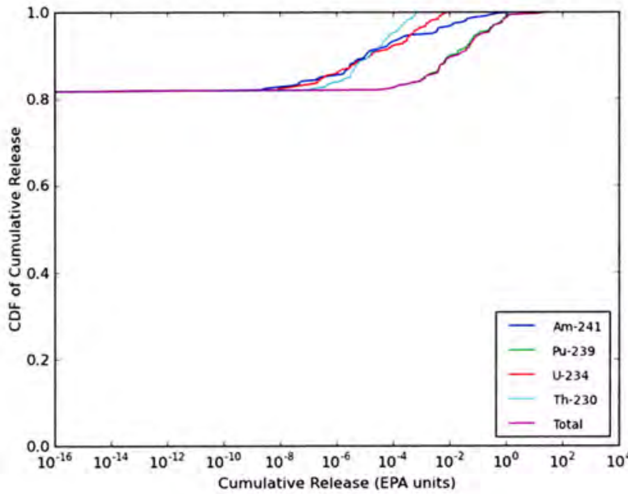
(c) CRA-2009 PABC

Figure 5 Normalized Cumulative Release (EPA Units) to the Culebra from the borehole for each isotope and the total for an E2 intrusion at 350 years; (a) CRA-2014 PA, (b) CRA-2014 BL, and (c) CRA-2009 PABC.

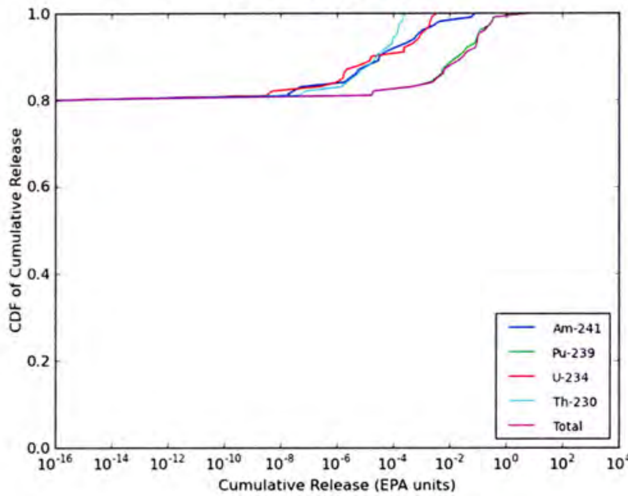
4.1.2.5 Scenario S5-BF: E2 Intrusion at 1000 Years

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

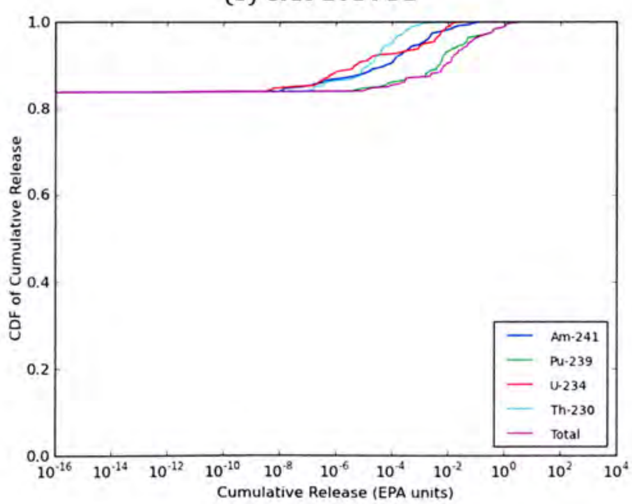
The releases in EPA units for each isotope and the total release are shown in Figure 6. Figure 21 shows the time-series plots for each vector across all replicates. Again, the time plots show greater variation in the occurrences of releases than the corresponding E1 intrusion plots. The 1000-year intrusion time allows for greater decay of the ^{241}Am than is found in the 350-year intrusion time of S4-BF, and a greater relative amount of ^{239}Pu than in S4-BF. The maximum activities for ^{241}Am, ^{239}Pu, ^{234}U, and ^{230}Th are 1.59, 20.64, 0.0083, and 0.0007 EPA units for the CRA-2014 PA, and 0.08, 8.18, 0.0035, and 0.0003 EPA units for the CRA-2014 BL. Releases are dominated by contributions from ^{239}Pu.



(a) CRA-2014 PA



(b) CRA-2014 BL



(c) CRA-2009 PABC

Figure 6 Normalized Cumulative Release (EPA Units) to the Culebra from the borehole for each isotope and the total for an E2 intrusion at 1000 years; (a) CRA-2014 PA, (b) CRA-2014 BL, and (c) CRA-2009 PABC.

4.1.3 Time Intrusion Runs

The time intrusion runs show the same pattern in terms of nuclide transport as do the isotope 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 6 shows the maximum normalized release in EPA units for each combination of intrusion type and time. The time series plots for each time across all three replicates are presented in Appendix A.

^{239}Pu for a 100-year intrusion of type E1 for the CRA-2014 PA shows the highest maximum activity (215.6 EPA units) of all the isotopes across all time intrusion runs, while ^{241}Am shows the highest maximum activity (123.1 EPA units) for the CRA-2014 PA. Under all other time intrusion scenarios and all analyses in Table 6, the maximum activity is from ^{239}Pu. ^{234}U and ^{230}Th never dominate the releases; however, because of ^{241}Am's relatively short half-life (approximately 432 yr), ^{234}U and ^{230}Th can occur at greater concentrations than ^{241}Am, particularly for intrusions close to the end of the 10,000-year horizon. This trend is shown in Table 6; cumulative release plots for the various time intrusion scenarios are provided in Appendix A.

As was done for the isotope runs in Section 4.1.2, we can calculate the average percentage of each isotope as a fraction of the average total release. Table 7 shows that the largest releases of ^{241}Am occur at short times in E1 intrusion, a consequence of the relatively short half-life of the species. For times 3000 years or later, ^{239}Pu comprises at least 97 percent (CRA-2014 PA and CRA-2014 BL) of the total observed activity. ^{234}U and ^{230}Th never dominate releases. Table 7 also demonstrates the large differences in the magnitude of releases between E1 and E2 intrusions; the average release for an E1 intrusion is more than an order of magnitude larger than the comparable average release for an E2 intrusion occurring at the same time.

Comparing the CRA-2014 PA and CRA-2014 BL with the CRA-2009 PABC results presented in Table 6 and Table 7, we see that the maximum releases in the CRA-2014 PA time intrusion runs for ^{239}Pu are uniformly larger than the corresponding maximum releases in the CRA-2009 PABC, although the releases in the CRA-2014 PA and CRA-2014 BL for ^{234}U are lower than their CRA-2009 PABC counterparts. With respect to the radionuclide distribution, ^{234}U and ^{230}Th in the CRA-2014 PA, and ^{241}Am in the CRA-2014 BL make up a smaller proportion of the average release compared to the CRA-2009 PABC; ^{239}Pu in the CRA-2014 PA makes up a larger proportion of the average release compared to the CRA-2009 PABC. The radionuclides in the CRA-2014 PA and CRA-2014 BL under the other time intrusions and analyses do not show a uniform trend compared to the CRA-2009 PABC.

Table 6 Maximum normalized release of each isotope at the Borehole/Culebra interface for time intrusion scenarios

Analysis	Intrusion	Time (yr)	Maximum Releases (EPA Units)				
			^{241}Am	^{239}Pu	^{234}U	^{230}Th	Total[a]
CRA-2009 PABC	E1	100	5.88E+01	4.27E+01	2.56E-01	2.67E-01	8.90E+01
		3000	1.54E+00	2.44E+01	1.78E-01	2.66E-01	2.62E+01
		5000	2.35E-01	2.10E+01	1.49E-01	2.27E-01	2.15E+01
		7000	1.23E-01	1.73E+01	1.19E-01	2.70E-01	1.77E+01
		9000	1.11E-01	1.02E+01	6.60E-02	1.99E-01	1.05E+01
	E2	100	4.31E+00	8.30E+00	4.56E-02	2.04E-02	1.26E+01
		3000	7.51E-03	2.34E+00	2.41E-02	8.44E-03	2.35E+00
		5000	8.51E-04	6.09E-01	9.34E-03	2.83E-03	6.10E-01
		7000	9.88E-05	2.07E-01	3.94E-03	9.62E-05	2.07E-01
		9000	1.34E-05	2.07E-01	1.56E-03	2.37E-06	2.07E-01
CRA-2014 BL	E1	100	8.63E+01	8.96E+01	4.33E-02	1.34E-01	1.66E+02
		3000	1.87E+00	6.37E+01	2.83E-02	1.55E-01	6.58E+01
		5000	1.98E-01	5.38E+01	2.25E-02	1.31E-01	5.42E+01
		7000	2.17E-02	4.31E+01	1.62E-02	1.04E-01	4.33E+01
		9000	2.22E-03	2.53E+01	1.32E-02	6.08E-02	2.54E+01
	E2	100	8.17E+00	9.76E+00	4.58E-03	2.23E-03	1.01E+01
		3000	4.20E-03	4.03E+00	2.24E-03	1.61E-04	4.03E+00
		5000	4.41E-04	1.11E+00	1.32E-03	1.56E-04	1.11E+00
		7000	4.78E-05	7.39E-02	1.32E-03	1.56E-04	7.41E-02
		9000	5.06E-06	7.18E-02	1.32E-03	1.56E-04	7.19E-02
CRA-2014 PA	E1	100	1.23E+02	2.16E+02	5.96E-02	1.53E-01	2.66E+02
		3000	1.04E+00	9.88E+01	3.84E-02	1.51E-01	9.97E+01
		5000	1.21E-01	9.14E+01	3.20E-02	1.28E-01	9.14E+01
		7000	1.51E-02	9.10E+01	2.52E-02	1.02E-01	9.11E+01
		9000	1.17E-02	3.43E+01	1.38E-02	5.93E-02	3.43E+01
	E2	100	1.57E+01	2.91E+01	1.08E-02	2.27E-03	4.47E+01
		3000	1.20E-01	2.07E+01	6.74E-03	6.14E-04	2.09E+01
		5000	1.12E-02	1.40E+01	6.68E-03	6.09E-04	1.40E+01
		7000	1.65E-03	1.38E+01	3.08E-03	3.02E-04	1.38E+01
		9000	2.21E-04	1.19E+01	9.28E-04	6.78E-05	1.19E+01

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

Table 7 Percentage of lumped isotopes relative to average release at the Borehole/Culebra interface for time intrusion scenarios

Analysis	Intrusion	Time (yr)	Percentage of Isotope in Average Release (%)				Average Release (EPA units)
			^{241}Am	^{239}Pu	^{234}U	^{230}Th	
CRA-2009 PABC	E1	100	6.95E+01	3.01E+01	3.01E-01	6.65E-02	3.10E+00
		3000	4.82E+00	9.41E+01	7.68E-01	2.91E-01	5.48E-01
		5000	8.10E-01	9.81E+01	7.98E-01	3.23E-01	4.05E-01
		7000	2.40E-01	9.86E+01	7.41E-01	4.26E-01	3.11E-01
		9000	3.59E-01	9.82E+01	6.83E-01	7.19E-01	1.21E-01
	E2	100	4.07E+01	5.85E+01	6.48E-01	1.01E-01	1.03E-01
		3000	3.58E-01	9.81E+01	1.30E+00	1.97E-01	1.94E-02
		5000	1.29E-01	9.80E+01	1.67E+00	2.45E-01	5.56E-03
		7000	7.64E-02	9.77E+01	2.15E+00	6.29E-02	8.80E-04
		9000	7.80E-03	9.92E+01	7.75E-01	1.67E-03	7.07E-04
CRA-2014 BL	E1	100	5.43E+01	4.56E+01	4.83E-02	3.56E-02	6.09E+00
		3000	2.58E+00	9.72E+01	9.36E-02	1.40E-01	1.50E+00
		5000	3.73E-01	9.94E+01	9.21E-02	1.46E-01	1.18E+00
		7000	5.54E-02	9.97E+01	8.63E-02	1.49E-01	9.24E-01
		9000	1.01E-02	9.97E+01	8.30E-02	1.61E-01	4.74E-01
	E2	100	3.96E+01	6.03E+01	9.00E-02	1.76E-02	2.31E-01
		3000	1.16E-01	9.97E+01	1.34E-01	1.70E-02	4.87E-02
		5000	4.07E-02	9.97E+01	2.11E-01	2.89E-02	1.47E-02
		7000	6.32E-02	9.82E+01	1.57E+00	2.14E-01	9.36E-04
		9000	7.53E-03	9.81E+01	1.66E+00	2.00E-01	8.36E-04
CRA-2014 PA	E1	100	5.54E+01	4.45E+01	5.20E-02	1.94E-02	6.53E+00
		3000	1.84E+00	9.80E+01	9.46E-02	6.24E-02	1.59E+00
		5000	2.21E-01	9.96E+01	9.29E-02	6.24E-02	1.40E+00
		7000	3.49E-02	9.98E+01	9.30E-02	6.02E-02	1.18E+00
		9000	1.39E-02	9.98E+01	8.89E-02	6.97E-02	5.92E-01
	E2	100	3.29E+01	6.70E+01	7.23E-02	1.08E-02	3.46E-01
		3000	4.45E-01	9.95E+01	5.89E-02	7.10E-03	1.46E-01
		5000	5.11E-02	9.99E+01	6.01E-02	7.00E-03	9.30E-02
		7000	1.24E-02	9.99E+01	5.13E-02	5.56E-03	5.27E-02
		9000	1.94E-03	1.00E+02	8.29E-03	1.09E-03	4.24E-02

4.1.4 Comparison to CRA-2009 PABC Results

The maximum and average releases obtained in the two analyses (CRA-2014 PA and CRA-2014 BL) performed here, as well as the CRA-2009 PABC calculations (Ismail and Garner, 2010), are shown in Figure 7 and Figure 8, respectively. Examining the maximum releases, we find that the maximum total releases in E1 intrusion for the CRA-2014 PA and CRA-2014 BL are uniformly larger than the corresponding cases from the CRA-2009 PABC. For E2 intrusion, difference of the maximum total releases between the CRA-2014 PA and the CRA-2009 PABC increases with the increasing intrusion time. However the maximum total releases in the CRA-2014 BL are roughly comparable to those in the CRA-2009 PABC. This implies that the higher actinide (An(III) and An(IV)) solubilities in the CRA-2014 PA and CRA-2014 BL compared to the CRA-2009 PABC (Kim, 2013) may not give a significant impact on the maximum total releases. Brine flow up the Borehole in the CRA-2014 PA increases compared to the CRA-2014 BL, higher than the CRA-2009 PABC (Camphouse, 2013a). The higher brine flow up the borehole may be associated with the difference in the maximum total releases among the CRA-2014 PA, CRA-2014 BL and CRA-2009 PABC.

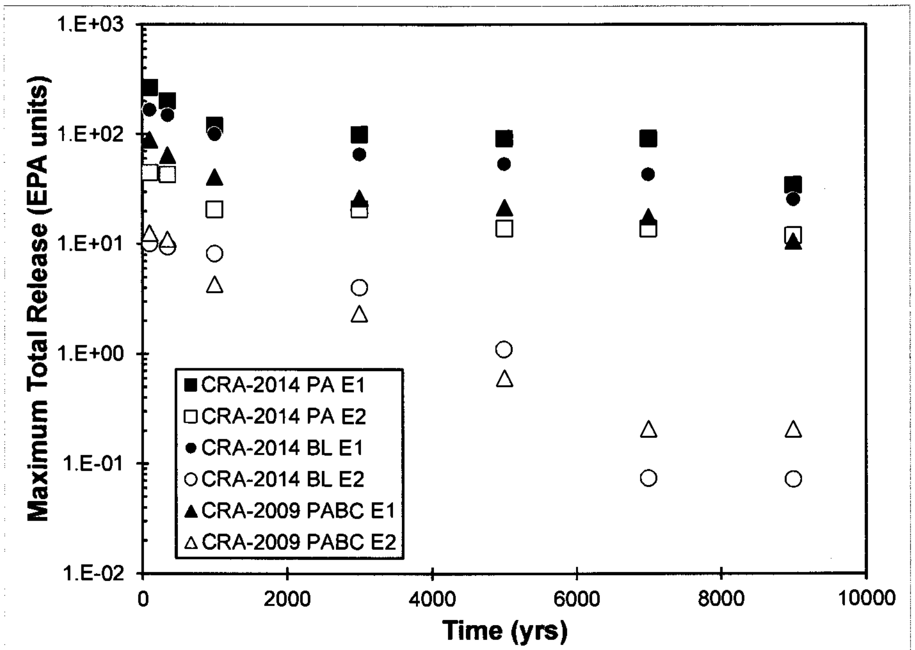


Figure 7 Maximum releases (in EPA units) as a function of time and intrusion type for the CRA-2014 PA, CRA-2014 BL and CRA-2009 PABC

Examining the average total releases in the two analyses, we see much more consistent behavior across the different intrusion times considered. The differences between the average total releases among the CRA-2014 PA, CRA-2014 BL and CRA-2009 PABC are much smaller than the difference in the maximum total releases.

Table 8 lists the number of vectors with non-zero releases for each of the intrusion scenarios examined. With two exceptions - the E2 scenario at 3000 and 5000 years - the number of vectors with releases in the CRA-2014 PA is greater than the number of vectors with releases in the CRA-2009 PABC. The increases in the E1 intrusion scenarios are larger than the comparable E2 intrusion scenarios.

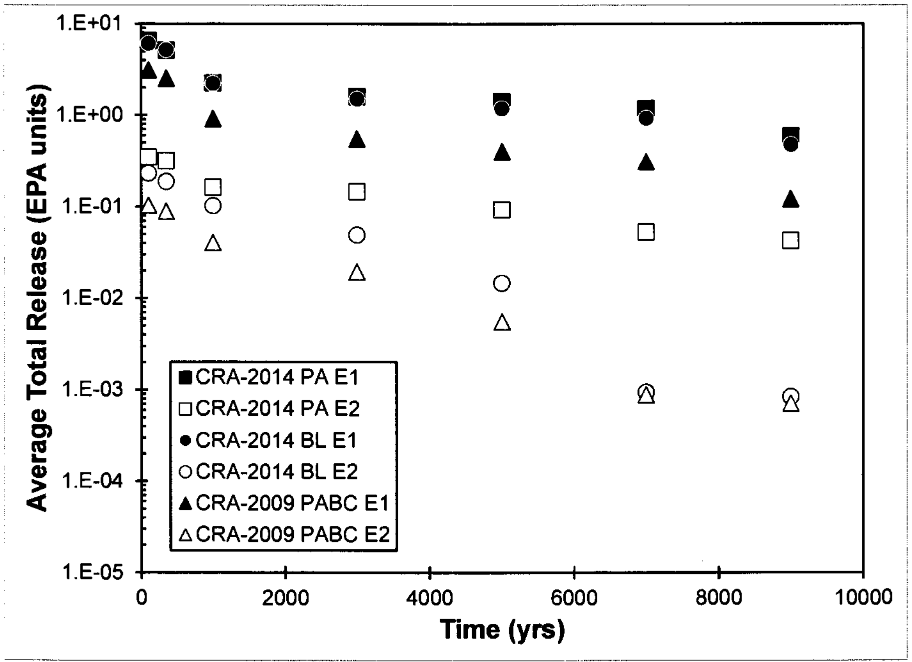


Figure 8 Average releases (in EPA units) as a function of time and intrusion type for the CRA-2014 PA, CRA-2014 PA BL and CRA-2009 PABC

Table 8 Number of vectors with releases for intrusion scenarios for the CRA-2014 PA, CRA-2014 BL and CRA-2009 PABC

Time (yr)	Number of Vectors with Releases E1 intrusion			Number of Vectors with Releases E2 intrusion		
	CRA-2009 PABC	CRA-2014 BL	CRA-2014 PA	CRA-2009 PABC	CRA-2014 BL	CRA-2014 PA
100	224	71	267	51	20	61
350	224	71	267	51	20	61
1000	177	57	241	49	20	55
3000	176	57	240	38	15	37
5000	174	57	241	32	13	22
7000	171	56	240	14	6	17
9000	165	54	235	3	3	9

4.2 PANEL

4.2.1 Scenario S6-BF: E1-E2 Intrusion

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

The PANEL results from Replicate 1 for the total releases up the borehole to the Culebra are shown in Figure 9, which displays the cumulative release plots of the releases for individual vectors as a function of time for the entire 10,000-year regulatory compliance period, given an E2 intrusion at 1000 years and an E1 intrusion at 2000 years.

Prior to 2000 years, only five vectors in the CRA-2014 PA and nearly twenty vectors in the CRA-2014 BL compared to only two vectors in the CRA-2009 PABC have radionuclides that move up the borehole to the Culebra. At 2000 years, the time of the E1 intrusion, radionuclides are washed up the borehole to the Culebra. The shape of the curves, with a rapid jump in cumulative releases at 2000 years followed by almost no increase in the ordinate value as time progresses, indicates that movement up the borehole to the Culebra is rapid and essentially complete at the time of the E1 intrusion. The same behavior is apparent for ^{241}Am, ^{239}Pu, ^{234}U, and ^{230}Th.

The cumulative releases up the borehole to the Culebra for Replicate 1 of S6-BF given an E1 intrusion at 100, 350, 1000, 4000, 6000, and 9000 years respectively are shown in Appendix A.3. In general, the results are as expected: most of the releases occur at the time of the initial intrusion, with very little change following the intrusion.

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

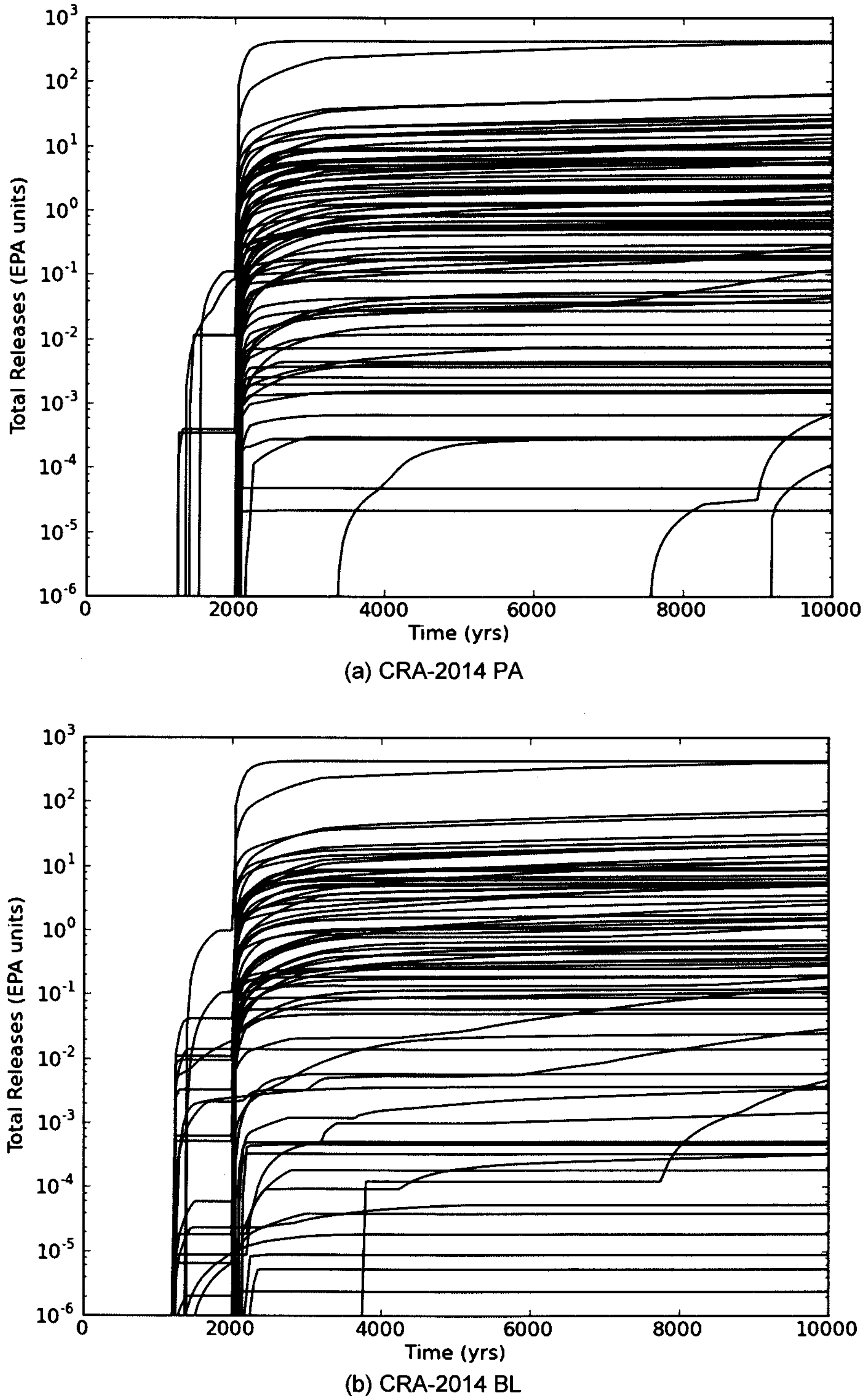
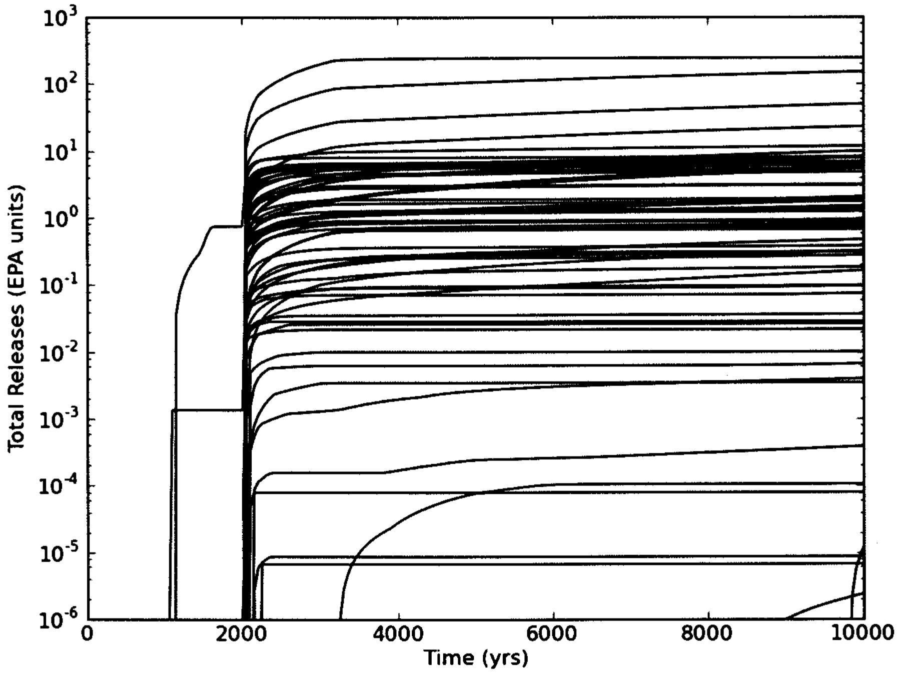


Figure 9(a,b) Total releases to the Culebra for Replicate 1, Scenario S6-BF in the (a) CRA-2014 PA, (b) CRA-2014 BL, and (c) CRA-2009 PABC.



(c) CRA-2009 PABC

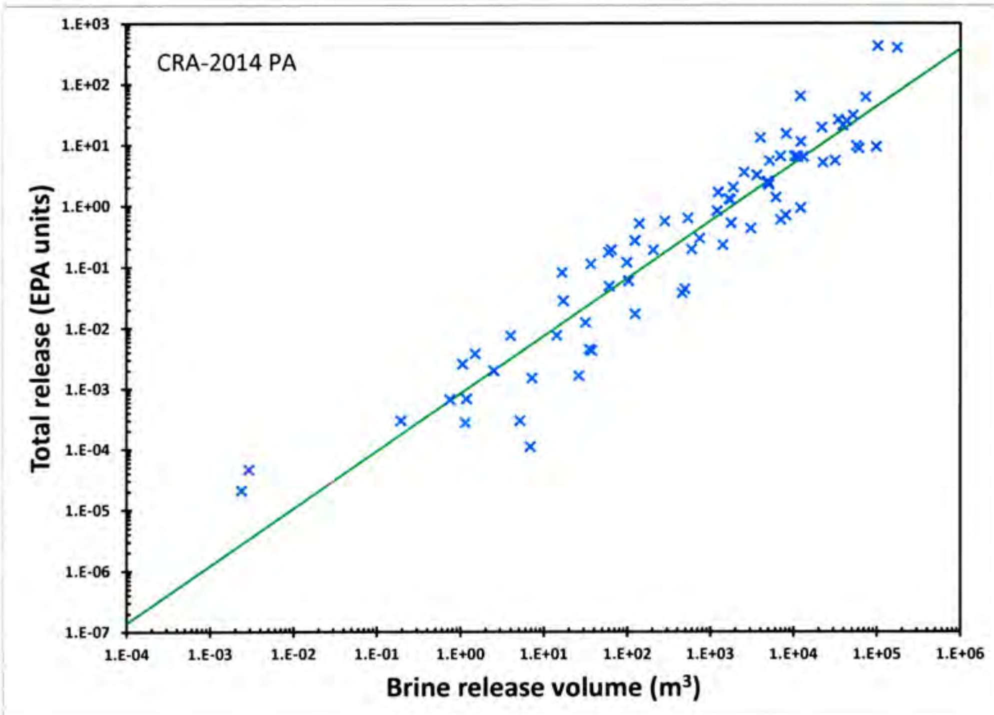
Figure 9(c) Total releases to the Culebra for Replicate 1, Scenario S6-BF in the (a) CRA-2014 PA, (b) CRA-2014 BL, and (c) CRA-2009 PABC.

4.2.2 Sensitivity Analysis

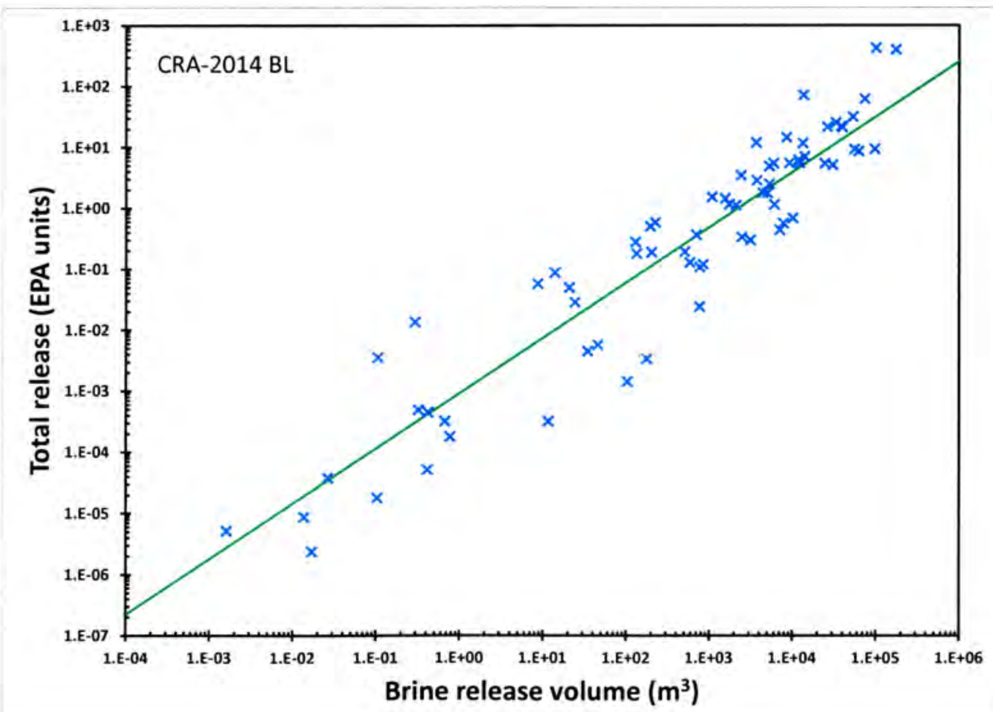
A SUMMARIZE was run to collect data from BRAGFLO CDB files (**ALG2_BF_CRA14_R1_S6_V*vvv*.CDB** and **ALG2_BF_CRA14BL_R1_S6_V*vvv*.CDB**, in library **CRA14_BFR1S6**, and **ALG2_BF_PABC09_R1_S6_V*vvv*.CDB** in library **PABC09_BFR1S6**, *vvv* = 001, 002, …, 100) and PANEL output files (**PANEL_INT_CRA14BV1_R1_S6_TI2000_V*vvv*.CDB** and **PANEL_INT_CRA14BL_R1_S6_TI2000_V*vvv*.CDB**, in library **CRA14_PANEL**, and **PANEL_INT_PABC09_R1_S6_TI2000_V*vvv*.CDB** in library **PABC09_PANEL**) in order to determine what variables have the most influence on the EPA units up the borehole to the Culebra in the S6-BF scenario. The sensitivity analysis was performed on the results for the cumulative EPA Units up the borehole to the Culebra at 10,000 years for the S6-BF scenario (E1 intrusion at 2000 years).

The strongest correlation identified in all cases was with the borehole permeability (BOREHOLE:BHPERM), which is a parameter used in BRAGFLO. This means that variability in the borehole permeability (a BRAGFLO input) is primarily responsible for variability in the total EPA Units up the borehole to the Culebra. Any variability caused by the PANEL input parameters was obscured by the BRAGFLO parameters.

By determining the relationship between EPA Units up the borehole to the Culebra (LDETOTAL) and the brine flow (BNBHUDRZ), it is possible to determine if other parameters can be expected to exert a significant influence on the potential releases up the borehole. Figure 10 shows a scatter plot of the total releases up the borehole to the Culebra (in EPA Units) versus the brine release volume. Because the resulting regression is linear on a log-log plot, this suggests a power-law relationship between the release volume and the total releases; computing the coefficients for the regression line, we find that $R \sim V^{0.944}$ for the CRA-2014 PA and $R \sim V^{0.906}$ for the CRA-2014 BL compared to $R \sim V^{0.842}$ for the CRA-2009 PABC, where R is the magnitude of total releases and V is the brine release volume. The regression coefficients r^2 = 0.971 for the CRA-2014 PA and 0.968 for the CRA-2014 BL suggest that there is a nearly direct correlation between the two variables. Consequently, other parameters are expected to have only a minor influence on the potential releases up the borehole. In addition, this would explain the reason for difference between maximum total releases among the CRA-2014 PA, CRA-2014 BL, and CRA-2009 PABC in section 4.1.4.

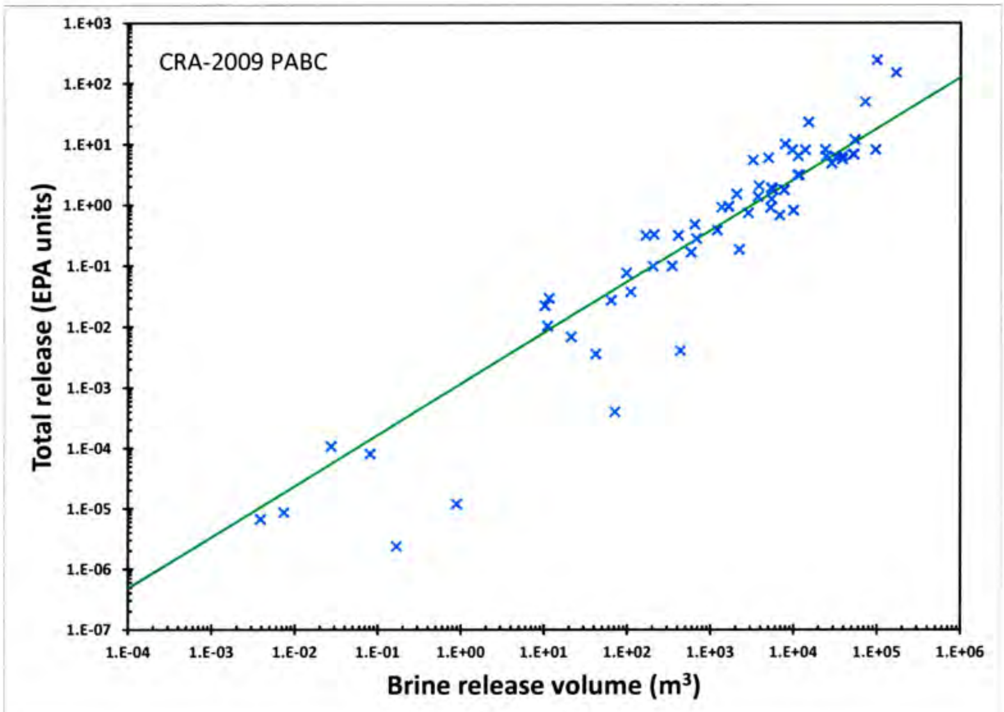


(a) CRA-2014 PA



(b) CRA-2014 BL

Figure 10(a,b) Sensitivity analysis for total releases as a function of brine release volume in the (a) CRA-2014 PA, (b) CRA-2014 BL, and (c) CRA-2009 PABC.



(c) CRA-2009 PABC

Figure 10(c) Sensitivity analysis for total releases as a function of brine release volume in the (a) CRA-2014 PA, (b) CRA-2014 BL, and (c) CRA-2009 PABC.

4.2.3 Comparison to CRA-2014 BL

As discussed in the previous section, the brine release volume is the dominant variable associated with predicting total releases. Consequently, by plotting the brine release volumes for the CRA-2014 PA versus the corresponding CRA-2014 BL brine release volumes, as shown in Figure 11, we can determine the source of any changes in the magnitude of releases. As can be seen from Figure 11, the brine volumes are essentially equal, and particularly so for releases of about 10^3 m^3 or more; discrepancies primarily show increases in volume from the CRA-2014 BL to the CRA-2014 PA. As a result, we may not expect roughly comparable releases for the CRA-2014 PA and CRA-2014 BL, with deviations between the two being the result of additional changes and modifications in the CRA-2014 PA relative to the CRA-2014 BL. The modifications included in the CRA-2014 PA can be found in Camphouse (Camphouse, 2013b).

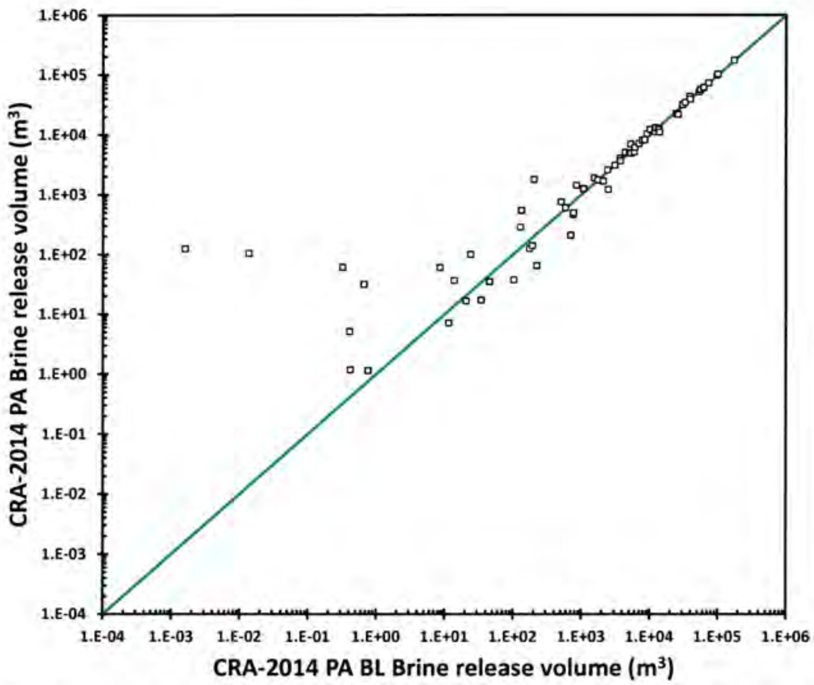


Figure 11 CRA-2014 PA versus CRA-2014 PA BL release volumes for Replicate 1, Scenario S6-BF

5 Summary

This analysis package describes the transport calculations that are part of the CRA-2014 PA and CRA-2014 BL as outlined in Camphouse (Camphouse, 2013b). Specifically, it covers the calculations to determine the mobilization and subsequent migration of radioisotopes throughout the repository, the shaft system, the Salado formation, and possible human intrusion boreholes.

The calculations presented in this report are based on the same process as the CRA-2009 PABC (Garner, 2010; Ismail and Garner, 2010). The primary changes affecting the results are the changes in the inventory and in the revised concentrations of dissolved actinides. Releases are larger in the CRA-2014 PA than in the CRA-2014 BL. However, these changes ultimately will have a negligible impact on repository performance, because material released to the Culebra must first make its way through the Culebra before reaching the accessible environment outside the LWB.

Calculations from PANEL show that brine release volumes between the CRA-2014 PA and CRA-2014 BL were essentially unchanged for release volumes larger than about 10^3 m^3, and any changes were for release volumes less than about 10^3 m^3.

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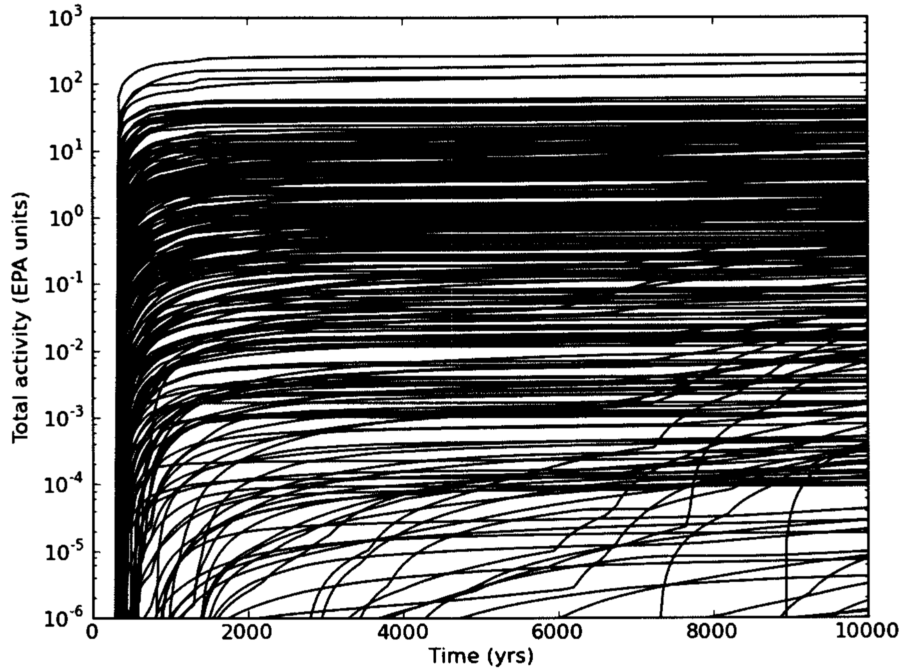
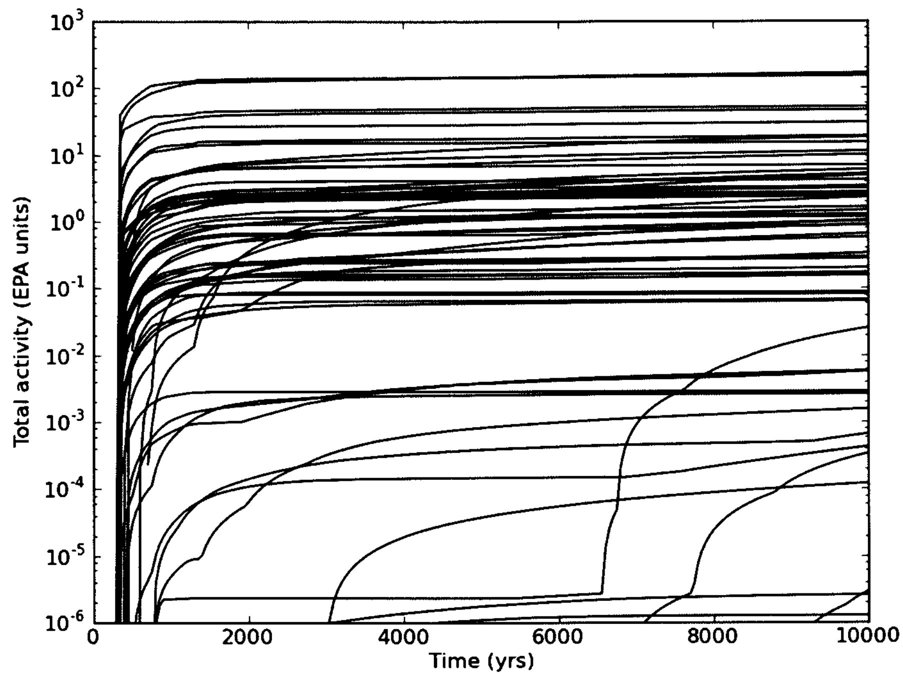
Appendix A Cumulative Release Plots

Appendix A.1 E1 intrusion scenario

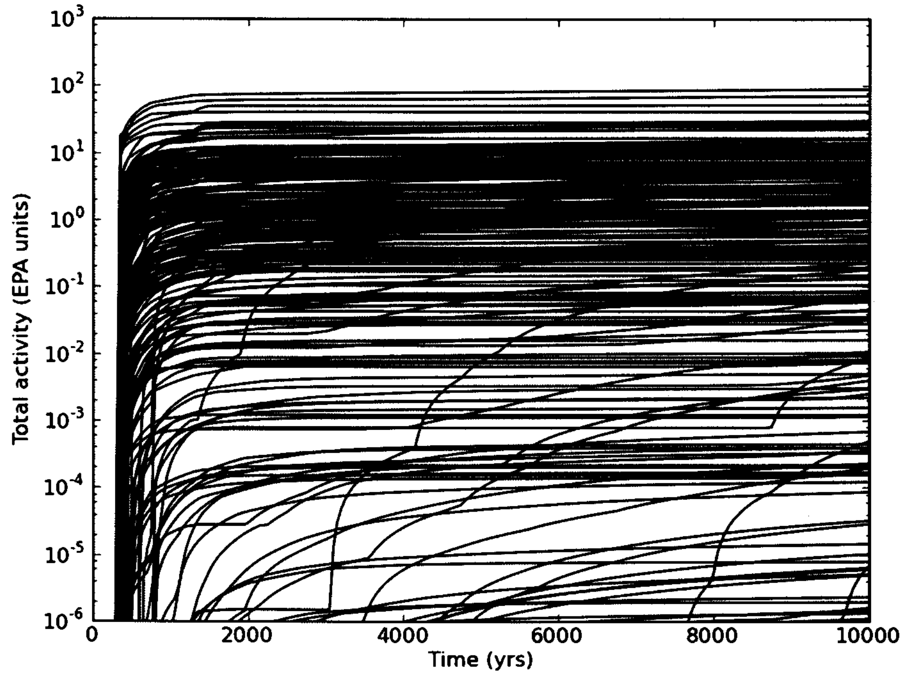


(a) CRA-2014 PA



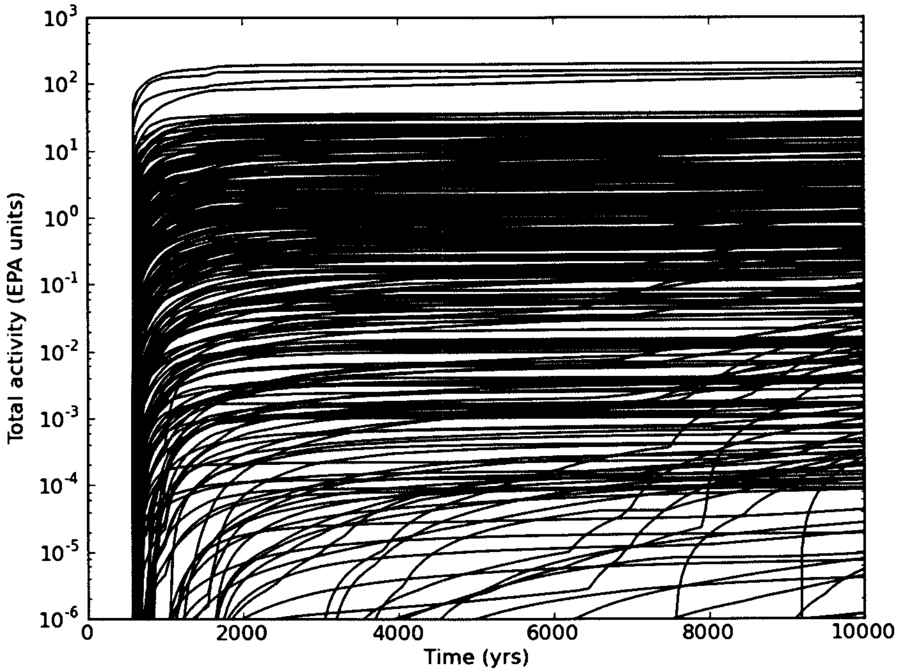
(b) CRA-2014 BL

Figure 12(a,b) Cumulative total releases to the Culebra for an E1 intrusion at 100 years in the (a) CRA-2014 PA, (b) CRA-2014 BL, and (c) CRA-2009 PABC.

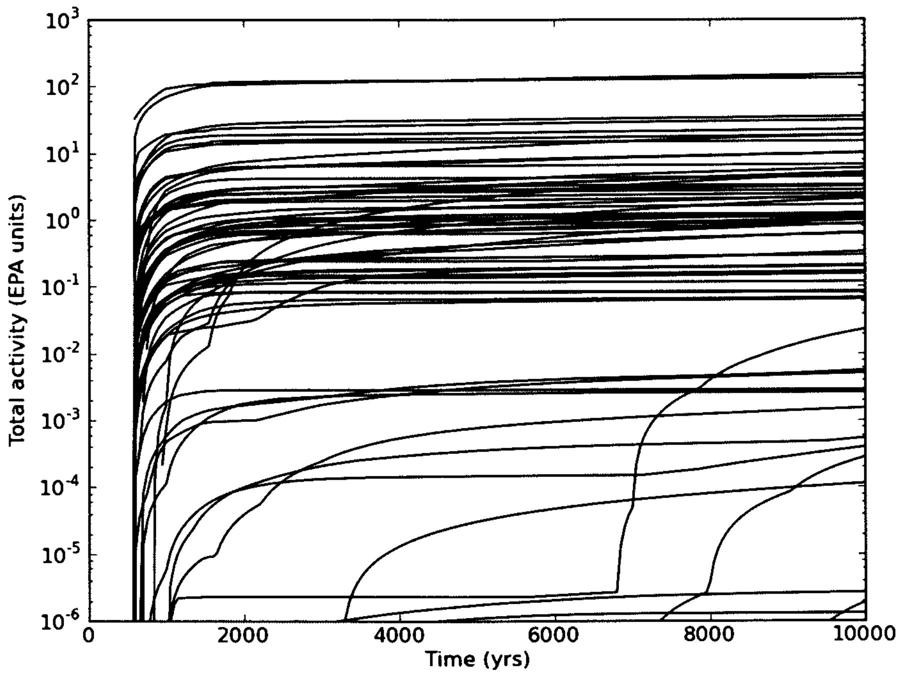


(c) CRA-2009 PABC

Figure 12(c) Cumulative total releases to the Culebra for an E1 intrusion at 100 years in the (a) CRA-2014 PA, (b) CRA-2014 BL, and (c) CRA-2009 PABC.

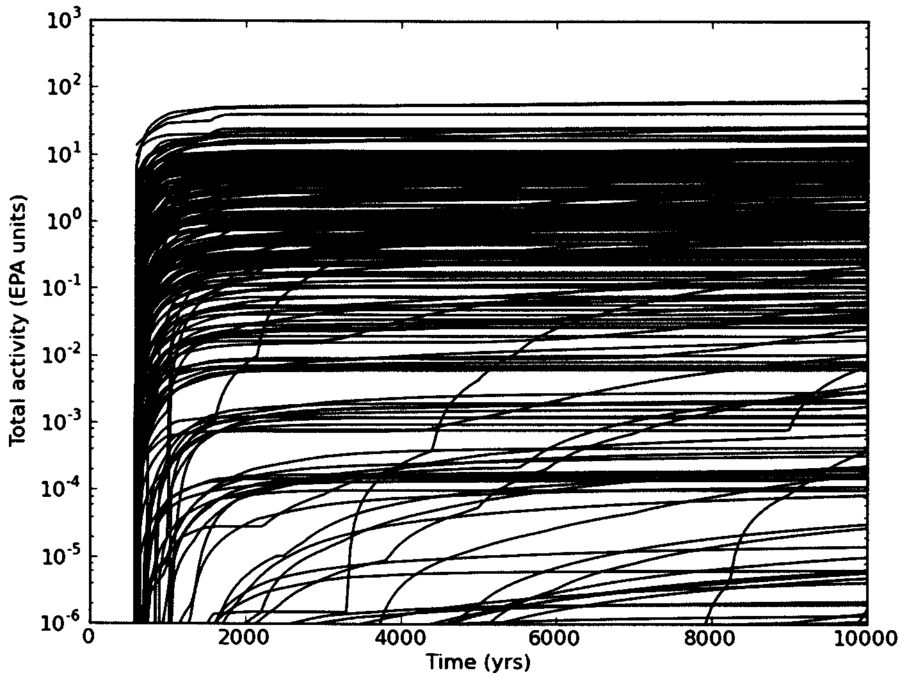


(a) CRA-2014 PA



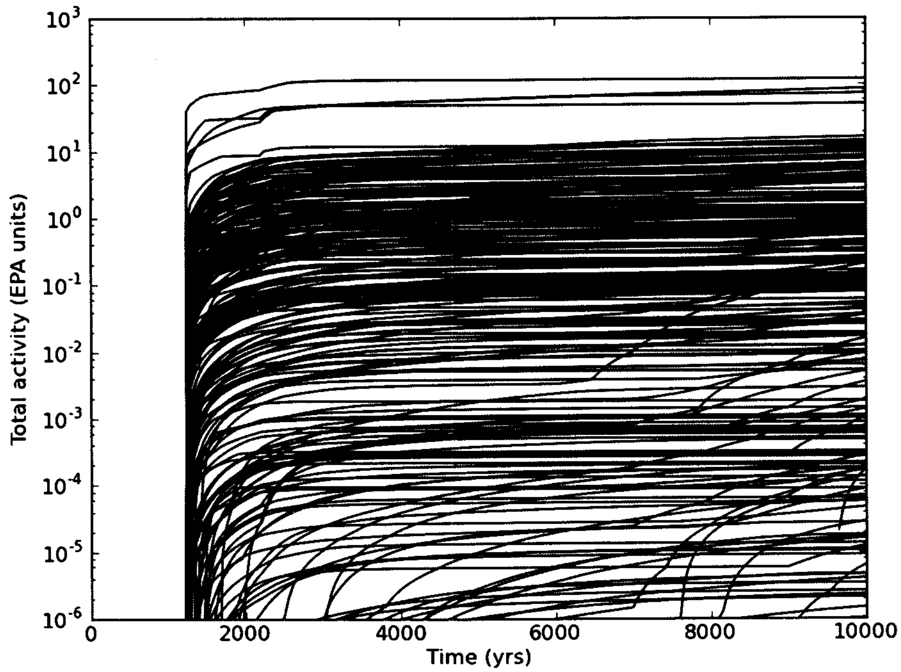
(b) CRA-2014 BL

Figure 13(a,b) Cumulative total releases to the Culebra for an E1 intrusion at 350 years in the (a) CRA-2014 PA, (b) CRA-2014 BL, and (c) CRA-2009 PABC.

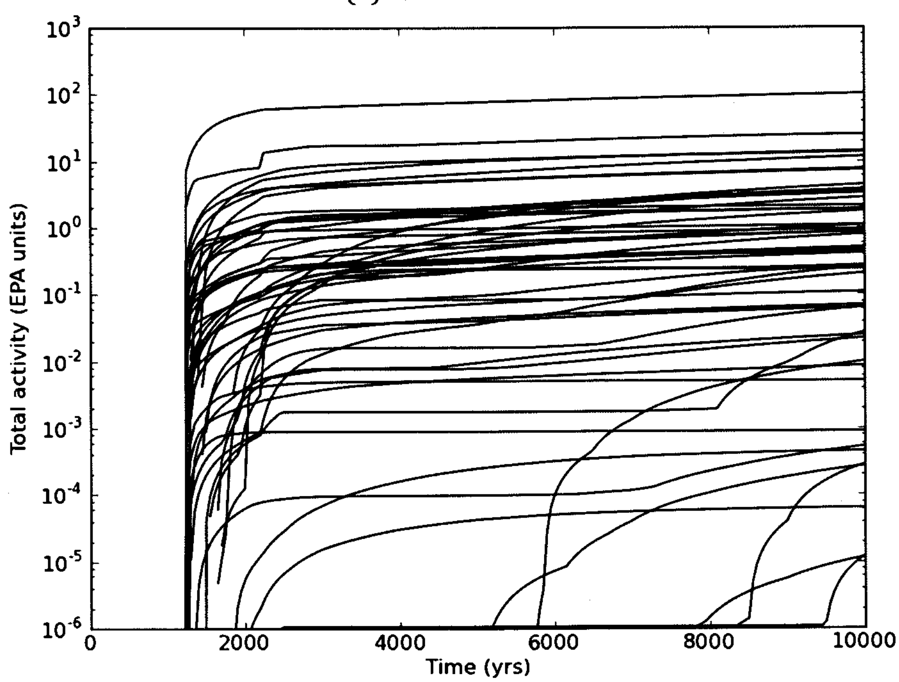


(c) CRA-2009 PABC

Figure 13(c) Cumulative total releases to the Culebra for an E1 intrusion at 350 years in the (a) CRA-2014 PA, (b) CRA-2014 BL, and (c) CRA-2009 PABC.

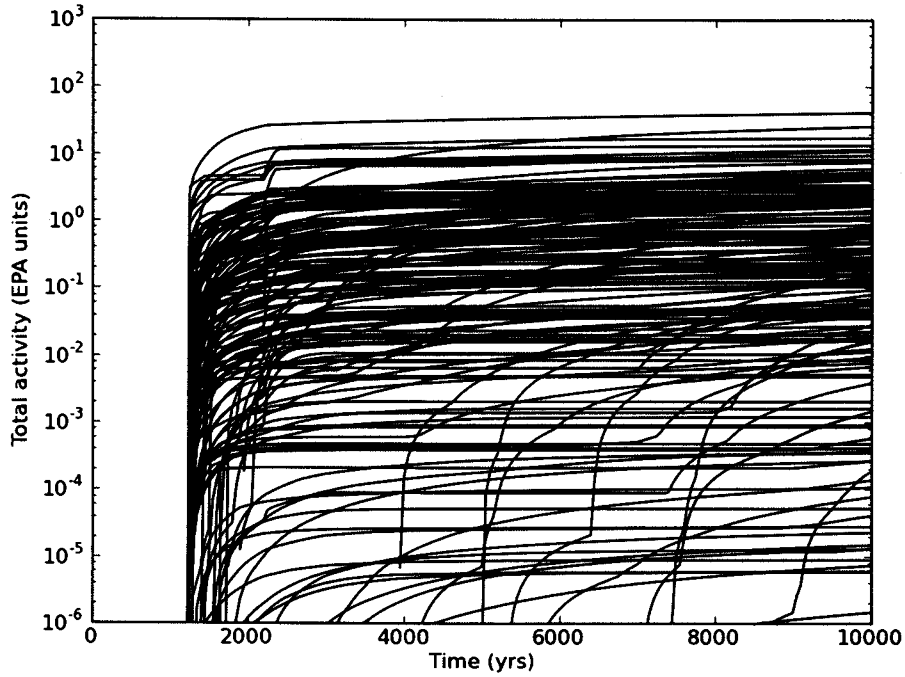


(a) CRA-2014 PA



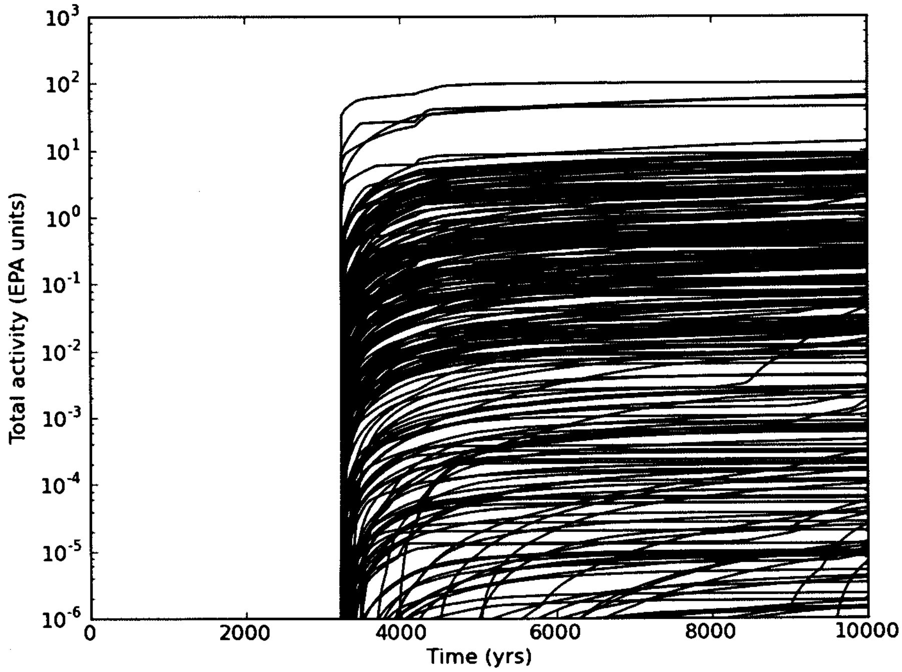
(b) CRA-2014 BL

Figure 14(a,b) Cumulative total releases to the Culebra for an E1 intrusion at 1000 years in the (a) CRA-2014 PA, (b) CRA-2014 BL, and (c) CRA-2009 PABC.

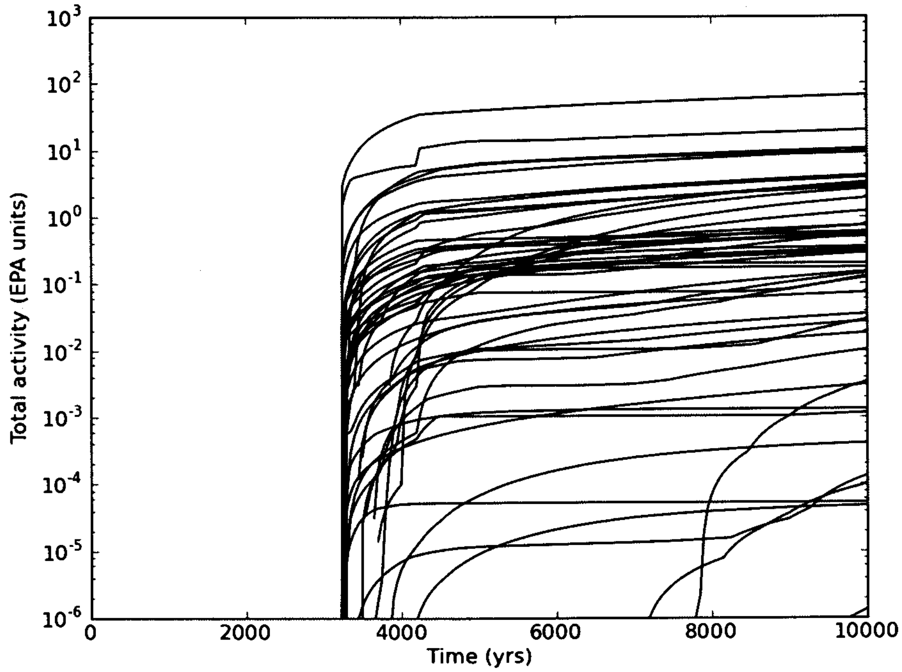


(c) CRA-2009 PABC

Figure 14(c) Cumulative total releases to the Culebra for an E1 intrusion at 1000 years in the (a) CRA-2014 PA, (b) CRA-2014 BL, and (c) CRA-2009 PABC.

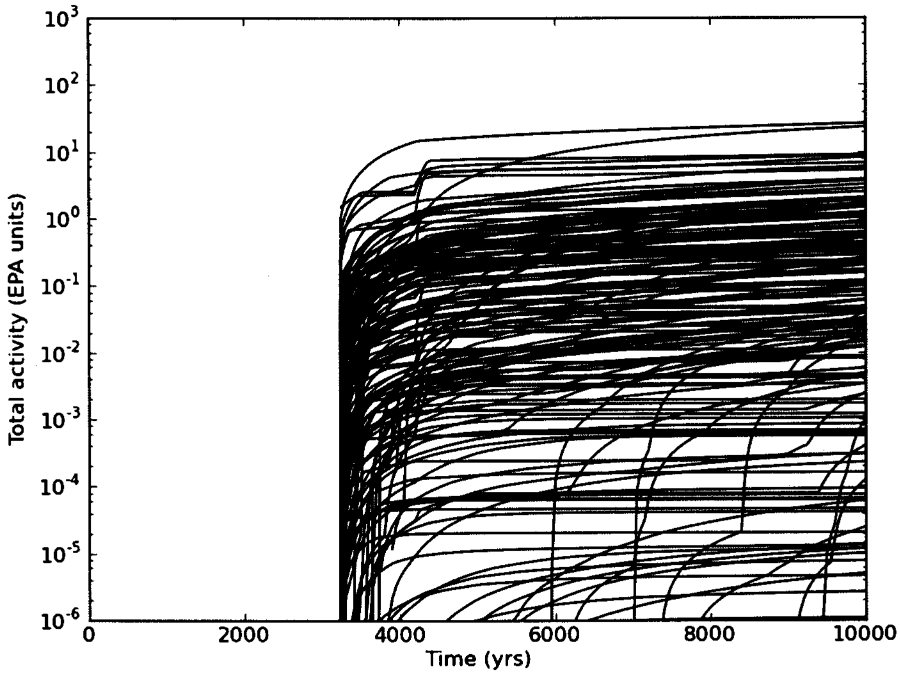


(a) CRA-2014 PA



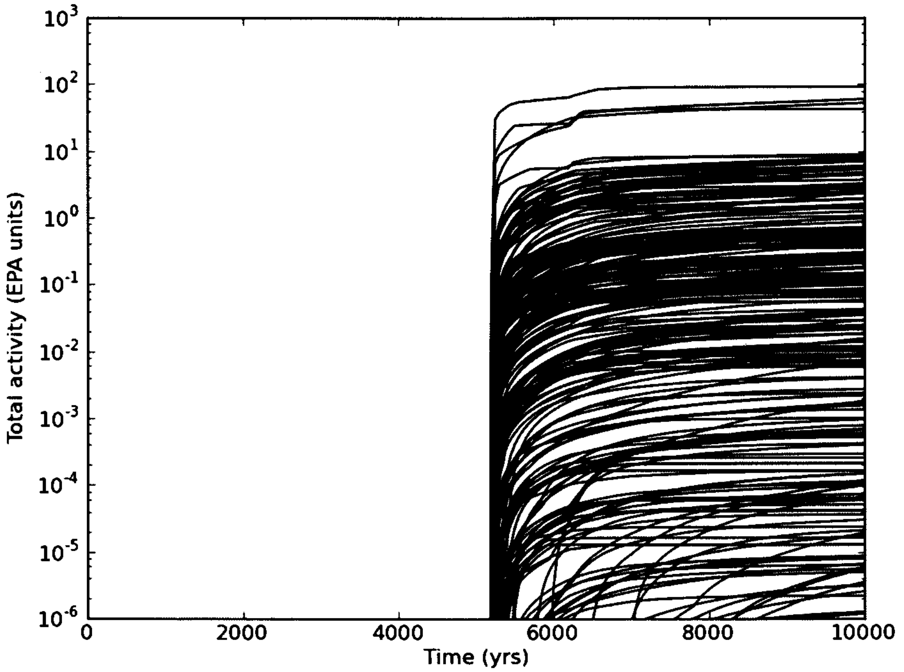
(b) CRA-2014 BL

Figure 15(a,b) Cumulative total releases to the Culebra for an E1 intrusion at 3000 years in the (a) CRA-2014 PA, (b) CRA-2014 BL, and (c) CRA-2009 PABC.

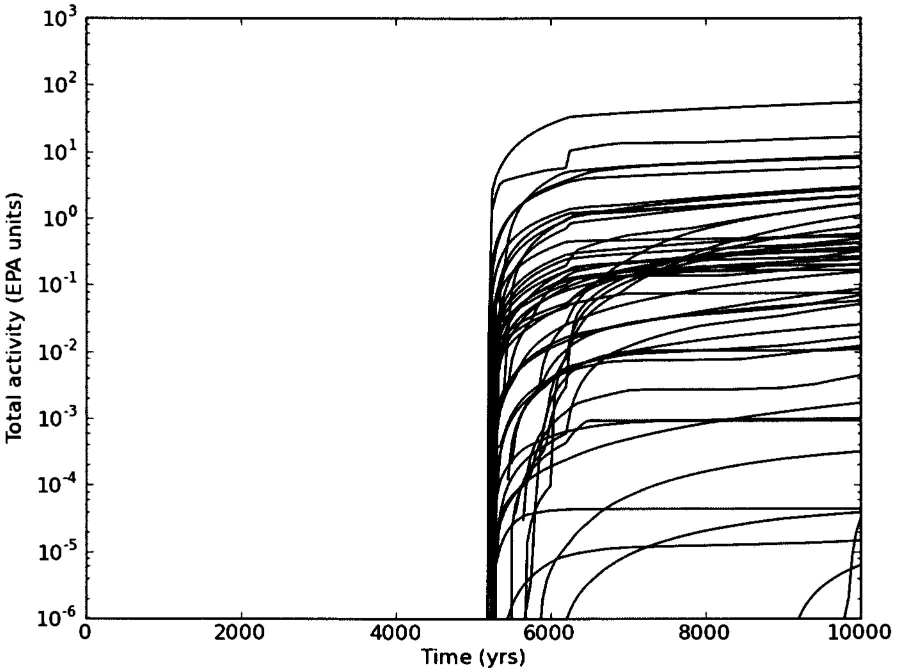


(c) CRA-2009 PABC

Figure 15(c) Cumulative total releases to the Culebra for an E1 intrusion at 3000 years in the (a) CRA-2014 PA, (b) CRA-2014 BL, and (c) CRA-2009 PABC.

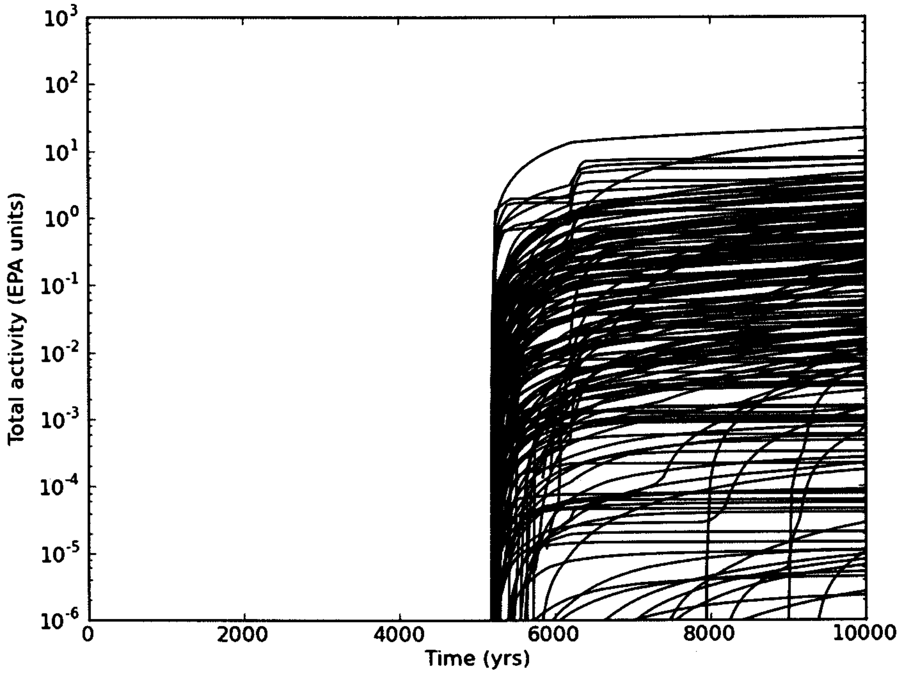


(a) CRA-2014 PA



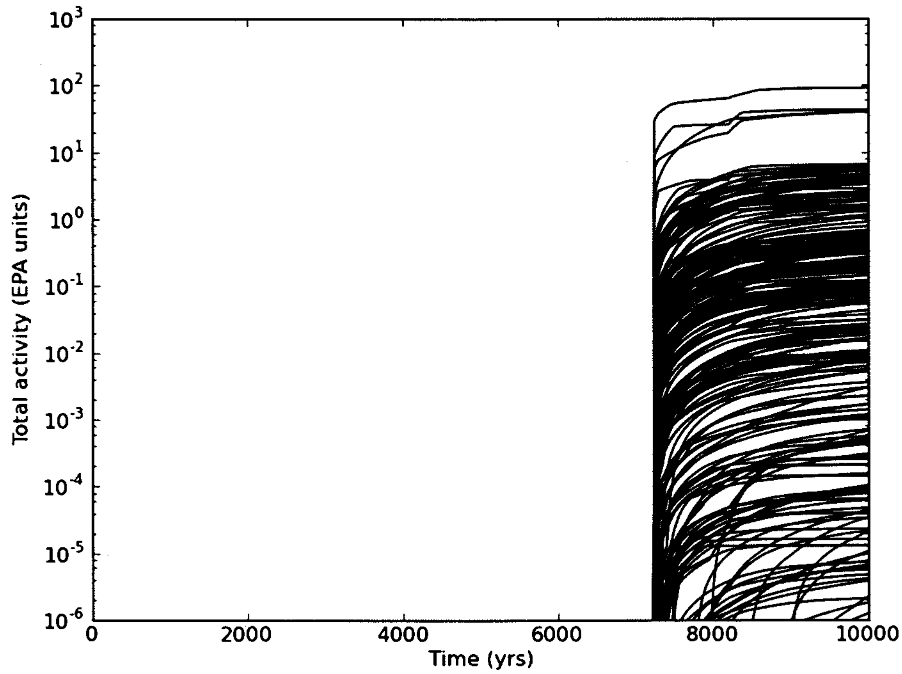
(b) CRA-2014 BL

Figure 16(a,b) Cumulative total releases to the Culebra for an E1 intrusion at 5000 years in the (a) CRA-2014 PA, (b) CRA-2014 BL, and (c) CRA-2009 PABC.

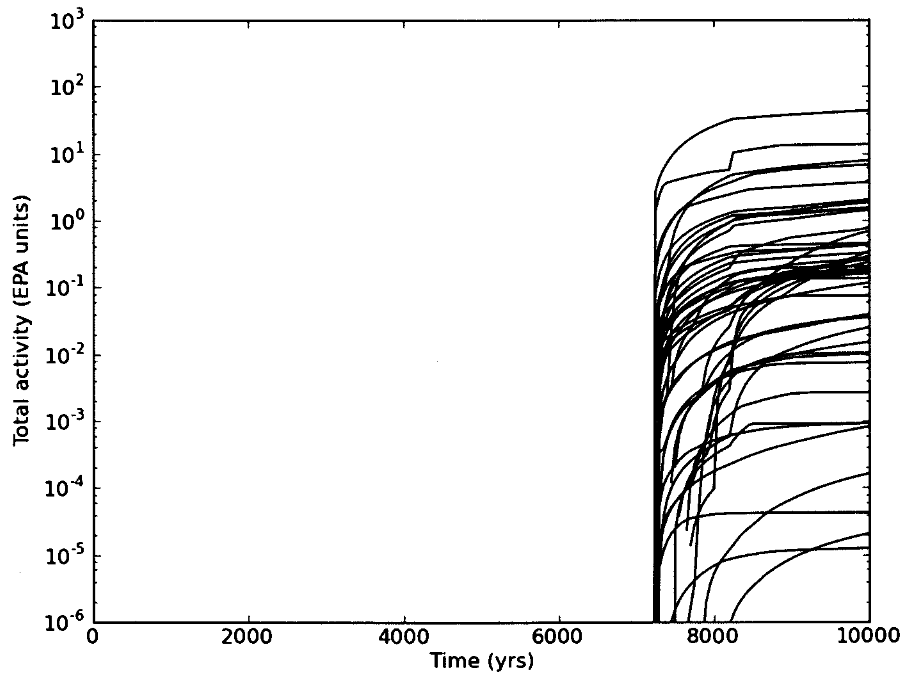


(c) CRA-2009 PABC

Figure 16(c) Cumulative total releases to the Culebra for an E1 intrusion at 5000 years in the (a) CRA-2014 PA, (b) CRA-2014 BL, and (c) CRA-2009 PABC.

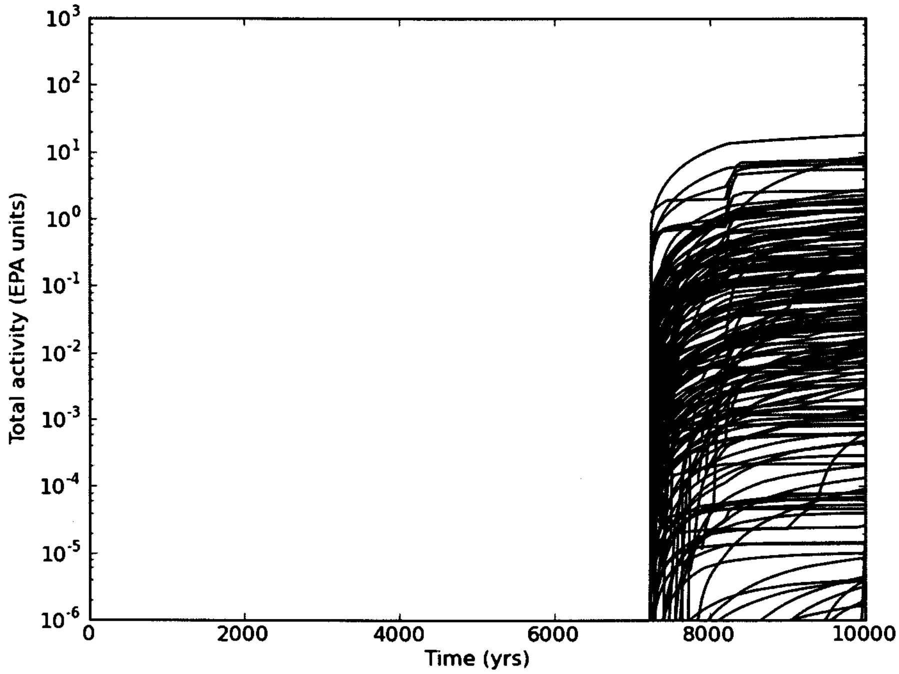


(a) CRA-2014 PA



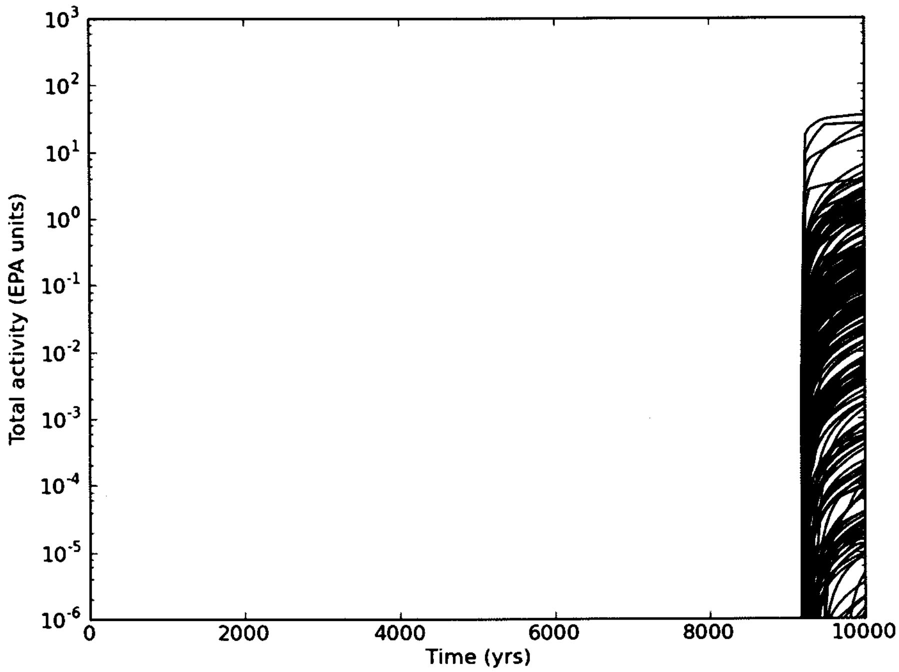
(b) CRA-2014 BL

Figure 17(a,b) Cumulative total releases to the Culebra for an E1 intrusion at 7000 years in the (a) CRA-2014 PA, (b) CRA-2014 BL, and (c) CRA-2009 PABC.

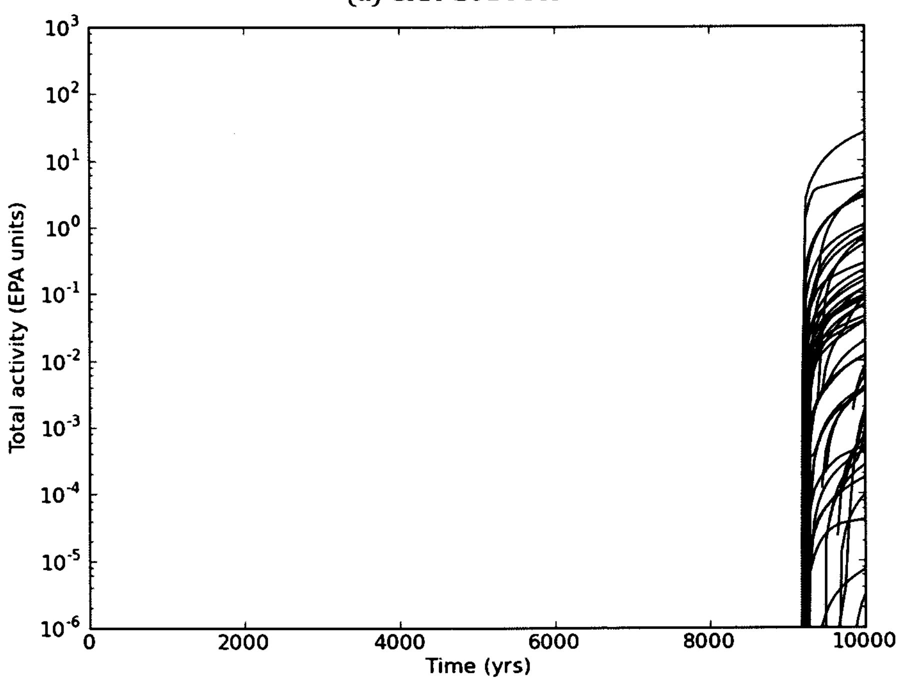


(c) CRA-2009 PABC

Figure 17(c) Cumulative total releases to the Culebra for an E1 intrusion at 7000 years in the (a) CRA-2014 PA, (b) CRA-2014 BL, and (c) CRA-2009 PABC.

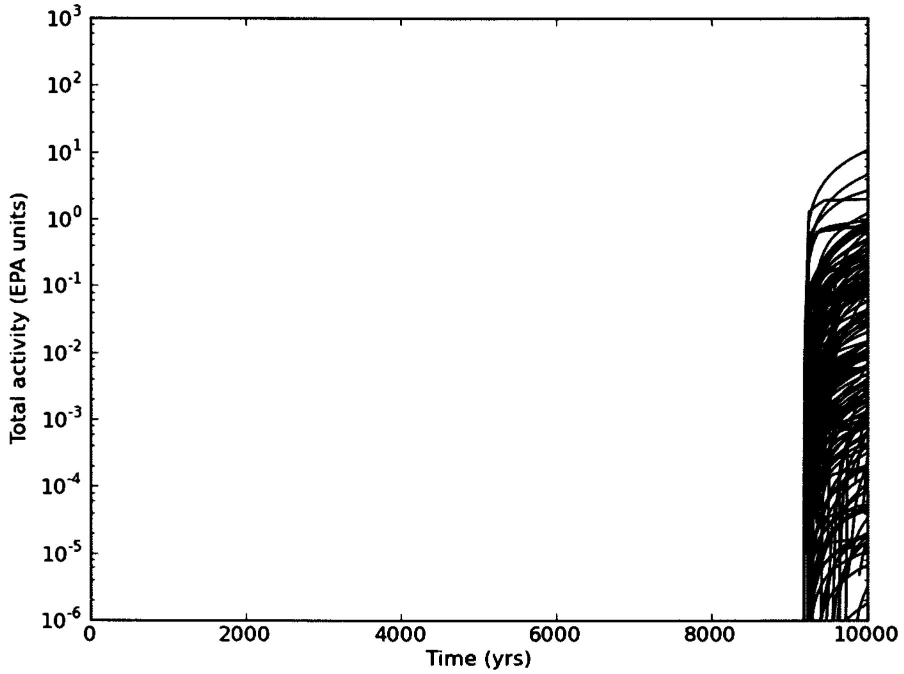


(a) CRA-2014 PA



(b) CRA-2014 BL

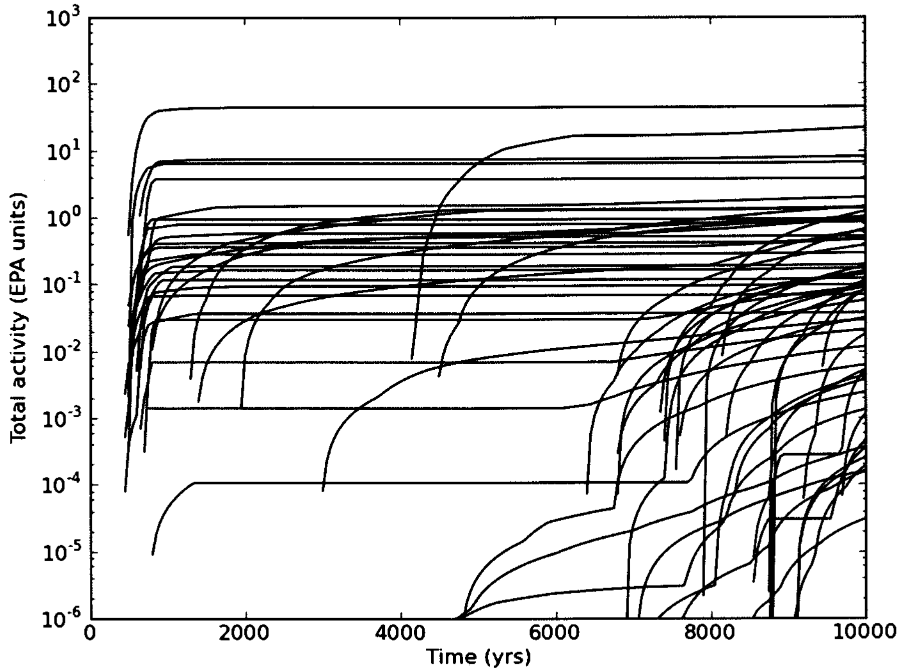
Figure 18(a,b) Cumulative total releases to the Culebra for an E1 intrusion at 9000 years in the (a) CRA-2014 PA, (b) CRA-2014 BL, and (c) CRA-2009 PABC.



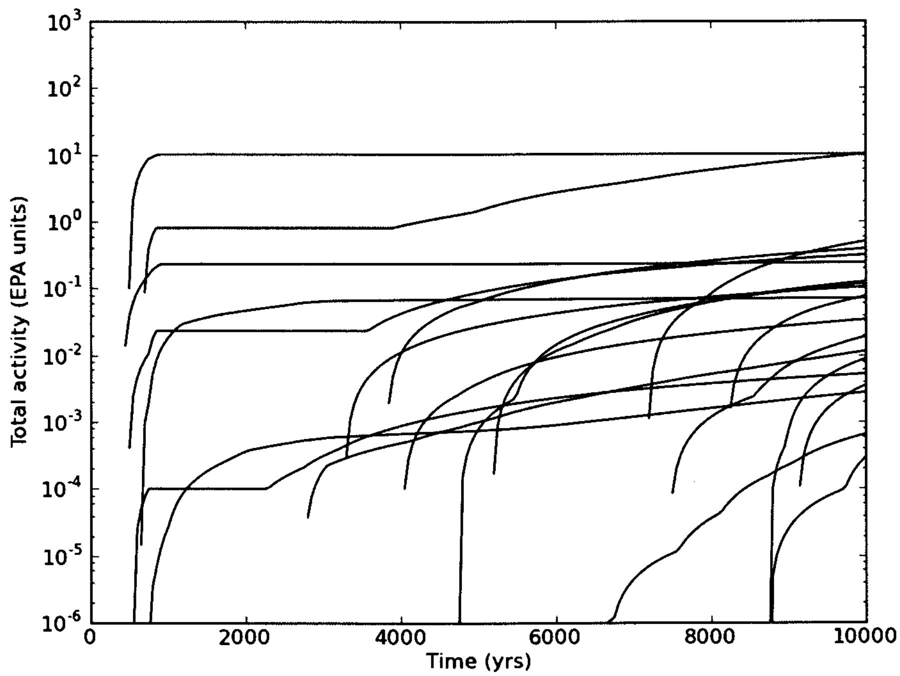
(c) CRA-2009 PABC

Figure 18(c) Cumulative total releases to the Culebra for an E1 intrusion at 9000 years in the (a) CRA-2014 PA, (b) CRA-2014 BL, and (c) CRA-2009 PABC.

Appendix A.2 E2 Intrusion Scenario

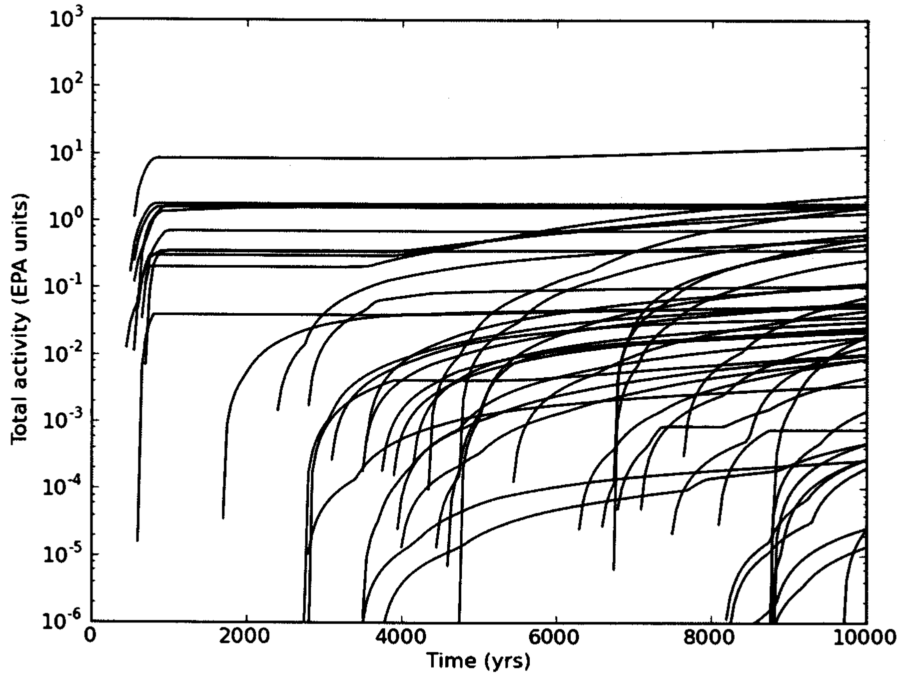


(a) CRA-2014 PA



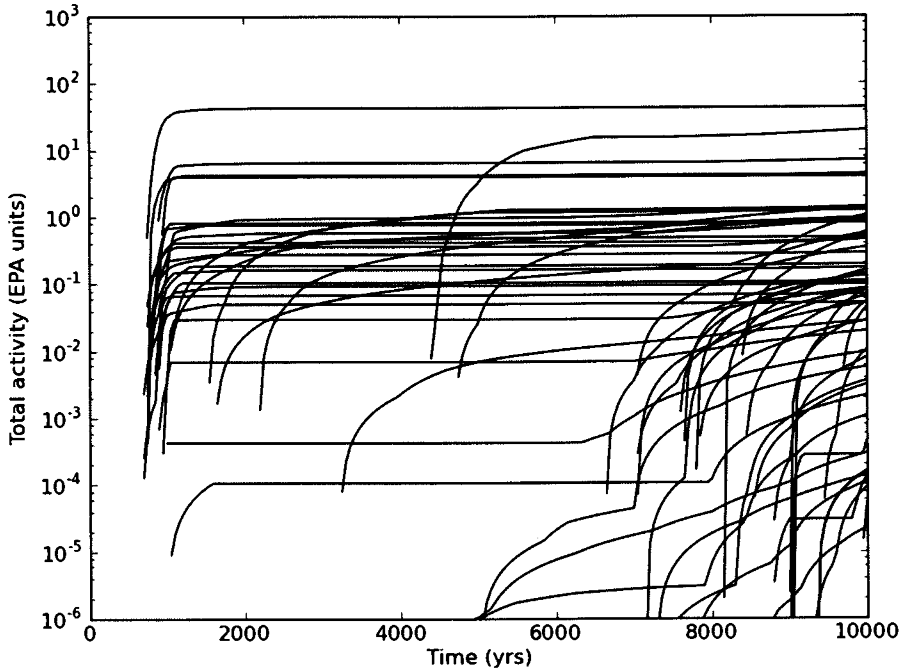
(b) CRA-2014 BL

Figure 19(a,b) Cumulative total releases to the Culebra for an E2 intrusion at 100 years in the (a) CRA-2014 PA, (b) CRA-2014 BL, and (c) CRA-2009 PABC.

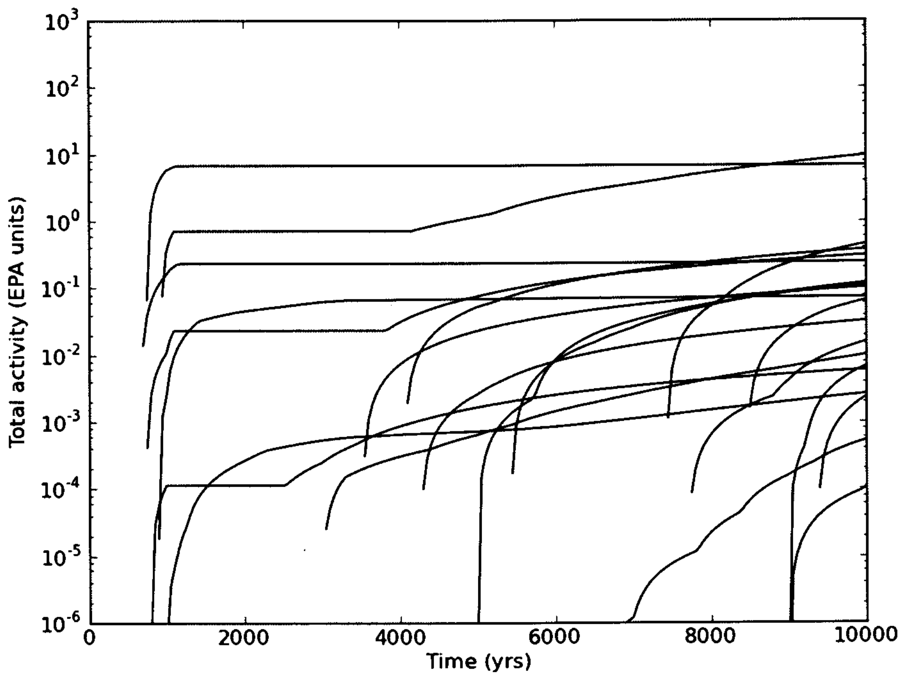


(c) CRA-2009 PABC

Figure 19(c) Cumulative total releases to the Culebra for an E2 intrusion at 100 years in the (a) CRA-2014 PA, (b) CRA-2014 BL, and (c) CRA-2009 PABC.

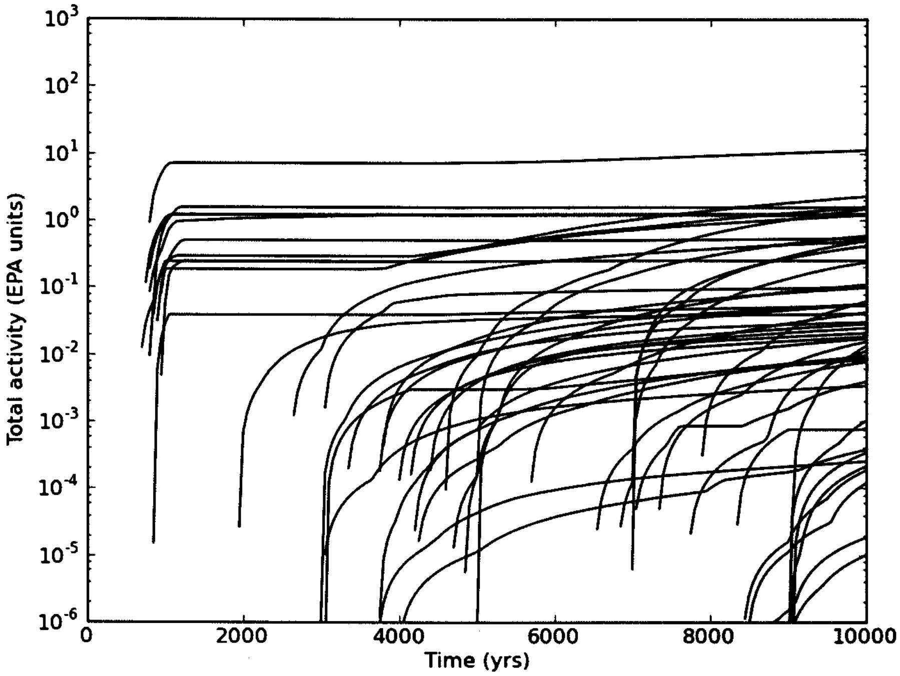


(a) CRA-2014 PA



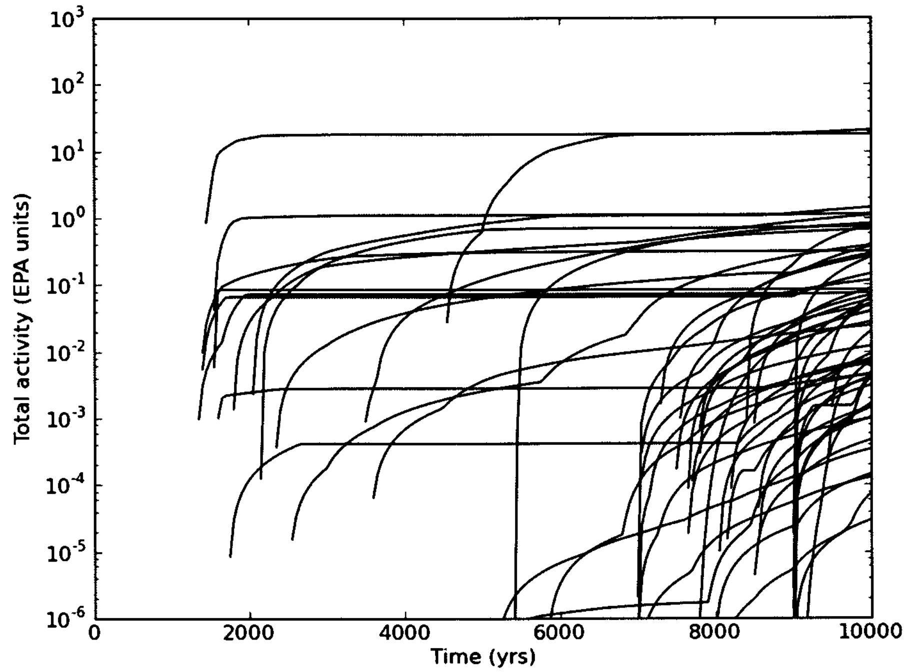
(b) CRA-2014 BL

Figure 20(a,b) Cumulative total releases to the Culebra for an E2 intrusion at 350 years in the (a) CRA-2014 PA, (b) CRA-2014 BL, and (c) CRA-2009 PABC.

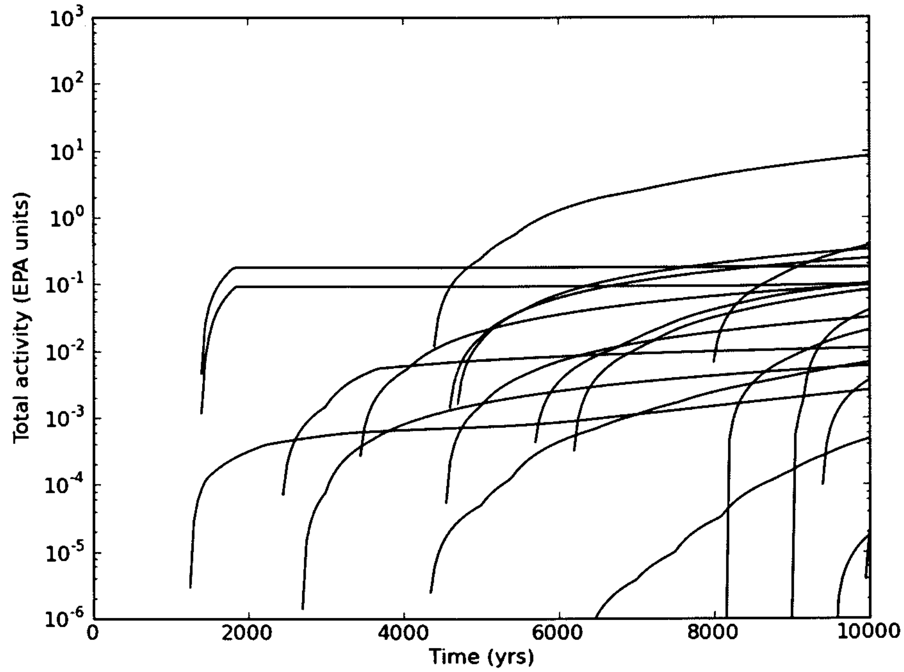


(c) CRA-2009 PABC

Figure 20(c) Cumulative total releases to the Culebra for an E2 intrusion at 350 years in the (a) CRA-2014 PA, (b) CRA-2014 BL, and (c) CRA-2009 PABC.

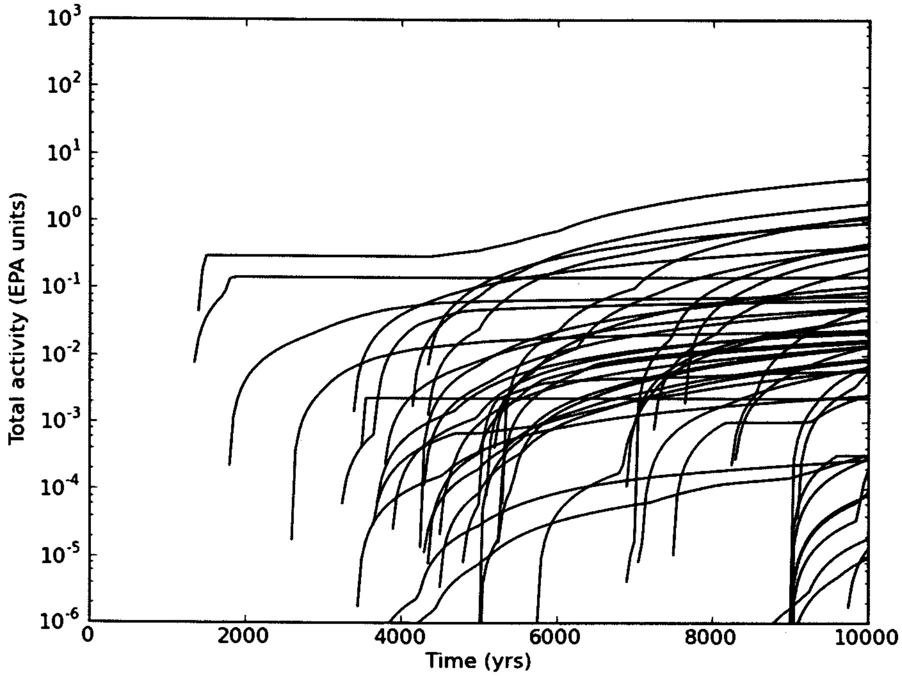


(a) CRA-2014 PA



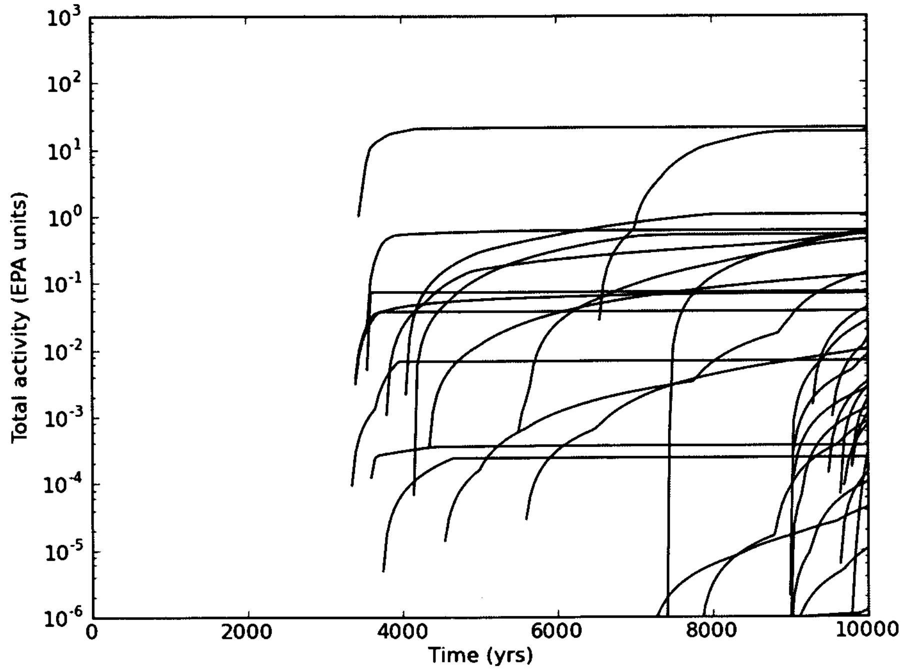
(b) CRA-2014 BL

Figure 21(a,b) Cumulative total releases to the Culebra for an E2 intrusion at 1000 years in the (a) CRA-2014 PA, (b) CRA-2014 BL, and (c) CRA-2009 PABC.

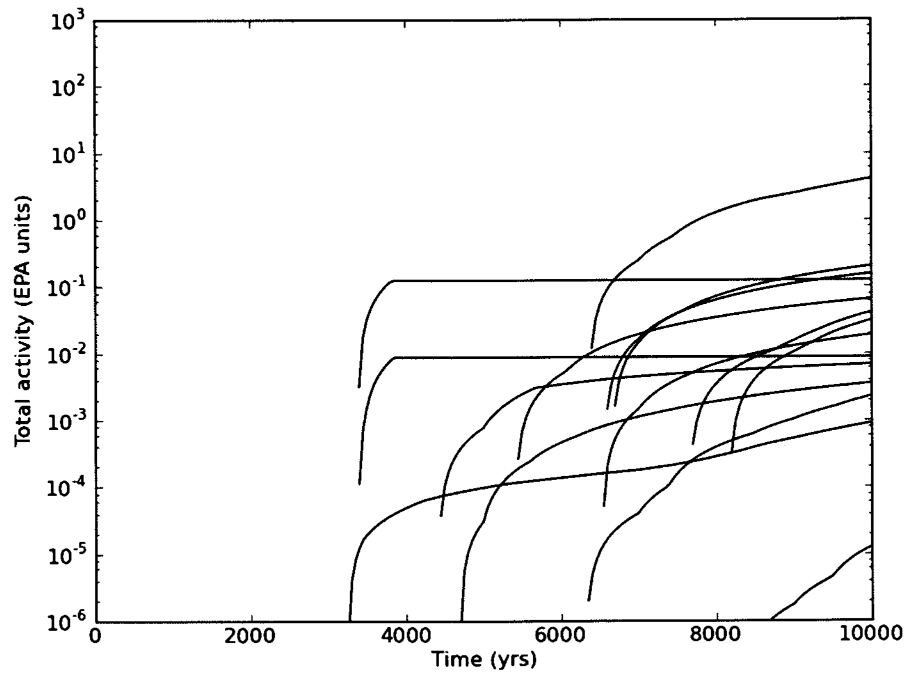


(c) CRA-2009 PABC

Figure 21(c) Cumulative total releases to the Culebra for an E2 intrusion at 1000 years in the (a) CRA-2014 PA, (b) CRA-2014 BL, and (c) CRA-2009 PABC.

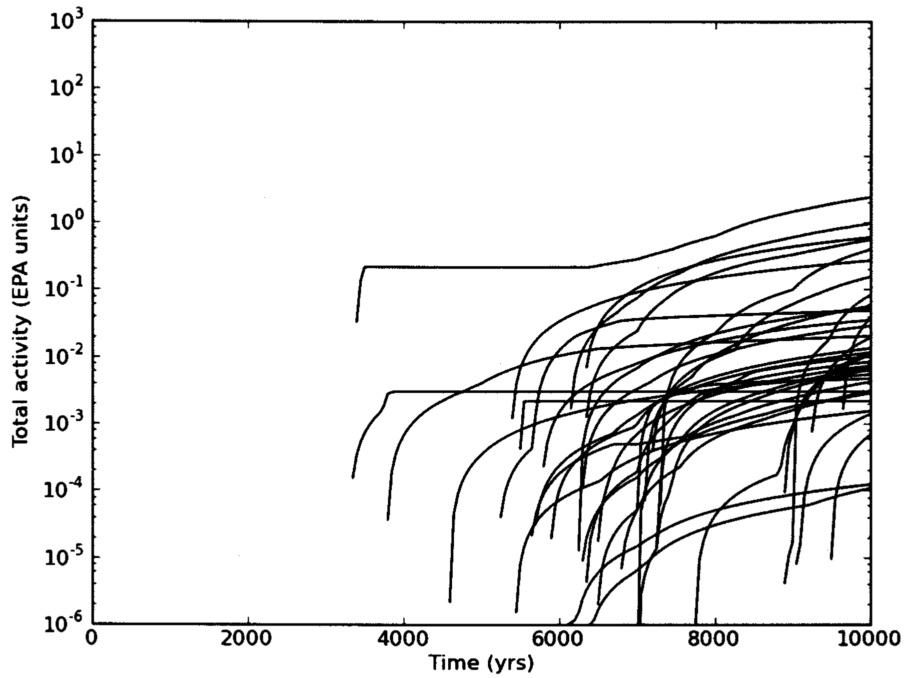


(a) CRA-2014 PA



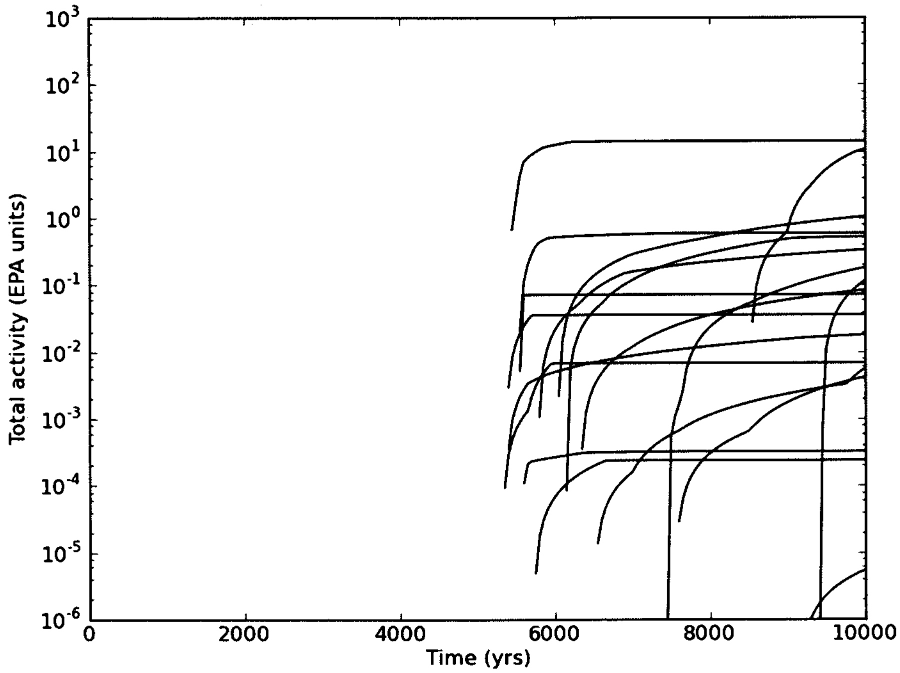
(b) CRA-2014 BL

Figure 22(a,b) Cumulative total releases to the Culebra for an E2 intrusion at 3000 years in the (a) CRA-2014 PA, (b) CRA-2014 BL, and (c) CRA-2009 PABC.

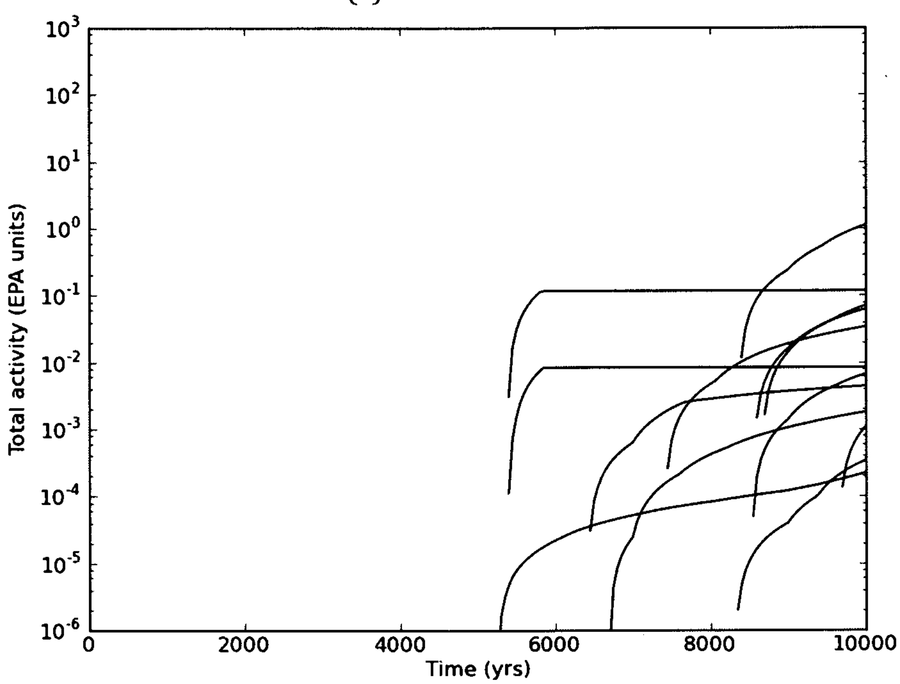


(c) CRA-2009 PABC

Figure 22(c) Cumulative total releases to the Culebra for an E2 intrusion at 3000 years in the (a) CRA-2014 PA, (b) CRA-2014 BL, and (c) CRA-2009 PABC.

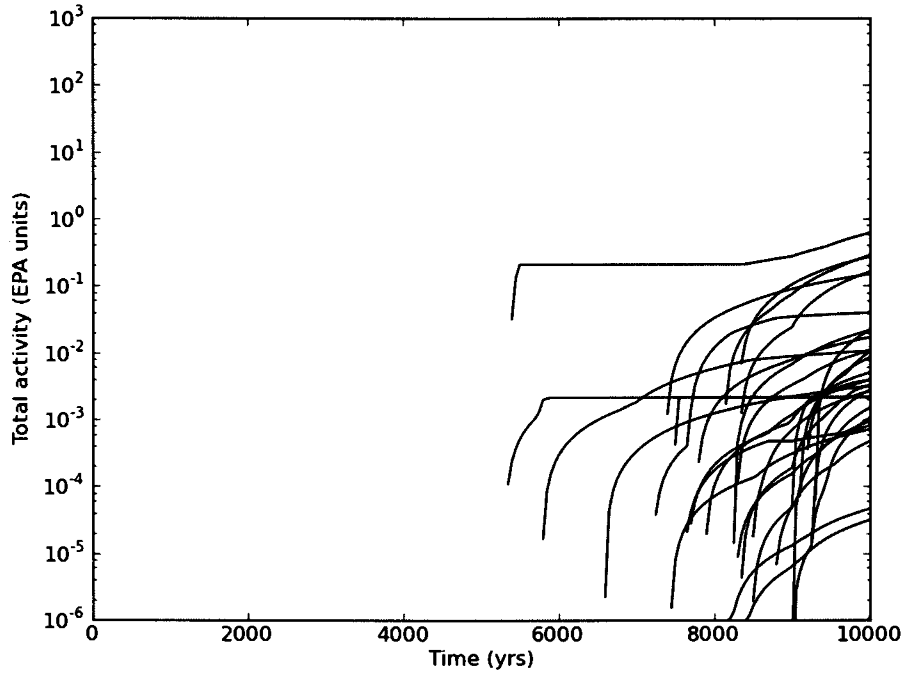


(a) CRA-2014 PA



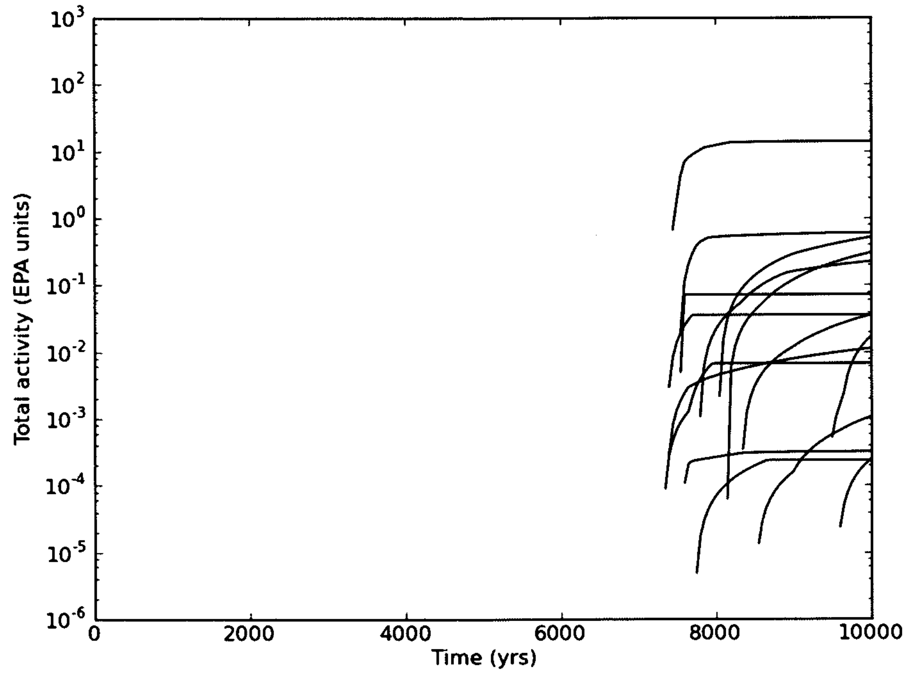
(b) CRA-2014 BL

Figure 23(a,b) Cumulative total releases to the Culebra for an E2 intrusion at 5000 years in the (a) CRA-2014 PA, (b) CRA-2014 BL, and (c) CRA-2009 PABC.

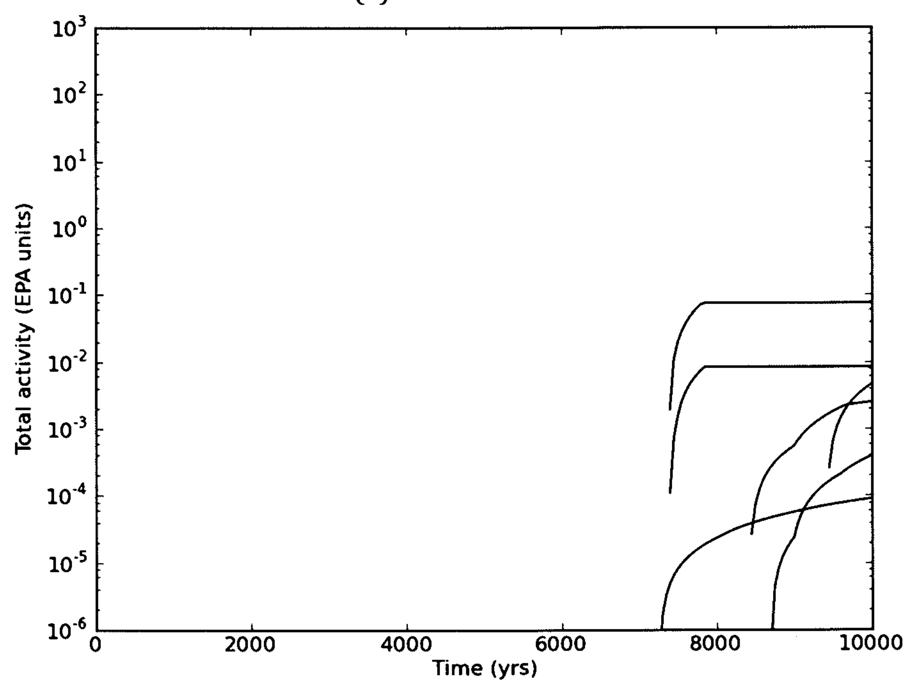


(c) CRA-2009 PABC

Figure 23(c) Cumulative total releases to the Culebra for an E2 intrusion at 5000 years in the (a) CRA-2014 PA, (b) CRA-2014 BL, and (c) CRA-2009 PABC.

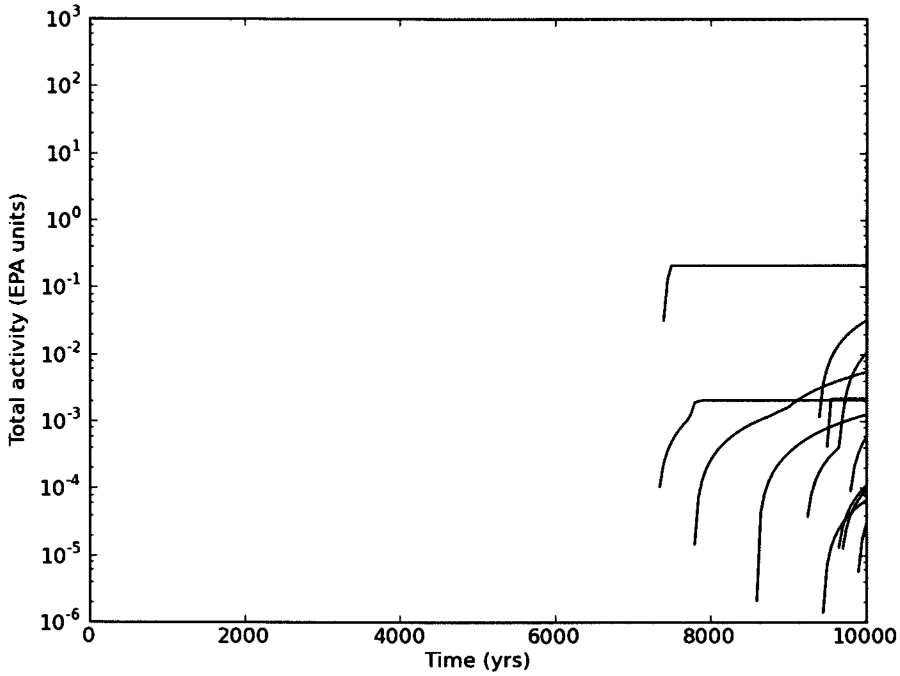


(a) CRA-2014 PA



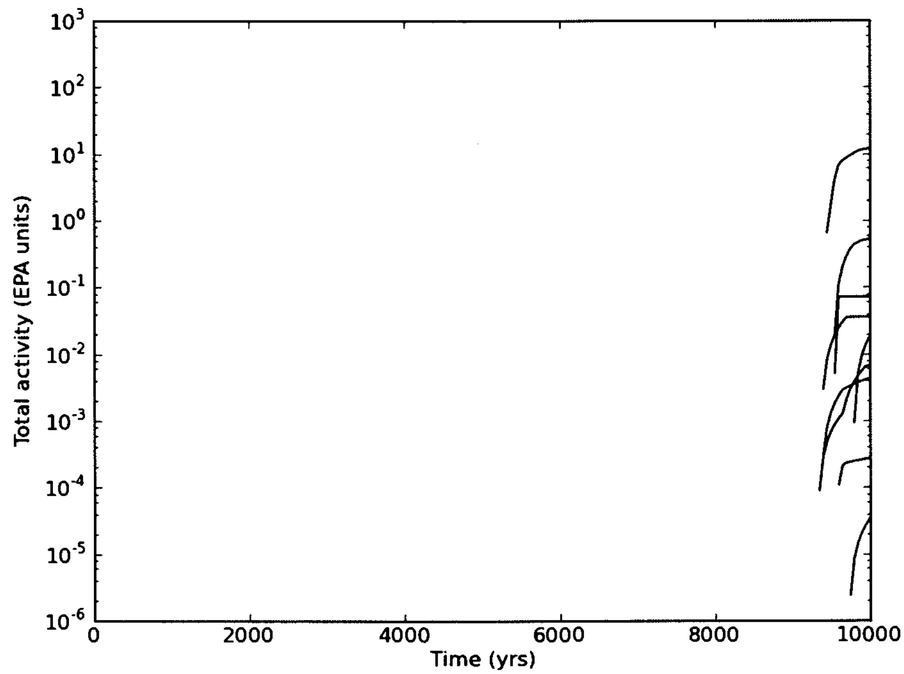
(b) CRA-2014 BL

Figure 24(a,b) Cumulative total releases to the Culebra for an E2 intrusion at 7000 years in the (a) CRA-2014 PA, (b) CRA-2014 BL, and (c) CRA-2009 PABC.

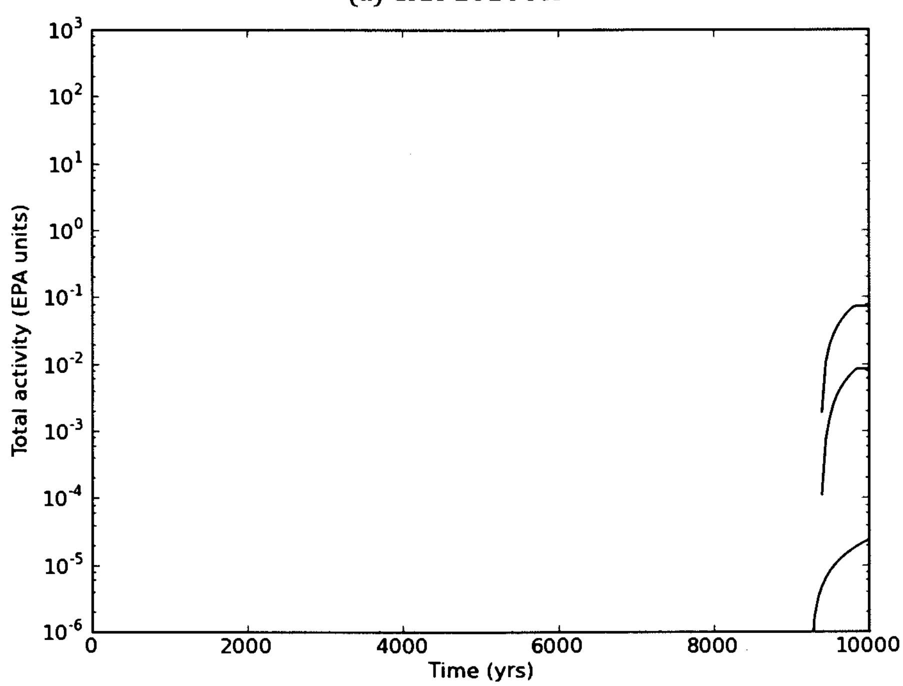


(c) CRA-2009 PABC

Figure 24(c) Cumulative total releases to the Culebra for an E2 intrusion at 7000 years in the (a) CRA-2014 PA, (b) CRA-2014 BL, and (c) CRA-2009 PABC.

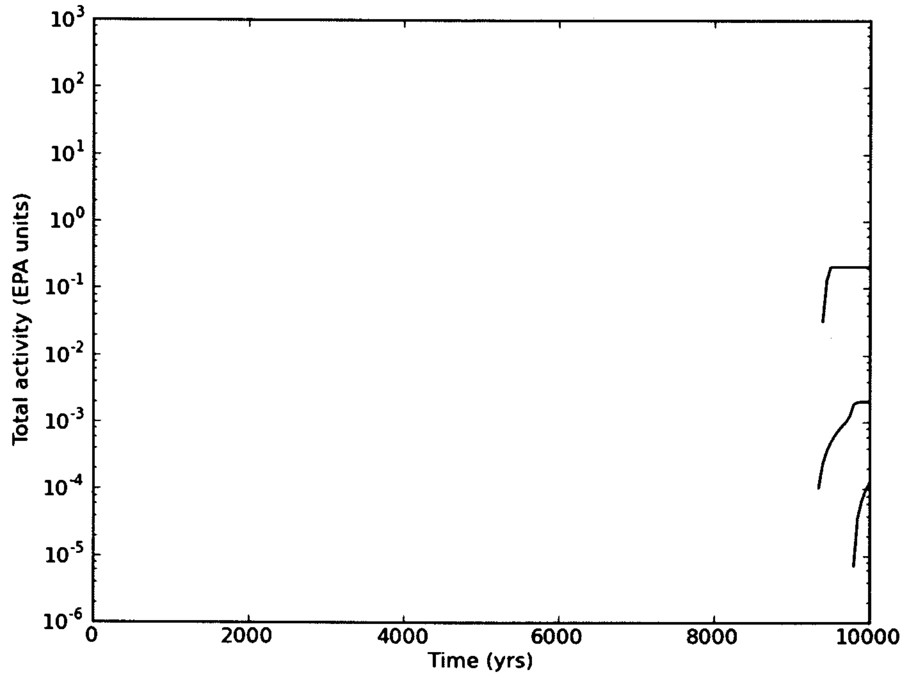


(a) CRA-2014 PA



(b) CRA-2014 BL

Figure 25(a,b) Cumulative total releases to the Culebra for an E2 intrusion at 9000 years in the (a) CRA-2014 PA, (b) CRA-2014 BL, and (c) CRA-2009 PABC.

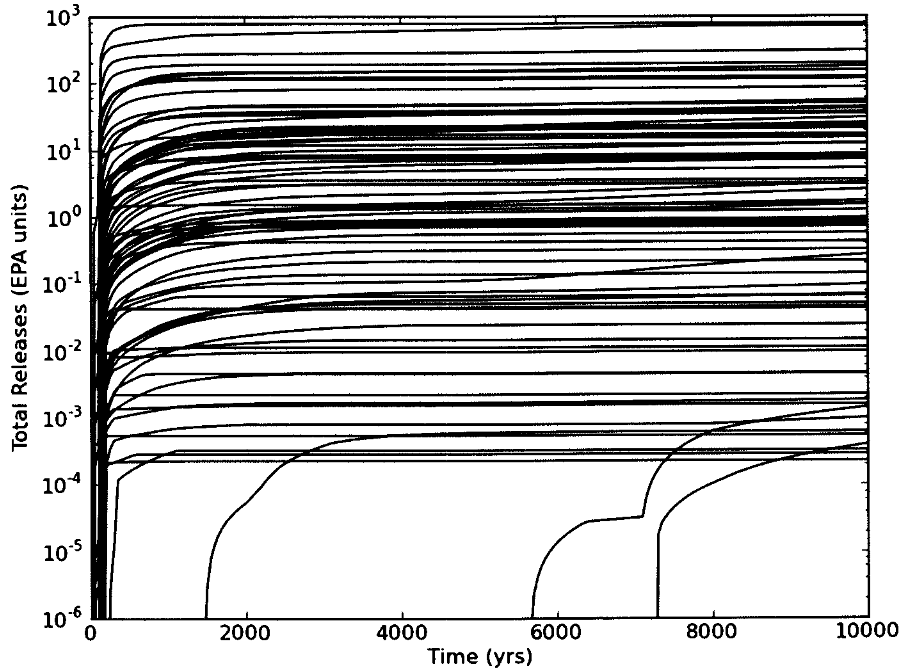


(c) CRA-2009 PABC

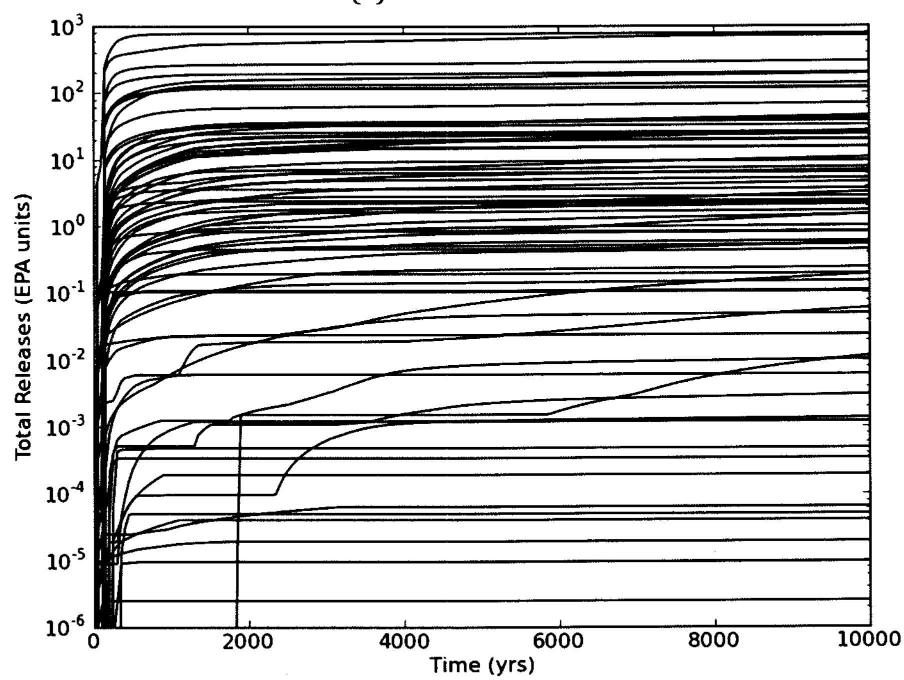
Figure 25(c) Cumulative total releases to the Culebra for an E2 intrusion at 9000 years in the (a) CRA-2014 PA, (b) CRA-2014 BL, and (c) CRA-2009 PABC.

Appendix A.3 E2-E1 Scenario

The results shown in this appendix are for Replicate 1 of S6-BF for each of the times indicated in the individual figures.

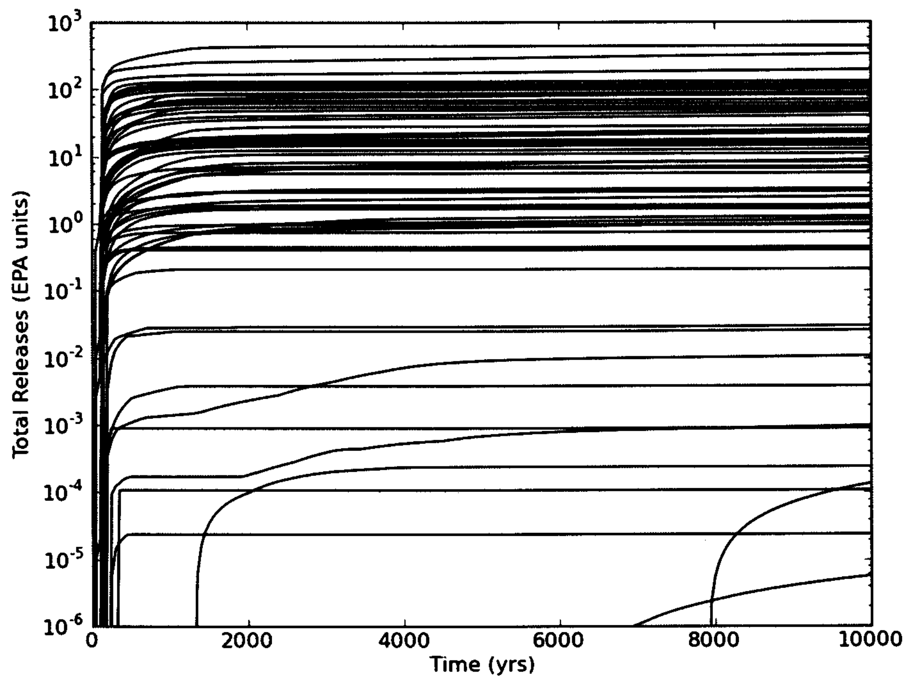


(a) CRA-2014 PA



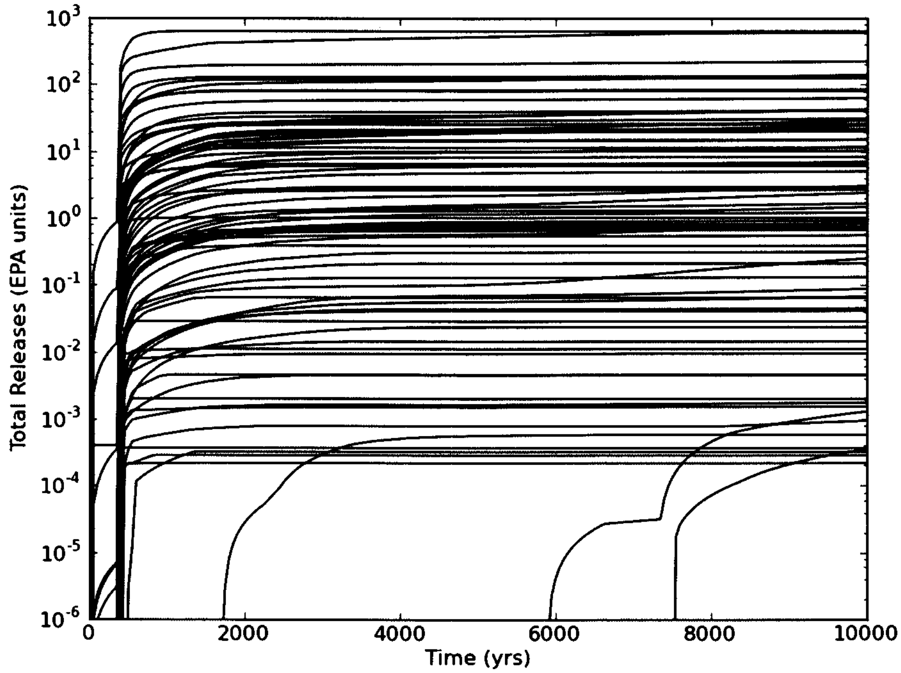
(b) CRA-2014 BL

Figure 26(a,b) Cumulative total releases to the Culebra for an E2-E1 intrusion at 100 years in the (a) CRA-2014 PA, (b) CRA-2014 BL, and (c) CRA-2009 PABC.

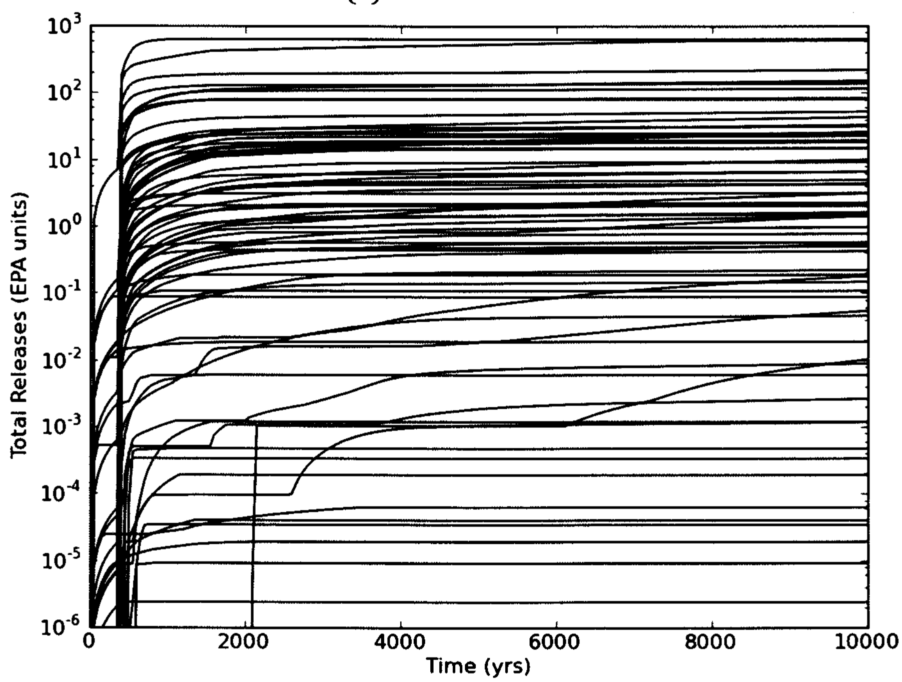


(c) CRA-2009 PABC

Figure 26(c) Cumulative total releases to the Culebra for an E2-E1 intrusion at 100 years in the (a) CRA-2014 PA, (b) CRA-2014 BL, and (c) CRA-2009 PABC.

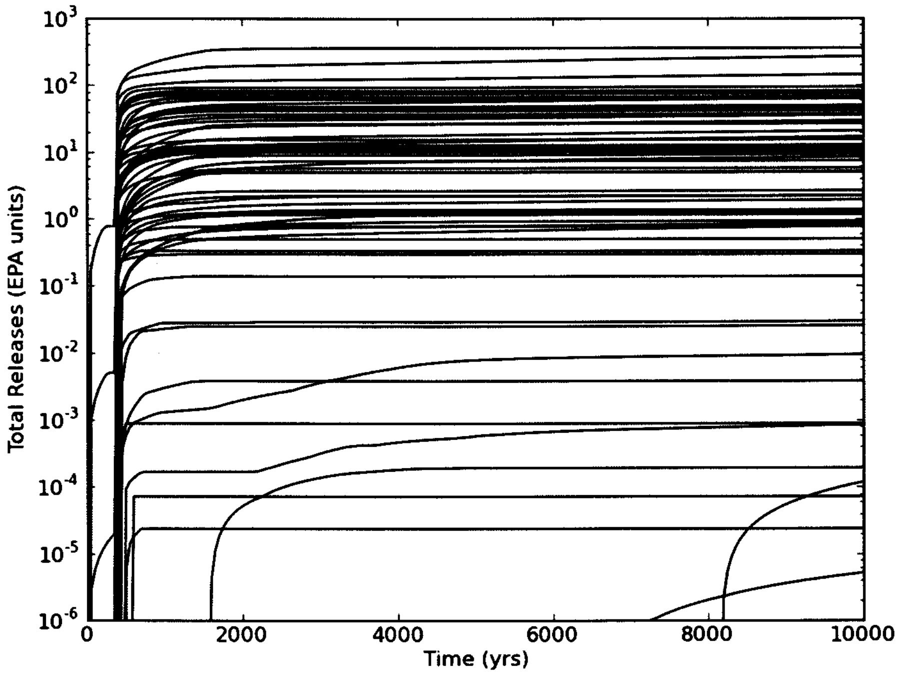


(a) CRA-2014 PA



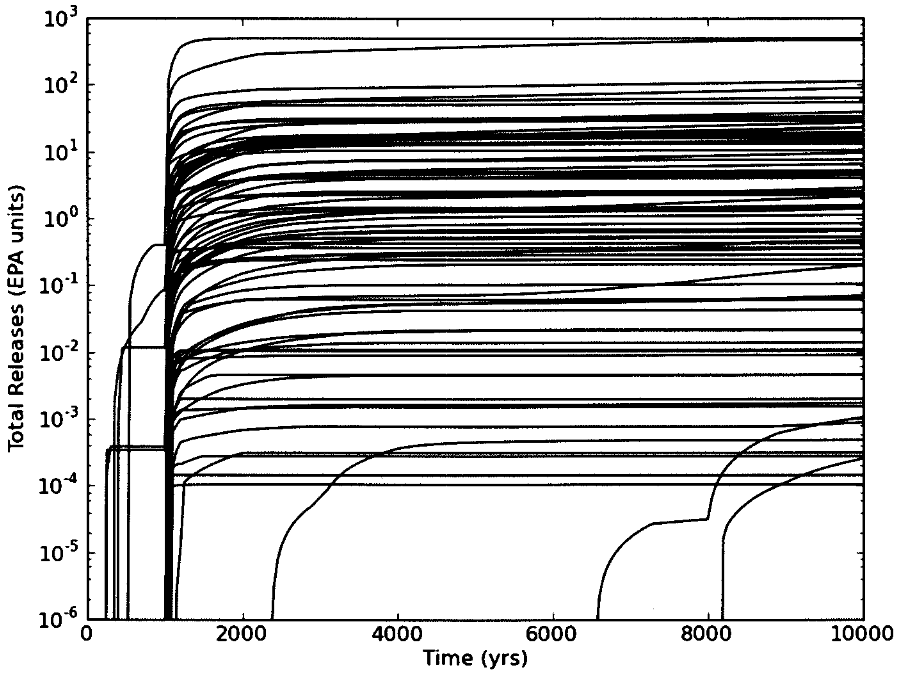
(b) CRA-2014 BL

Figure 27(a,b) Cumulative total releases to the Culebra for an E2-E1 intrusion at 350 years in the (a) CRA-2014 PA, (b) CRA-2014 BL, and (c) CRA-2009 PABC.

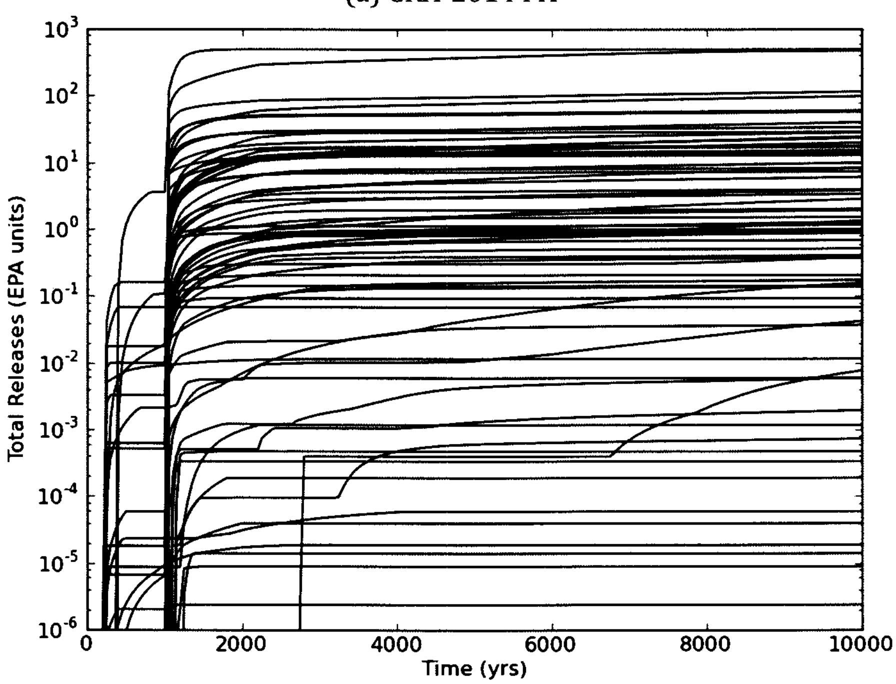


(c) CRA-2009 PABC

Figure 27(c) Cumulative total releases to the Culebra for an E2-E1 intrusion at 350 years in the (a) CRA-2014 PA, (b) CRA-2014 BL, and (c) CRA-2009 PABC.

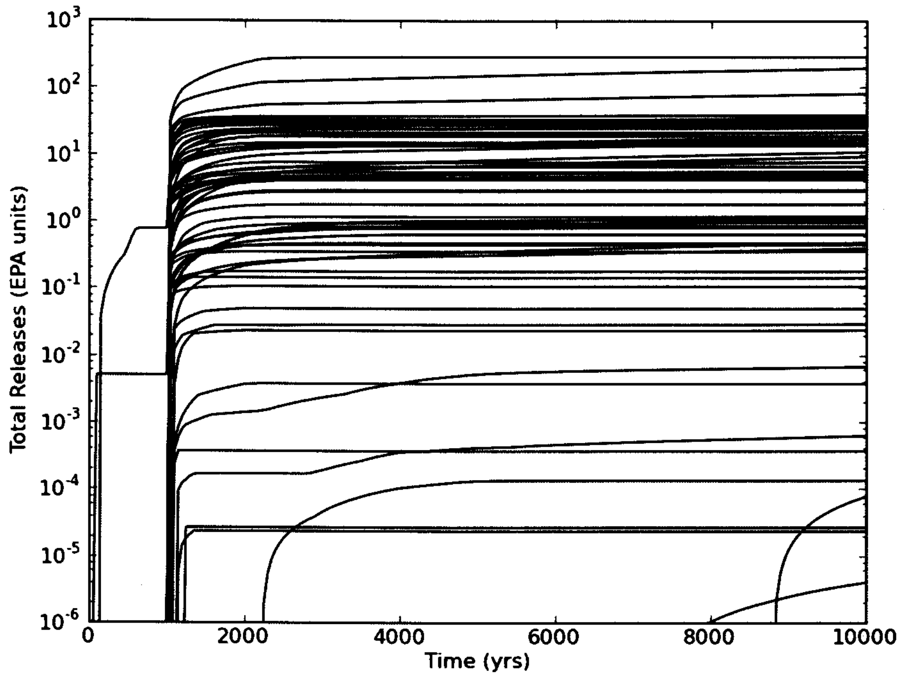


(a) CRA-2014 PA



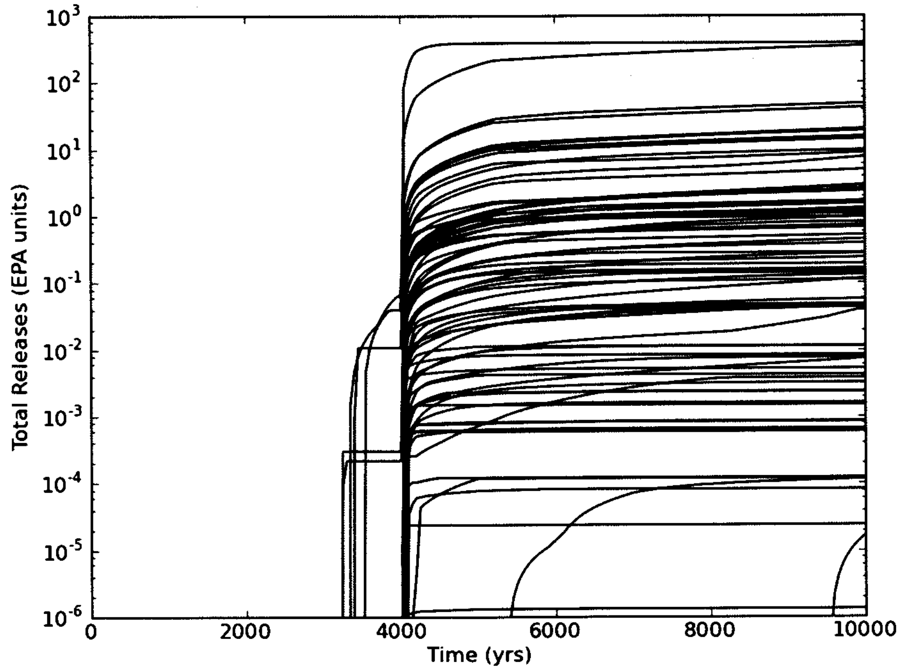
(b) CRA-2014 BL

Figure 28(a,b) Cumulative total releases to the Culebra for an E2-E1 intrusion at 1000 years in the (a) CRA-2014 PA, (b) CRA-2014 BL, and (c) CRA-2009 PABC.

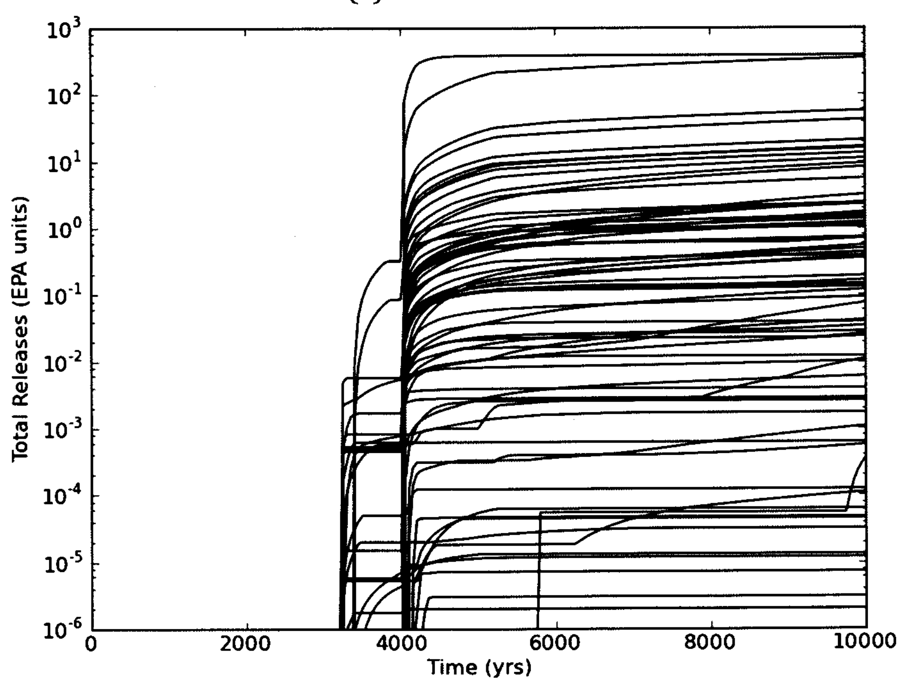


(c) CRA-2009 PABC

Figure 28(c) Cumulative total releases to the Culebra for an E2-E1 intrusion at 1000 years in the (a) CRA-2014 PA, (b) CRA-2014 BL, and (c) CRA-2009 PABC.

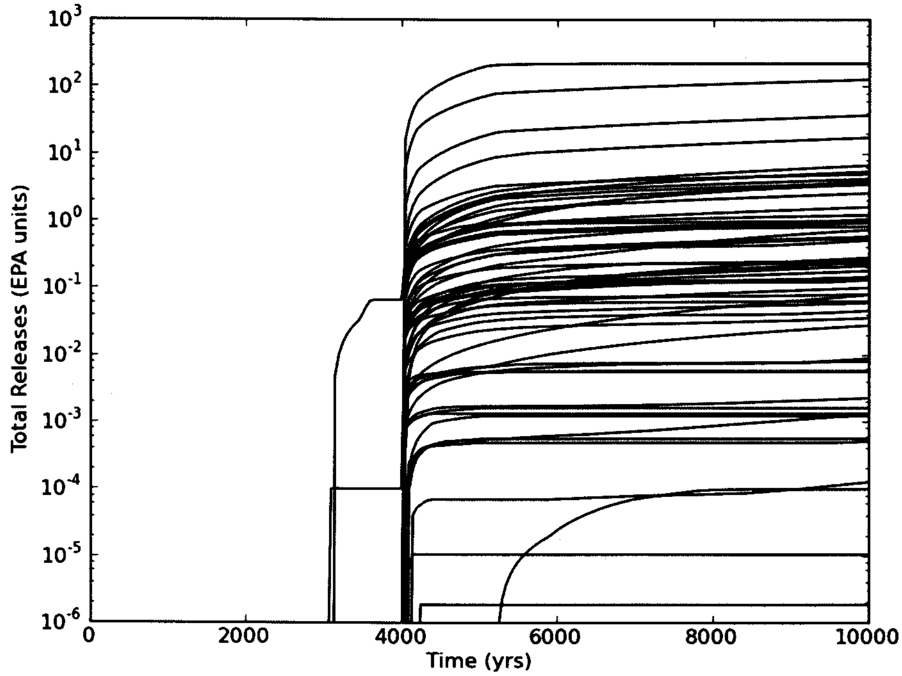


(a) CRA-2014 PA



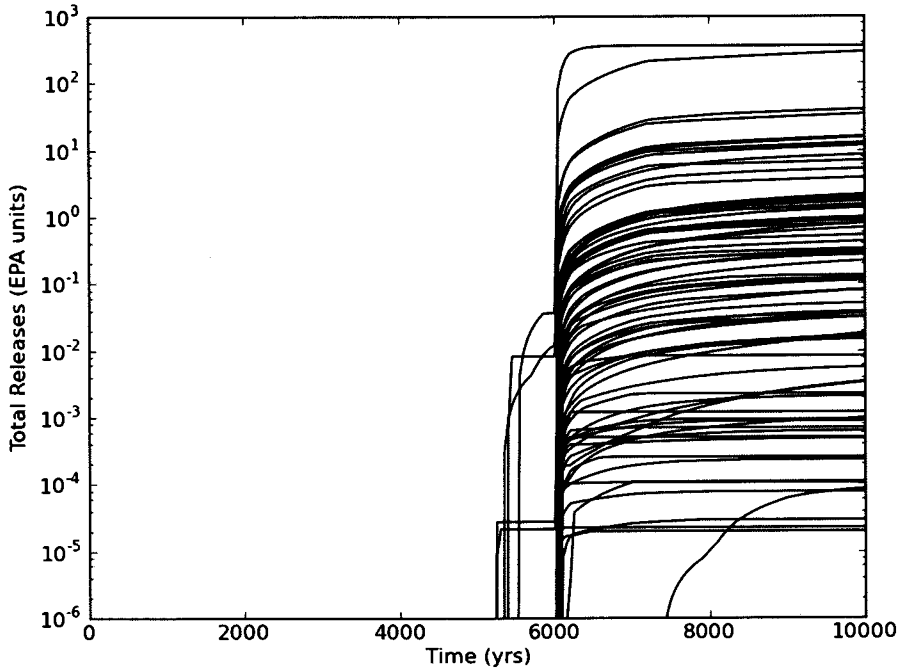
(b) CRA-2014 BL

Figure 29(a,b) Cumulative total releases to the Culebra for an E2-E1 intrusion at 4000 years in the (a) CRA-2014 PA, (b) CRA-2014 BL, and (c) CRA-2009 PABC.

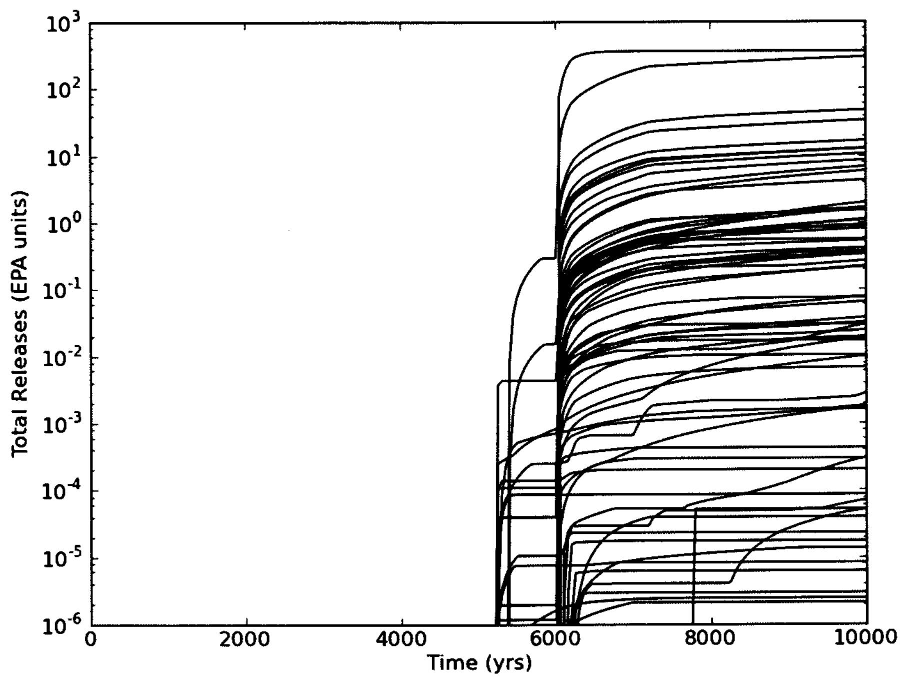


(c) CRA-2009 PABC

Figure 29(c) Cumulative total releases to the Culebra for an E2-E1 intrusion at 4000 years in the (a) CRA-2014 PA, (b) CRA-2014 BL, and (c) CRA-2009 PABC.

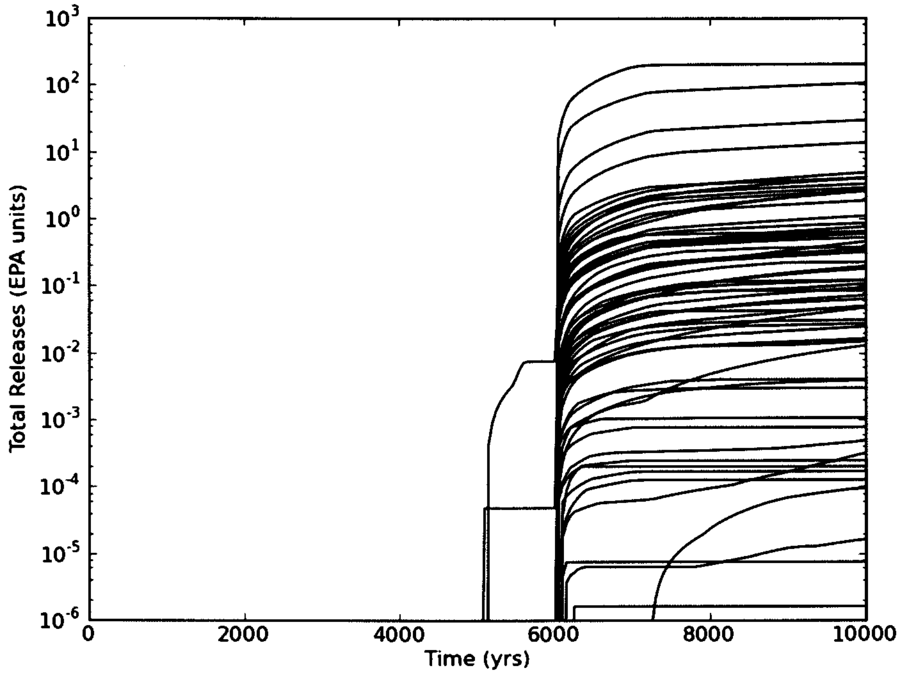


(a) CRA-2014 PA



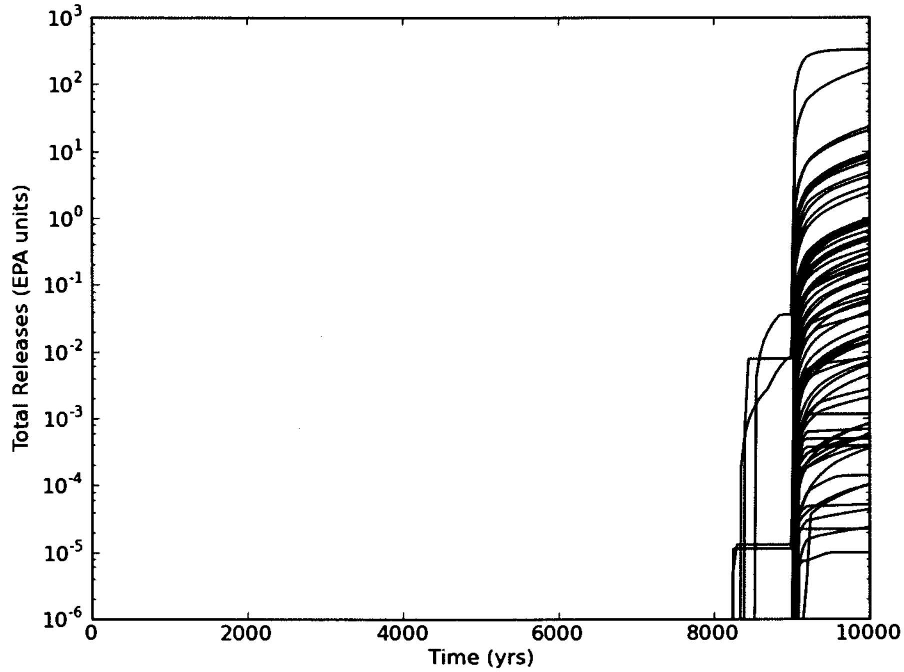
(b) CRA-2014 BL

Figure 30(a,b) Cumulative total releases to the Culebra for an E2-E1 intrusion at 6000 years in the (a) CRA-2014 PA, (b) CRA-2014 BL, and (c) CRA-2009 PABC.

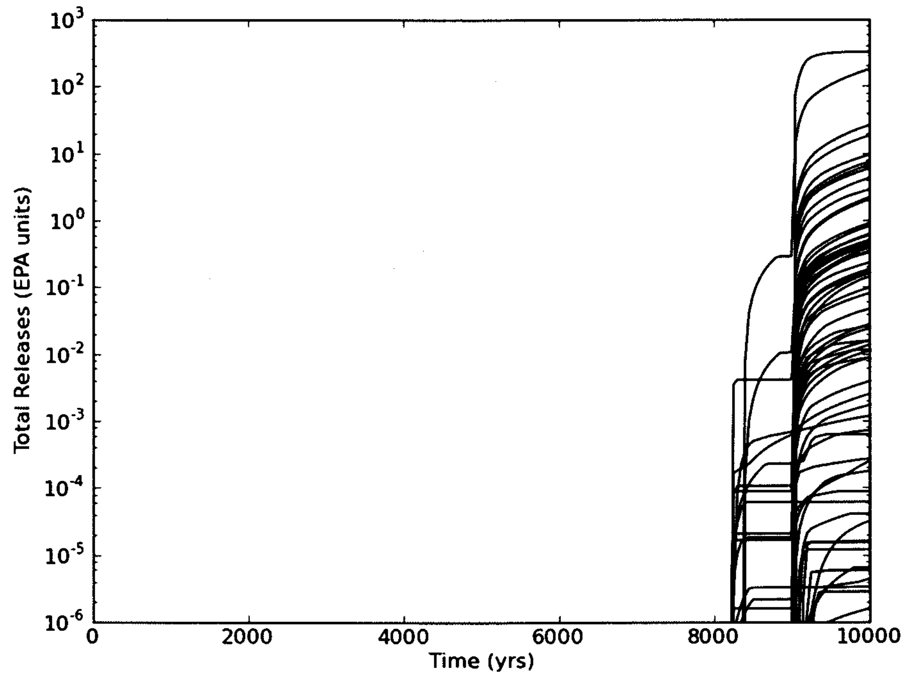


(c) CRA-2009 PABC

Figure 30(c) Cumulative total releases to the Culebra for an E2-E1 intrusion at 6000 years in the (a) CRA-2014 PA, (b) CRA-2014 BL, and (c) CRA-2009 PABC.

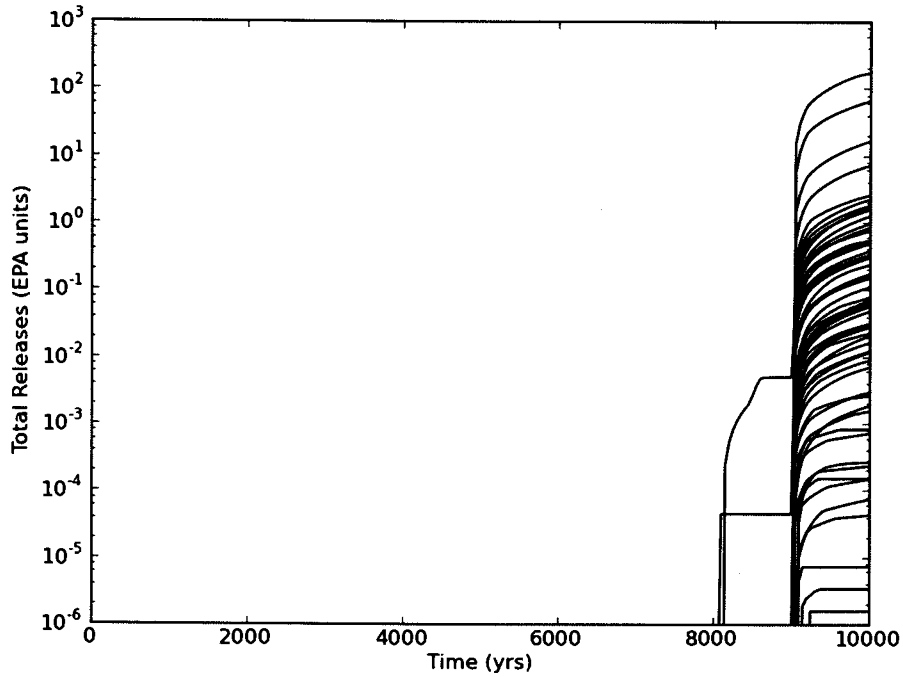


(a) CRA-2014 PA



(b) CRA-2014 BL

Figure 31(a,b) Cumulative total releases to the Culebra for an E2-E1 intrusion at 9000 years in the (a) CRA-2014 PA, (b) CRA-2014 BL, and (c) CRA-2009 PABC.



(c) CRA-2009 PABC

Figure 31(c) Cumulative total releases to the Culebra for an E2-E1 intrusion at 9000 years in the (a) CRA-2014 PA, (b) CRA-2014 BL, and (c) CRA-2009 PABC.

Appendix B Python Scripts Used to Analyze NUTS Results

A set of Python scripts has been used both to process the output files from NUTS and PANEL, as well as to generate most of the plots contained in this report. The script source codes along with the code output files, will be stored in an archived zip file, **Salado_Transport_CRA14PA.zip**, which will be available in class ANALYSIS of CMS library **LIBCRA14_NUT**. The results of the code were confirmed by visual inspection and hand calculations where appropriate.

Appendix B.1 nuts_analysis_v2.py

The original script *nuts_analysis.py* from CMS library **LIBPABC09_NUT** is slightly upgraded to *nuts_analysis_v2.py* that is stored in **Salado_Transport_CRA14PA.zip**. The upgraded script performs a number of different functions on output files: **SUM_NUT_*analysis*_R*r*_S*s*_T*ttttt*.TBL**, where ***analysis*** is the designation given to the analysis plan in the CMS system (***analysis*** = CRA14 or PABC09), **R*r*** is the replicate number (***r*** = 1, 2, 3), **S*s*** is the scenario number (***s*** = 1, 2, 3, 4, 5), and **T*ttttt*** is the intrusion time (***ttttt*** = 00100, 00350, 01000, 03000, 05000, 07000, 09000); these files are stored in CMS library **LIB*analysis*_SUM**. For the CRA-2014 PA and CRA-2014 BL, the different commands are used to produce output text files and plots that will be stored in **Salado_Transport_CRA14PA.zip** in CMS library **LIBCRA14_NUT**. The routines in this Python module were used to prepare the tables and graphs for the analysis of results from NUTS (all tables plus Figure 3 through Figure 8 and Figure 12 through Figure 25).

```
#!/usr/bin/python
#
# Ahmed E. Ismail
# SNL
# December 2009
# version 1.0
#
# Modified: Sungtae Kim
# May 2013
# version 2.0
#
# nuts_analysis_v2.py
#
# This collection of Python scripts processes output file from NUTS
# and PANEL, and uses this information to produce summary statistics
# and plots used in the preparation of the Salado Transport Analysis
# Package.

import os
import glob
import subprocess
import collections
import matplotlib.pyplot as mpl
from numpy import sum

# List of radionuclides studied in this report. (Change as needed.)
nuclide = ["Am-241", "Pu-239", "U-234", "Th-230", "Total"]

# Divisors for each radionuclide analyzed, as defined by the EPA.
epa_divisor = [100.0, 100.0, 100.0, 10.0]

def remove_vms(pattern="*.*"):
#
#    remove_vms(pattern) removes the ";N" extension from one or more
#    files specified by pattern, which is passed as a string to the glob module.
#    And make files readable in pc
#
#    pattern = *.* in order to be able to read file name with the ";N"
#
    for file in glob.glob(pattern):
        if ";" in file:
            trunk = file.split(";")[0]
            os.rename(file,trunk)
            f0 = open(trunk,'r')
```

```
            lines = f0.readlines()
            f0.close()
            f1 = open(trunk,'w')
            for l in lines:
                f1.write(l)
            f1.close()
    return


def read_screened(pattern="*.OUT", output_file="screened_list.dat"):
#
#    read_screened(pattern, output_file) processes SCREEN.EXE output
#    files specified by pattern through the read_screen_info function,
#    and writes the output to a file. The filename is an optional
#    argument; "screened_list.dat" is used as a default.
#
#    Vectors with markerbed releases are marked with an "M."
#
#    pattern = *.out  (NUT_SCN & SCREEN.EXE generate .OUT files)
#
    output = open(output_file, "w")
    for file in glob.glob(pattern):
        repl, scen, vector_list = read_screen_info(file)
        output.write('Replicate %s, Scenario %s:\n' % (repl, scen))
        list_string = ''
        for item, key in enumerate(sorted(vector_list)):
            if item != 0:
                list_string += ", "
            list_string += "%s" % (key, )
            if vector_list[key] == 2:
                list_string += "M"
        output.write(list_string + "\n")
        output.write("Count: %d\n\n" % (len(vector_list), ))
    output.close()
    return


def read_screen_info(file):
#
#    read_screen_info(file) parses the data stored in a SCREEN.EXE
#    output file to determine the vectors that will be passed on for
#    isotope and time intrusion calculations. The arguments returned by
#    the function is a dictionary whose keys are the vector numbers,
#    and whose stored values are the type of vector (borehole versus
#    markerbed releases, or used only for support of an intrusion
#    vector).
#
#   screen_out file name is SCREEN_NUT_SCN_'analysis'_Rr_Ss.OUT
    repl, scen = file[-8], file[-5]
    data = open(file, "r")
    v_list = collections.defaultdict(int)

    for line in data:
        if 'NONUNION_BEGIN' in line:
            break
    for line in data:
        if 'NONUNION_END' in line:
            break
        values = line.split()
        v_list[int(values[0])] = 2 if 'Markerbed' in values[1] else 1

    for line in data:
        if 'UNION_BEGIN' in line:
            break
    for line in data:
        if 'UNION_END' in line:
            break
        values = line.split()
        if int(values[0]) not in v_list:
            v_list[int(values[0])] = 3
```

```
    data.close()
    return repl, scen, v_list


def find_max(pattern, wuf):
#
#    find_max(pattern, wuf) calls find_maximum_epa for each file
#    globbed from pattern, using the wuf specified as the second
#    argument (or a default value if none is provided).
#
#    pattern = *.TBL (the SUMMARIZE output files)
#
    for file in glob.glob(pattern):
        find_maximum_epa(file, wuf)
    return


def find_maximum_epa(file, wuf):
#
#    find_maximum_epa takes the SUMMARIZE file specified by the
#    variable file and uses it to compute the maximum releases observed
#    for each species as a function of time across the individual
#    vectors, and then creates a file that lists all of the maxima
#    across all vectors.
#
#    file = *.TBL file name (SUM_NUT_PABC09_Rr_Ss_Ttttt.TBL)
#    r=1,2,3  s=1,2,3,4,5   tttt=00100,00350,01000,03000,05000,07000,09000
#
    handle = file[8:-4]
    input = open(file, "r")
    output = open(handle + ".out", "w")
    summary = open(handle + ".sum", "w")

    max_epa = [0.0 for i in range(4)]
    max_loc = [0 for i in range(4)]
    norm_term = [0.0 for i in range(4)]
    max_vec_epa, max_vec = 0.0, 0

    [input.readline() for i in range(4)]
    while True:
        line = input.readline()
        if line == "":
            break
        values = line.split()
        if len(values) == 0:
            output.write("%3s  %10.5g  %10.5g  %10.5g  %10.5g  %10.5g\n" %
                         (vec_id, norm_term[0], norm_term[1], norm_term[2],
                          norm_term[3], activity))
            continue
        activity = 0
        vec_id = values[0]
        for item, term in enumerate(values[2:6]):
            norm_term[item] = float(term) / (wuf * epa_divisor[item])
            activity += norm_term[item]
            if norm_term[item] > max_epa[item]:
                max_epa[item], max_loc[item] = norm_term[item], vec_id
        if activity > max_vec_epa:
            max_vec_epa, max_vec = activity, vec_id

    for act, loc, rn in zip(max_epa, max_loc, nuclide):
        summary.write("  %12.6g   %3s  %s\n" % (act, loc, rn))
    summary.write("  %12.6g   %3s  %s\n" % (max_vec_epa, max_vec, "Total"))

    input.close()
    output.close()
    summary.close()
    return


def concat_max_results(scen, time_list=None, analysis="PABC09"):
#
```

```
#    concat_max_results(scen, time_list, analysis) takes the results of
#    find_maximum_epa for a given scenario and set of times, and
#    produces a unified file showing all of the releases across all
#    vectors in all of the files.
#
    if scen == 1:
        handles = ["_S" + str(scen)]
    else:
        handles = ["_S" + str(scen) + "_T" + time for time in time_list]

    for handle in handles:
        max_epa = [0.0 for i in range(len(nuclide))]
        max_loc = [0 for i in range(len(nuclide))]
        max_rep = [0 for i in range(len(nuclide))]
        output = open(analysis + handle + ".max", "w")
        summary = open(analysis + handle + ".maxsum", "w")

        for i in range(1, 4):
            input_out = open(analysis + "_R" + str(i) + handle + ".out", "r")
            for line in input_out:
                output.write(line)
            input_out.close()
            input_sum = open(analysis + "_R" + str(i) + handle + ".sum", "r")
            for j in range(len(nuclide)):
                values = input_sum.readline().split()
                term = float(values[0])
                if term > max_epa[j]:
                    max_epa[j], max_loc[j], max_rep[j] = term, values[1], i
            input_sum.close()

        for j in range(len(nuclide)):
            summary.write("  %12.6g  %3d  %3s  %s\n" % (max_epa[j], max_rep[j],
                                                        max_loc[j], nuclide[j]))

        output.close()
        summary.close()
    return


def pct_act(pattern):
#
#    pct_act calls calc_pct_activity for each file globbed from the
#    specified pattern.
#
    output = open("percent.dat", "w")
    for file in glob.glob(pattern):
        string = calc_pct_activity(file)
        output.write(string)
    output.close()


def calc_pct_activity(file):
#
#    calc_pct_activity(file) takes an output file from
#    concat_max_results, and uses it to determine the percentage
#    composition of releases for the given conditions.
#

    def is_positive(x):
        #
        # is_positive(x) returns True if any element of x is positive;
        # otherwise, False is returned.
        #
        for value in x:
            if value > 0.0:
                return True
        else:
            return False

    # Determine output based on the input filename.
    handle = file[7:-4]
```

```
    input = open(file, "r")
    [input.readline() for i in range(4)]

    sp_act = [0.0 for i in nuclide[:-1]]
    count = 0
    while True:
        line = input.readline()
        if line == "":
            break
        values = line.split()
        if is_positive(values[1:5]):
            count += 1
            for i, value in enumerate(values[1:5]):
                sp_act[i] += float(value)

    total_act = sum(sp_act)
    if total_act > 0.0:
        sp_act = [100.0 * x / total_act for x in sp_act]
        avg_act = total_act / count
        return "%s  %10.5f  %10.5f  %10.5f  %10.5f  %10.5g \n" \
            % (handle, sp_act[0], sp_act[1], sp_act[2], sp_act[3], avg_act)
    else:
        return "%s         nan         nan         nan         nan           0 \n" \
            % handle


def make_plots(pattern, wuf):
#
#    make_plots(pattern, wuf) calls make_vector_plots for each file
#    globbed from the specified pattern, using the wuf value specified
#    in the second argument (or the default if not given explicitly).
#
    for file in glob.glob(pattern):
        make_vector_plots(file, wuf)


def make_vector_plots(file, wuf):
#
#    make_vector_plots(file, wuf) reads the data in a .TBL file
#    produced by ALGEBRACDB and SUMMARIZE and uses that information to
#    construct the horsetail plots showing the total releases as a
#    function of time. The resulting file is passed along to
#    concat_plot_results, which actually constructs the plots.
#

    # Determine output filenames based on the input filename.
    handle = file[8:-4]
    input = open(file, "r")
    output = open(handle + ".plot.dat", "w")

    vec_act = [[] for i in range(101)]
    has_activity = [False for i in range(101)]
    times = []

    # Throw away the header in the .TBL file
    [input.readline() for i in range(4)]
    while True:
        line = input.readline()
        if line == "":
            break
        values = line.split()
        if len(values) == 0:
            continue

        # We need to determine the set of times which will be plotted,
        # but this only needs to be done once per file.
        vec_id = int(values[0])
        if vec_id == 1:
            times.append(values[1])

        # Compute activity of vector
```

```
            activity = 0
            for item, term in enumerate(values[2:len(nuclide) + 1]):
                activity += float(term) / (wuf * epa_divisor[item])
            vec_act[vec_id].append(activity)
            if activity > 0.0:
                has_activity[vec_id] = True

    # Produce output file
    time_string = " ".join(times)
    output.write(time_string + "\n")
    for x in range(101):
        if has_activity[x]:
            string = " ".join([" %11.6g " % activity for activity in vec_act[x]])
            output.write(string + "\n")

    input.close()
    output.close()
    return


def concat_plot_results(scen, ymin, ymax, time_list=None, analysis="PABC09"):
#
#    concat_plot_results(scen, time_list, analysis) takes files from
#    scenario scen of the calculations defined by analysis over the
#    times specified in time_list, and plots the full set of
#
    # Scenario 1, if needed, does not have intrusion times, so make
    # sure they're not added to the list if the routine is called for
    # Scenario 1.
    if scen != 1:
        handles = ["_S" + str(scen) + "_T" + time for time in time_list]
    else:
        handles = ["_S" + str(scen)]

    for handle in handles:
        fig = mpl.figure()
        total_vectors = 0
        # Read each of the three files for a given scenario and time
        # combination, and create "horsehair" plots for each
        # vector provided.
        for i in range(1, 4):
            input = open(analysis + "_R" + str(i) + handle + ".plot.dat", "r")
            lines = input.readlines()
            times = [float(x) for x in lines[0].split()]
            # Plot the releases on a semilog-y axis.
            for line in lines[1:]:
                total_vectors += 1
                activities = [float(x) for x in line.split()]
                mpl.semilogy(times, activities, 'k')

            # Finish the plot details.
            mpl.axis([0, 10000, ymin, ymax])
            mpl.xlabel('Time (yrs)')
            mpl.ylabel('Total activity (EPA units)')
            mpl.savefig(analysis + handle + ".png")
            input.close()

        # We keep track of the total number of vectors with measurable
        # releases for each scenario and intrusion time combination.
        print handle, total_vectors


def plot_cdf_of_releases(filename, plot_min=1.0e-16):
#
#    plot_cdf_of_releases(filename, plot_min) takes the results from
#    concat_max_results specified by filename, and uses it to construct
#    a graphical cdf of the releases for a given scenario and time
#    combination. plot_min is an optional parameter that specifies the
#    smallest value of releases that will be shown on the plot.
#
```

```
    # Read the file produced by concat_max_results to get the
    # cumulative releases for each nuclide, as well as the cumulative
    # total release, for all vectors.
    input = open(filename, "r")
    releases = [[] for x in range(len(nuclide))]
    for line in input:
        values = line.split()[1:]
        for i in range(len(nuclide)):
            releases[i].append(float(values[i]))
    input.close()

    # For each nuclide, sort the vectors according to release
    # size. Plot vectors larger than a cutoff, and count those that
    # are smaller than the cutoff and use it as the starting point for
    # the cdf.
    fig = mpl.figure()
    legend_pos = 2
    for i in range(len(nuclide)):
        releases[i].sort()
        orig_len = len(releases[i])
        plot_releases = [x for x in releases[i] if x > plot_min]
        n_plotted = len(plot_releases)
        plot_releases.insert(0, plot_min)
        cdf = [float(orig_len - n_plotted + j) / orig_len for j in range(n_plotted + 1)]
        # Change the display location of the legend if it's going to
        # overlap the CDF's; this is only an issue if lots of vectors
        # have no releases (or at most releases smaller than the
        # cutoff).
        if cdf[0] > 0.7:
            legend_pos = 4
        mpl.semilogx(plot_releases, cdf, label=nuclide[i])

    # These commands control the plot display.
    mpl.axis([plot_min, 1.0e4, 0, 1])
    legend = mpl.legend(loc = legend_pos)
    for label in legend.get_texts():
        label.set_fontsize("small")
    mpl.xlabel('Cumulative Release (EPA units)')
    mpl.ylabel('CDF of Cumulative Release')
    mpl.savefig(filename.split(".")[0] + ".cdf.png")
    mpl.show()
    return


def max_marker(pattern):

    filelist = glob.glob(pattern)
    for no, file in enumerate(filelist):
        vec = 0
        max_marker = 0.0
        input = open(file, "r")
        [input.readline() for i in range(4)]
        while True:
            line = input.readline()
            if line == "":
                break
            data = line.split()
            if len(data) == 0:
                continue
            elif max_marker < float(data[-1]):
                vec, max_marker = data[0], float(data[-1])
        input.close()

        print "File/Vector = ", file, vec
        print "Maximum release = ", max_marker
```

Appendix B.2 Verification of SCREEN.FOR

The utility SCREEN.FOR has been used to determine which vectors will be considered for further processing in the isotope and time-intrusion scenarios in NUTS.

For the CRA-2014 PA, the compiled executable SCREEN.EXE was taken from the **LIB-CRA1BC_NUT** library and used without change. Since no new version of SCREEN.EXE was built for CRA-2014 PA and SCREEN.EXE is run as part of the run control process, no new verification files were created for the CRA-2014 PA. The previous verification, performed for the CRA-2009 PA (Ismail and Garner, 2008), is therefore the most recent possible test of the existing verification files. Verification of SCREEN.FOR for the present analysis has therefore been performed by visual comparison of the output of selected vectors screened in or excluded by SCREEN.FOR to the data in the original ***.TBL** files which are used as inputs to SCREEN.FOR.