540572

Sandia National Laboratories
Waste Isolation Pilot Plant

Analysis Package for PANEL: CRA-2004 Performance Assessment Baseline Calculation

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Acronyms

AP	Analysis Plan
CCA	Compliance Certification Application
CFR	Code of Federal Regulations
CH	Contact Handled
CMS	Configuration Management System
CPR	Cellulose, Plastic, and Rubber
CRA	Compliance Recertification Application
DBR	Direct Brine Release
DCL	Digital Command Language
DOE	US Department of Energy
DRZ	Disturbed Rock Zone
EPA	Environmental Protection Agency
ERDA	Energy Research and Development Administration
FMT	Fracture-Matrix Transport
GWB	Generic Weep Brine
LANL	Los Alamos National Laboratory
LHS	Latin Hypercube Sampling
PA	Performance Assessment
PABC	Performance Assessment Baseline Calculation
PAPDB	Performance Assessment Parameter Database
PAVT	Performance Assessment Verification Test
PC	Personal Computer
POD	Parameter Output Database
RH	Remote Handled
SNL	Sandia National Laboratories
TRU	Transuranic
WIPP	Waste Isolation Pilot Plant

1. INTRODUCTION

1.1 BACKGROUND

The Waste Isolation Pilot Plant (WIPP) is located in southeastern New Mexico and has been developed by the U.S. Department of Energy (DOE) for the geologic (deep underground) disposal of transuranic (TRU) waste (U.S. DOE 1980, 1990, 1993). In 1992, Congress designated the U.S. Environmental Protection Agency (EPA) as WIPP's official certifier, and mandated that once DOE demonstrated to EPA's satisfaction that WIPP complied with Title 40 of the Code of Federal Regulations (CFR), Part 191 (U.S. DOE, 1996, U.S. EPA 1996), EPA would certify the repository. To show compliance with the regulations, the DOE had their scientific advisor, Sandia National Laboratories (SNL) develop a computational modeling system to predict the future performance of the repository for 10,000 years after closure. SNL has developed a system, called WIPP Performance Assessment (PA), which examines failure scenarios, quantifies their likelihoods, estimates potential releases to the surface or the site boundary, and evaluates the potential consequences, including uncertainties. The regulation also requires that these models be maintained and updated with new information to be part of a recertification process that occurs at five-year intervals after the first waste is received at the site.

The WIPP PA consists of a suite of numerical models or "codes" designed to predict conditions in and around the repository over a period of 10,000 years. One model that is run for the PA is the PANEL code (Garner 2005a). PANEL's PA role is to estimate the mobilized radioactive contaminant load in the brine phase of the brine/gas mixture that seeps or flows through the repository's waste panels (Garner 2003b).

This report documents the PANEL simulations and results that support the baseline PA calculations for the first recertification of the repository as described below. The calculations to be completed for the baseline PA are outlined in the analysis plan AP-122 (Kanney and Leigh 2005). PANEL is run as part of the work scope defined in AP-122.

1.2 COMPLIANCE CERTIFICATION APPLICATION

In October 1996, DOE submitted the Compliance Certification Application (CCA) to the EPA, which included the results of the WIPP PA system. During the review of the CCA, EPA mandated an additional Performance Assessment Verification Test (PAVT), which revised selected CCA inputs to the PA (SNL 1997). The PAVT analysis ran the full suite of WIPP PA codes and confirmed the conclusions of the CCA analysis that the repository design met the regulations. Following the receipt of the PAVT analysis, EPA ruled in May 1997 that WIPP had met the regulations for permanent disposal of transuranic waste. Several lawsuits in opposition to the EPA's ruling were filed in court and were eventually dismissed. The first shipment of radioactive waste from the nation's nuclear weapons complex arrived at the WIPP site in late March 1999, starting the five-year clock for the site's required recertification. The results of CCA PA analyses were subsequently summarized in a SNL report (Helton, et. al. 1998).

1.3 2004 COMPLIANCE RECERTIFICATION APPLICATION

The first Compliance Recertification Application (CRA-2004) was submitted to the EPA by the DOE in March 2004 (U.S. DOE 2004). During its review of CRA-2004, the EPA raised several questions regarding its completeness and technical adequacy (Cotsworth 2004 a-d, Gitlin 2005). The DOE and SNL responded to EPA questions in writing (Detwiler 2004 a-f, Piper 2004, Triay 2005, Patterson 2005, U.S. DOE 2004) and by engaging in technical meetings with EPA staff. The result of these technical interactions was that the EPA insisted that SNL revise the CRA-2004 PA analysis and run a new PA analysis, which would be considered the PA new baseline following recertification. The PANEL results of this revised calculation (CRA-2004 PABC) are the subject of this report.

1.4 OBJECTIVES FOR THE CRA-2004 PABC PANEL ANALYSIS

The EPA required that DOE revise the CRA-2004 analysis and present results before EPA would judge the CRA-2004 complete (Cotsworth 2005). The EPA noted a number of technical changes and corrections to the CRA-2004 PA that it deemed necessary. Additionally, the EPA stated that a number of modeling assumptions used in CRA-2004 have not been sufficiently justified and that alternative modeling assumptions must be used. The issues and changes affecting the PANEL portion of WIPP PA include the following:

1) Changes in the probability of microbial gas generation in the repository were made.
2) Actinide solubilities were updated.
3) Implementation of uncertainty for the actinide solubilities was updated.
4) Inventory information was updated.

Minor corrections are also made in the CRA-2004 PABC to the PANEL code's method for setting the default brine volume (Garner 2005a).

2. UPDATES FROM CRA-2004 TO CRA-2004 PABC THAT AFFECT PANEL CALCULATIONS

2.1 PROBABILITY FOR MICROBIAL DEGRADATION OF DIFFERENT ORGANIC MATERIALS

During a technical exchange with EPA in January 2005, EPA expressed concerns about the parameter that defines the probability that microbial gas generation will occur in the WIPP. Advances in microbiology have found microbes existing in a wide variety of so-called "extreme" environments that were previously not considered to be conducive to supporting microbes. Based on these scientific advances, the EPA argued that the probability that microbial activity and resulting microbial gas generation would occur in the WIPP should be changed from 0.5, which corresponds to microbial activity in 50% of the vectors, to 1.0 which means that microbial activity could occur in every vector. The importance of microbial activity for PANEL is described in section 2.2.

2.2 ACTINIDE SOLUBILITY UPDATE

The Fracture-Matrix Transport (FMT) code (Babb and Novak 1997 and addenda; Wang 1998) is used to calculate actinide solubilities in WIPP brines. The EPA requested (Cotsworth 2005) parameter changes related to the FMT calculations for actinide solubility in the CRA-2004 PABC. In particular, organic-ligand concentrations for the CRA-2004 PABC were recalculated by Brush and Xiong (2005, Table 4). The other chemical conditions agreed upon for the CRA-2004 PABC solubility calculations include: (1) use of Generic Weep Brine (GWB) (Snider 2003) and Energy Research and Development Administration (WIPP Well) 6 (ERDA-6) (Popielak et. al. 1983) to simulate Salado and Castile brines, respectively; (2) the assumption that instantaneous, reversible equilibria among GWB or ERDA-6, major Salado minerals such as halite (NaCl) and anhydrite ($CaSO_4$), and the MgO hydration and carbonation products brucite ($Mg(OH)_2$) and hydromagnesite ($Mg_5(CO_3)_4(OH)_2 \cdot 4H_2O$) will control chemical conditions, such as f_{CO_2}, pH, and brine composition; and (3) elimination of separate, slightly different chemical conditions characteristic of the absence of microbial activity from the calculations (since all vectors are assumed to have microbial degradation for CRA-2004 PABC).

The EPA also specified that a revised estimate of 1×10^{-3} M be used for the solubility of U(VI) in WIPP brines for the CRA-2004 PABC source term. The EPA specified this value during a DOE-EPA teleconference on March 2, 2005 (Brush 2005).

Actinide solubilities calculated by FMT are represented in the remainder of this document as

$$\left(S_{brine}^{red/ox}\right) \quad (1)$$

and are defined for a particular actinide oxidation state (+III, +IV, +V, +VI) and a particular brine (Salado or Castille). Table 2 and Table 3 show the way that actinide solubilities are designated as parameters in WIPP PA. The tables show which actinide solubility parameters were updated for CRA-2004 PABC and which actinide solubility parameters were not updated for the CRA-2004 PABC.

Table 1. Actinide Solubility Parameters that were re-calculated for the CRA-2004 PABC(a)

Material	Property	Description	CRA-2004	CRA-2004 PABC	Units
SOLMOD3	SOLCOH	Solubility of +III actinides in Castile brine, including organic ligands with a brucite-hydromagnesite buffer	1.69E-07	2.88E-07	moles/liter
SOLMOD3	SOLSOH	Solubility of +III actinides in Salado brine, including organic ligands with a brucite-hydromagnesite buffer	3.07E-07	3.87E-07	moles/liter
SOLMOD4	SOLCOH	Solubility of +IV actinides in Castile brine, including organic ligands with a brucite-	2.47E-08	6.79E-08	moles/liter

		hydromagnesite buffer			
SOLMOD4	SOLSOH	Solubility of +IV actinides in Salado brine, including organic ligands with a brucite-hydromagnesite buffer	1.19E-08	5.64E-08	moles/liter
SOLMOD5	SOLCOH	Solubility of +V actinides in Castile brine, including organic ligands with a brucite-hydromagnesite buffer	5.08E-06	8.24E-07	moles/liter
SOLMOD5	SOLSOH	Solubility of +V actinides in Salado brine, including organic ligands with a brucite-hydromagnesite buffer	1.02E-06	3.55E-07	moles/liter
SOLMOD6	SOLCOH	Solubility of +VI actinides in Castile brine, including organic ligands with a brucite-hydromagnesite buffer	8.80E-06	1.00E-03	moles/liter
SOLMOD6	SOLSOH	Solubility of +VI actinides in Salado brine, including organic ligands with a brucite-hydromagnesite buffer	8.70E-06	1.00E-03	moles/liter

(a)Corresponds to $\left(s_{brine}^{red/ox}\right)$ in Equation 1.

Table 2. Actinide Solubility Parameters that Were Used in CRA-2004 but are not Used in CRA-2004 PABC[a]

Material	Property	Description
SOLMOD3	SOLCOC	Solubility of +III actinides in Castile brine, including organic ligands with a brucite-calcium carbonate buffer
SOLMOD3	SOLSOC	Solubility of +III actinides in Salado brine, including organic ligands with a brucite-calcium carbonate buffer
SOLMOD4	SOLCOC	Solubility of +IV actinides in Castile brine, including organic ligands with a brucite-calcium carbonate buffer
SOLMOD4	SOLSOC	Solubility of +IV actinides in Salado brine, including organic ligands with a brucite-calcium carbonate buffer
SOLMOD5	SOLCOC	Solubility of +V actinides in Castile brine, including organic ligands with a brucite-calcium carbonate buffer
SOLMOD5	SOLSOC	Solubility of +V actinides in Salado brine, including organic ligands with a brucite-calcium carbonate buffer
SOLMOD6	SOLCOC	Solubility of +VI actinides in Castile brine, including organic ligands with a brucite-calcium carbonate buffer
SOLMOD6	SOLSOC	Solubility of +VI actinides in Salado brine, including organic ligands with a brucite-calcium carbonate buffer

[a]These parameters are not used in the CRA-2004 PABC because all vectors are considered to have the potential for microbial gas generation. In the presence of microbial gas generation, the system is buffered by brucite-hydromagnesite (U.S. DOE 2004 Appendix BARRIERS, Subsection BARRIERS-2.3.2.3.)

2.3 SOLUBILITY UNCERTAINTY UPDATE

Xiong et al. (2004) re-established the uncertainty range and probability distribution for An(III), An(IV), and An(V) solubility predictions in response to an EPA request (Cotsworth 2004c) to update the ranges and distributions established by Bynum (1996a, 1996b, 1996c) for the PA calculations for the CCA. Xiong et al. (2004) concluded that (1) the An(III) thermodynamic speciation and solubility model implemented in FMT slightly overpredicted the measured An(III) solubilities; (2) the An(IV) model in FMT significantly underpredicted the measured An(IV) solubilities; (3) the An(V) model in FMT slightly overpredicted the measured An(V) solubilities; and (4) overall, the An(III), An(IV), and An(V) models in FMT together significantly underpredicted the measured An(III), An(IV), and An(V) solubilities. Xiong et al. (2004) used the thermodynamic database FMT_040628.CHEMDAT for their analysis. Because the An(IV) model in FMT significantly underpredicted the measured An(IV) solubilities, Nowak (2005) identified the value of the dimensionless standard chemical potential (μ^0/RT) for $Th(OH)_4(aq)$ in FMT_040628.CHEMDAT, -622.4700, as the cause of this problem; and recommended that μ^0/RT for $Th(OH)_4(aq)$ be changed from -622.4700 to -626.5853. Xiong (2005) made this change and released the corrected version of the database, FMT_050405.CHEMDAT.

Xiong et al. (2005) used FMT_050405.CHEMDAT to establish a revised uncertainty range and probability distribution for An(IV) solubility predictions and a revised composite range and distribution for An(III), An(IV), and An(V) solubility predictions. Xiong et al. (2005) did not revise the ranges and distributions for An(III) and An(V) solubility predictions established by Xiong et al. (2004).

The EPA specified that a fixed value be used for U(VI). In the CCA PA, the PAVT, and the CRA-2004 PA, the uncertainty range of -2.0 to +1.4 orders of magnitude was applied to the U(VI) solubility estimate of Hobart and Moore (1996). For the CRA-2004 PABC the U(VI) solubility is fixed at 1×10^{-3} M.

Actinide solubilities calculated by FMT are modified by a variability factor (M) as shown in Equation 2. $S_{brine}^{red/ox} = \left(s_{brine}^{red/ox}\right) \bullet \left(10^{M}\right)$ is the solubility estimate for a given vector. M is a function of the oxidation state and is a sampled value as shown in Table 4.

$$S_{brine}^{red/ox} = \left(s_{brine}^{red/ox}\right) \bullet \left(10^{M}\right) \quad (2)$$

Table 4 shows the actinide solubility variability parameters that were not used in the CRA-2004 PABC.

Table 3. Actinide Solubility Uncertainty Parameters for the CRA-2004 PABC

Material	Property	CRA-2004 Value	CRA-2004 PABC Value[b]	Units	Distribution Type
SOLMOD3	SOLVAR[a]	NA	-3.07E-02	NONE	Cumulative
SOLMOD4	SOLVAR	NA	7.50E-02	NONE	Cumulative
GLOBAL	OXSTAT[c]	5.00E-01	5.00E-01	NONE	Uniform

[a]Variability parameter for actinide solubility (M in Equation 2) [b] For a cumulative distribution, the distribution is represented in the WIPP Performance Assessment Parameter Database (WIPP PAPDB 2003) with a single value that is the median value. The reader can reference Garner (2005b) and Garner (2005c) for the conversion to the cumulative distribution. Appendix D shows the distribution in more detail. (c) If GLOBAL:OXSTAT is less than or equal to .5, Pu will be in oxidation state +III. If it is greater than .5, the oxidation state for Plutonium will be +IV.

Table 4. Actinide Solubility Uncertainty Parameters That Were Not Updated for the CRA-2004 PABC[a]

Material	Property	Description
SOLAM3	SOLCIM	Variability parameter[b] for Am(+III) in Castille brine
SOLAM3	SOLSIM	Variability parameter[b] for Am(+III) in Salado brine
SOLPU3	SOLCIM	Variability parameter[b] for Pu(+III) in Castille brine
SOLPU3	SOLSIM	Variability parameter[b] for Pu(+III) in Salado brine
SOLPU4	SOLCIM	Variability parameter[b] for Pu(+IV) in Castille brine
SOLPU4	SOLSIM	Variability parameter[b] for Pu(+IV) in Salado brine
SOLTH4	SOLCIM	Variability parameter[b] for Th(+IV) in Castille brine
SOLTH4	SOLSIM	Variability parameter[b] for Th(+IV) in Salado brine
SOLU4	SOLCIM	Variability parameter[b] for U(+IV) in Castille brine
SOLU4	SOLSIM	Variability parameter[b] for U(+IV) in Salado brine
SOLU6	SOLCIM	Variability parameter[b] for U(+VI) in Castille brine
SOLU6	SOLSIM	Variability parameter[b] for U(+VI) in Salado brine

[a] These parameters were not updated in the WIPP PAPDB because a simplified model using only two variability parameters was implemented for CRA-2004 PABC. However, the input to PANEL is still via these parameters. Steps were added to the *ALGEBRACDB* input file (see Appendix B) which write the values of SOLMOD3:SOLVAR into SOLAM3: SOLCIM, SOLAM3:SOLSIM, SOLPU3:SOLCIM, and SOLPU3:SOLSIM. ALGEBRACDB also writes SOLMOD4:SOVAR values into SOLPU4:SOLCIM, SOLPU4:SOLSIM, SOLTH4:SOLCIM, SOLTH4:SOLSIM, SOLU4:SOLCIM, SOLU4:SOLSIM. Also it sets SOLU6:SOLCIM and SOLU6:SOLSIM to zero. [b] M in Equation 2.

2.4 INVENTORY UPDATE

The EPA requested (Cotsworth 2005) that the waste inventory used for the CRA-2004 PABC is updated to reflect corrections and changes that have occurred while the completeness review of CRA-2004 was being performed. The update to the CRA-2004 inventory was conducted by Los Alamos National Laboratory (LANL) under AP-113, *Analysis Plan For Inventory Reconciliation: Compliance Recertification Application* (Crawford and Leigh 2005). Calculation of the parameters needed for the CRA-2004 PABC PA were conducted by SNL under AP-119, *Analysis Plan For Deriving Radionuclide Inventory Information for Performance Assessment Calculations: Post CRA Performance Assessment Baseline Calculation* (Leigh 2005). Table 5 shows the updated inventory values that are relevant for the PANEL calculations.

Table 5. Updated Radionuclide Inventory Values That Are Relevant to the PANEL Calculations for the CRA-2004 PABC.

Material	Property	CRA-2004 Value	CRA-2004 PABC Value	Units
BOREHOLE	WUF[a]	2.48E+00	2.32E+00	Curies
AM241	INVCHD[b]	4.42E+05	5.01E+05	Curies
AM241	INVRHD[c]	1.58E+04	1.65E+04	Curies
AM241L	INVCHD	4.59E+05	5.15E+05	Curies
AM241L	INVRHD	1.66E+04	1.74E+04	Curies
AM243	INVCHD	2.10E+01	7.75E+01	Curies
AM243	INVRHD	7.42E-01	1.13E+00	Curies
CF252	INVCHD	4.64E-05	3.85E-05	Curies
CF252	INVRHD	3.95E-06	1.98E-05	Curies
CM243	INVCHD	1.82E-01	1.82E-01	Curies
CM243	INVRHD	2.25E-01	2.32E-01	Curies
CM244	INVCHD	3.39E+03	1.81E+03	Curies
CM244	INVRHD	7.94E+01	3.20E+02	Curies
CM245	INVCHD	8.59E-03	6.13E-03	Curies
CM245	INVRHD	1.06E-02	1.10E-02	Curies
CM248	INVCHD	9.14E-02	6.51E-02	Curies
CM248	INVRHD	1.83E-03	9.16E-03	Curies
CS137	INVCHD	4.61E+03	3.52E+03	Curies
CS137	INVRHD	1.74E+05	2.03E+05	Curies
NP237	INVCHD	9.25E+00	1.13E+01	Curies
NP237	INVRHD	8.22E-01	8.32E-01	Curies
PA231	INVCHD	1.21E+00	8.69E-01	Curies
PA231	INVRHD	6.55E-04	8.26E-04	Curies
PB210	INVCHD	4.94E+00	3.59E+00	Curies
PB210	INVRHD	1.42E-05	3.02E-05	Curies
PM147	INVCHD	3.86E-04	3.74E-04	Curies
PM147	INVRHD	7.47E-02	1.30E-01	Curies
PU238	INVCHD	1.25E+06	1.13E+06	Curies
PU238	INVRHD	2.80E+03	2.96E+03	Curies
PU238L	INVCHD	1.25E+06	1.13E+06	Curies
PU238L	INVRHD	2.80E+03	2.96E+03	Curies
PU239	INVCHD	6.59E+05	5.77E+05	Curies
PU239	INVRHD	5.37E+03	5.24E+03	Curies
PU239L	INVCHD	7.66E+05	6.71E+05	Curies
PU239L	INVRHD	7.05E+03	6.83E+03	Curies
PU240	INVCHD	1.07E+05	9.38E+04	Curies
PU240	INVRHD	1.67E+03	1.58E+03	Curies
PU241	INVCHD	5.14E+05	4.20E+05	Curies
PU241	INVRHD	2.39E+04	2.80E+04	Curies

Table 5. Updated Radionuclide Inventory Values That Are Relevant to the PANEL Calculations for the CRA-2004 PABC (continued)

Material	Property	CRA-2004 Value	CRA-2004 PABC Value	Units
PU242	INVCHD	2.66E+01	1.22E+01	Curies
PU242	INVRHD	4.74E-01	4.80E-01	Curies
PU244	INVCHD	1.32E-06	1.26E-06	Curies
PU244	INVRHD	1.10E-03	5.53E-03	Curies
RA226	INVCHD	6.28E+00	4.56E+00	Curies
RA226	INVRHD	4.99E-05	9.34E-05	Curies
RA228	INVCHD	7.63E+00	2.88E+00	Curies
RA228	INVRHD	2.51E-01	1.06E+00	Curies
SR90	INVCHD	2.68E+04	2.62E+04	Curies
SR90	INVRHD	1.15E+05	1.50E+05	Curies
TH229	INVCHD	5.25E+00	4.65E+00	Curies
TH229	INVRHD	1.39E-01	5.64E-01	Curies
TH230	INVCHD	1.69E-01	1.69E-01	Curies
TH230	INVRHD	6.67E-03	1.07E-02	Curies
TH230L	INVCHD	5.42E+00	4.82E+00	Curies
TH230L	INVRHD	1.46E-01	5.75E-01	Curies
TH232	INVCHD	6.61E+00	2.50E+00	Curies
TH232	INVRHD	2.18E-01	9.20E-01	Curies
U233	INVCHD	1.24E+03	1.10E+03	Curies
U233	INVRHD	3.41E+01	1.27E+02	Curies
U234	INVCHD	2.97E+02	3.13E+02	Curies
U234	INVRHD	2.20E+01	3.08E+01	Curies
U234L	INVCHD	1.54E+03	1.41E+03	Curies
U234L	INVRHD	5.61E+01	1.58E+02	Curies
U235	INVCHD	1.34E+00	3.92E+00	Curies
U235	INVRHD	9.42E-01	1.09E+00	Curies
U236	INVCHD	2.31E-01	1.56E+00	Curies
U236	INVRHD	1.42E+00	1.32E+00	Curies
U238	INVCHD	2.44E+01	7.91E+01	Curies
U238	INVRHD	1.30E+02	1.38E+02	Curies

(a) f_w in Equation 10. (b)INVCHD is the inventory in contact-handled (CH) TRU waste. (c)INVRHD is the inventory in remote-handled (RH) TRU waste.

2.5 PANEL IMPLEMENTATION

SNL originated the PANEL code for use in WIPP PA. PANEL version 3.60 was used in the CCA. Subsequently, PANEL was revised to Version 4.00 (Garner 1998a and Garner 1998b) to simplify the PA calculation sequence, and to accommodate a change in the software that maintains the WIPP PAPDB. In preparation for the CRA-2004, PANEL was further revised to Version 4.02 to accommodate an increase in the number of sampled parameters for radionuclide solubilities (Garner 2003a). For the CRA-2004 PABC, PANEL was revised (Garner 2005a) to set the default volume of a panel via MATSET. PANEL 4.03 was validated according to the requirement of NP 19-1 (Garner 2003c) and used in the CRA-2004 PABC calculations.

3. THEORETICAL BASIS FOR PANEL CALCULATIONS

WIPP PA deals with uncertainty in several ways. There is uncertainty in the appropriate value to assign to certain physical properties, like solubility, which is called subjective uncertainty. Subjective uncertainty is dealt with in WIPP PA (and in PANEL) by running multiple realizations in which the values of uncertain parameters are varied. For the WIPP PA, LHS (Vugrin 2005a) is used to create a "replicate" of 100 distinct parameter sets ("vectors") that span the full range of parameter uncertainty. To ensure that these LHS replicates are representative, a total of three replicates are run for a total of 300 separate vectors. Another type of uncertainty is what is called "stochastic" uncertainty, or the uncertainty in what will happen in the future. To deal with this type of uncertainty, WIPP PA employs a Monte Carlo method of sampling on random "futures". A future is defined as one possible sequence of events, or scenario. There are six scenarios defined for WIPP PA (see Table 6). The total number of PANEL simulations that have to be run for a WIPP PA calculation is 300 vectors x 6 scenarios = 1800 PANEL model runs.

Table 6. WIPP PA modeling scenarios

Scenario	Description
S1	Undisturbed Repository
S2	E1 intrusion at 350 years
S3	E1 intrusion at 1000 years
S4	E2 intrusion at 350 years
S5	E2 intrusion at 1000 years
S6	E2 intrusion at 1000 years; E1 intrusion at 2000 years.

E1: Borehole penetrates through the repository and into a hypothetical pressurized brine reservoir in the Castile Formation. E2: Borehole penetrates the repository, but does not encounter brine in the Castile. (Nemer and Stein 2005)

In WIPP PA scenarios, brine is assumed to enter the repository panels in either of two very different ways, namely: (a) by natural seepage from the surrounding Salado formation, and (b) by various locally-enhanced flows induced by hypothetical exploratory boreholes. In the case of the undisturbed scenario (S1), Salado brine can seep through the disturbed rock zone from the surrounding undisturbed halite and marker beds. In the case of a repository breached by an exploratory borehole (S2-S5), Castile and/or Culebra brine could flow into and through the repository via the pipe-like channels created by the borehole(s). An E1 intrusion assumes that a borehole passes through the repository and encounters a brine pocket in the Castile; an E2 intrusion is a borehole that does not encounter a brine pocket. The most intense flow (of Castile brine) would occur if a borehole that penetrates a waste panel also penetrates a deep pressurized brine pocket. The S6 scenario assumes that both an E1 and an E2 intrusion occur in the same waste panel. In this scenario, brine can flow from the Castile, through the waste in the panel, and then continue up an earlier, open borehole to the Culebra (Nemer and Stein 2005).

PANEL's PA role is to estimate the mobilized radioactive contaminant load in the brine phase of the brine/gas mixture that seeps or flows through the repository's waste panels. Mobilization by any process, for example dissolution or suspension on colloids, is modeled as taking place

instantaneously. The contaminants introduced into the brine are the aged radioisotopes that are assumed to reside in the repository at the time of closure plus any progeny of those radioisotopes that may have been produced through radioactive decay.

For WIPP PA, PANEL calculates: 1) decay and production over time for specified radionuclides, 2) concentrations of mobilized radionuclides, and 3) radionuclide quantities up the borehole to the Culebra for the S6 scenario. For each of these functions, an individual PANEL run is made. Thus, PANEL has three types of runs, the DECAY run type, the CONCENTRATION run type, and the STANDARD run type.

The following is a brief overview of the conceptual models implemented in PANEL for each of these run types. The conceptual models implemented in PANEL for the CRA-2004 PABC are unchanged from those used in the CCA, the PAVT, and CRA-2004.

3.1 RADIOACTIVE DECAY

The natural time scales associated with deep, tight-media, groundwater flows are typically centuries, and WIPP intrusion scenarios include temporal lapses of millennia prior to the hypothesized breaching of repository waste panels by boreholes. Moreover, EPA regulations extend to 10,000 years after decommissioning. On these time scales, radioisotopes of interest exhibit significant natural decay by which they transform to other radioactive and non-radioactive isotopes and/or compounds in a well-established way (Kaplan 1964). Thus, it is required to quantify the decay process and maintain a running record of the decayed contents of the repository as well as all the products of decay from the time of closure onward to 10,000 years.

This is performed in PANEL for all three run types: DECAY, CONCENTRATION, or STANDARD. If the user wishes to obtain an output file with the decayed values, the DECAY run type has to be used. The DECAY run type decays the radionuclide inventory for 10,000 years and outputs the results.

The equations that quantify the decay-and-growth cycle of isotopes were first described by Bateman (1910) and traditionally bear his name. Bateman's equations state that the rate at which the mass of a radioisotope decreases by natural radioactive decay is proportional to the present available mass of that radioisotope. In single decays, the constant of proportionality is the natural logarithm of 2 divided by the half-life of the isotope in question. If the isotope in question is other than the first isotope in the chain, its mass will also increase at a rate proportional to the present mass of its parent isotope. In simple decay chains, the constant of proportionality is the natural logarithm of 2 divided by the half-life of the parent. In multiple (i.e., bifurcated) chains, the decay algebra is slightly more complicated. However, the simple decay chains used in WIPP PAs have no bifurcations. The formulation and solution for Bateman's equations in PANEL are given in Section 4.4 of the PANEL User's Manual (Garner 2003b).

PANEL solves the Bateman equations at each time step (50 year time steps). In addition to the radionuclide inventory that is an input for this calculation (shown in Table 6), PANEL needs the atomic weight and half-life of the radionuclides. These values are shown in Table 7 and have not

changed since the CCA. In the DECAY mode, PANEL decays those radionuclides shown in Table 7.

Table 7. Atomic Weights and Radionuclide Half-lives for CRA-2004 PABC

Material	Property	CRA-2004 PABC Value	Units	Material	Property	CRA-2004 PABC Value	Units
AM241	ATWEIGH	2.41E-01	kg/mole	PU240	ATWEIGH	2.40E-01	kg/mole
AM241	HALFLIFE	1.36E+10	s	PU240	HALFLIFE	2.06E+11	s
AM243	ATWEIGH	2.43E-01	kg/mole	PU241	ATWEIGH	2.41E-01	kg/mole
AM243	HALFLIFE	2.33E+11	s	PU241	HALFLIFE	4.54E+08	s
CF252	ATWEIGH	2.52E-01	kg/mole	PU242	ATWEIGH	2.42E-01	kg/mole
CF252	HALFLIFE	8.33E+07	s	PU242	HALFLIFE	1.22E+13	s
CM243	ATWEIGH	2.43E-01	kg/mole	PU244	ATWEIGH	2.44E-01	kg/mole
CM243	HALFLIFE	8.99E+08	s	PU244	HALFLIFE	2.61E+15	s
CM244	ATWEIGH	2.44E-01	kg/mole	RA226	ATWEIGH	2.26E-01	kg/mole
CM244	HALFLIFE	5.72E+08	s	RA226	HALFLIFE	5.05E+10	s
CM245	ATWEIGH	2.45E-01	kg/mole	RA228	ATWEIGH	2.28E-01	kg/mole
CM245	HALFLIFE	2.68E+11	s	RA228	HALFLIFE	2.11E+08	s
CM248	ATWEIGH	2.48E-01	kg/mole	SR90	ATWEIGH	8.99E-02	kg/mole
CM248	HALFLIFE	1.07E+13	s	SR90	HALFLIFE	9.19E+08	s
CS137	ATWEIGH	1.37E-01	kg/mole	TH229	ATWEIGH	2.29E-01	kg/mole
CS137	HALFLIFE	9.47E+08	s	TH229	HALFLIFE	2.32E+11	s
NP237	ATWEIGH	2.37E-01	kg/mole	TH230	ATWEIGH	2.30E-01	kg/mole
NP237	HALFLIFE	6.75E+13	s	TH230	HALFLIFE	2.43E+12	s
PA231	ATWEIGH	2.31E-01	kg/mole	TH232	ATWEIGH	2.32E-01	kg/mole
PA231	HALFLIFE	1.03E+12	s	TH232	HALFLIFE	4.43E+17	s
PB210	ATWEIGH	2.10E-01	kg/mole	U233	ATWEIGH	2.33E-01	kg/mole
PB210	HALFLIFE	7.04E+08	s	U233	HALFLIFE	5.00E+12	s
PM147	ATWEIGH	1.47E-01	kg/mole	U234	ATWEIGH	2.34E-01	kg/mole
PM147	HALFLIFE	8.28E+07	s	U234	HALFLIFE	7.72E+12	s
PU238	ATWEIGH	2.38E-01	kg/mole	U235	ATWEIGH	2.35E-01	kg/mole
PU238	HALFLIFE	2.77E+09	s	U235	HALFLIFE	2.22E+16	s
PU239	ATWEIGH	2.39E-01	kg/mole	U236	ATWEIGH	2.36E-01	kg/mole
PU239	HALFLIFE	7.59E+11	s	U236	HALFLIFE	7.39E+14	s
U238	HALFLIFE	1.41E+17	s	U238	ATWEIGH	2.38E-01	kg/mole

3.2 POTENTIAL FOR DISSOLUTION AND MOBILIZATION

PANEL calculates what is in essence the potential for dissolution and mobilization of an actinide in a brine. It is called a potential here because it is basically the limit on how much material can be dissolved and/or mobilized in a brine if the inventory of the material is unlimited. This

potential would be equal to the solubility in the absence of colloids. In the presence of colloids, the potential includes dissolved species and mobilized colloidal species. Like solubility, the units for the mobilization potential is moles/liter.
The dissolved component of the mobilization potential is calculated using Equation 2 from Section 2.3. The base solubility value, $\left(s_{brine}^{red/ox}\right)$, is one of the values from Table 2, depending on the oxidation state of the actinide and the brine type for the vector. Since microbial activity is present for all vectors in the CRA-2004 PABC, the buffer is brucite/hydromagnesite (U.S. DOE 2004 Appendix BARRIERS, Subsection BARRIERS-2.3.2.3.). The variable, *M*, is sampled from one of the distributions shown in Table 4 depending on the oxidation state of the actinide.

Once the dissolution potential is known, the colloidal mobilization potentials are determined by means of proportionality factors or by constants. The mobilization potential for humic colloids is calculated using Equation 3 (U.S. DOE 2004 Appendix SOTERM).

$$H_{brine}^{red/ox} = \begin{cases} \left(S_{brine}^{red/ox}\right) \bullet \left(h_{brine}^{red/ox}\right) & if \left(S_{brine}^{red/ox}\right) \bullet \left(h_{brine}^{red/ox}\right) \le \left(H_{elem}^{\max}\right) \\ \left(H_{elem}^{\max}\right) & if \left(S_{brine}^{red/ox}\right) \bullet \left(h_{brine}^{red/ox}\right) > \left(H_{elem}^{\max}\right) \end{cases} \quad (3)$$

$H_{brine}^{red/ox}$ is the mobilization potential for humic colloids. $\left(S_{brine}^{red/ox}\right)$ is defined in Equation 2. $\left(h_{brine}^{red/ox}\right)$ is a factor for humic colloids that is defined for each oxidation state and brine type as shown in Table 8. $\left(H_{elem}^{\max}\right)$ is the maximum allowed for mobilized humic colloids for the element (also shown in Table 8). None of the values in Table 8 were updated for the CRA-2004 PABC.

The mobilization potential for mineral fragment colloids is as shown in Equation 4.

$$MF_{brine}^{red/ox} = \left(mf_{brine}^{red/ox}\right) \quad (4)$$

$MF_{brine}^{red/ox}$ is the mobilization potential for mineral fragment colloids. $\left(mf_{brine}^{red/ox}\right)$ is a constant value for each element that is independent of brine type as shown in Table 9. None of the values in Table 9 were updated for the CRA-2004 PABC.

The mobilization potential for intrinsic colloids is as shown in Equation 5.

$$IC_{brine}^{red/ox} = \left(ic_{brine}^{red/ox}\right) \quad (5)$$

$IC_{brine}^{red/ox}$ is the mobilization potential for intrinsic colloids. $\left(ic_{brine}^{red/ox}\right)$ is a constant value for each element that is independent of brine of type as shown in Table 10. None of the values in Table 10 were updated for the CRA-2004 PABC.

The mobilization potential for microbial colloids is zero if there is no microbial activity. However all vectors have microbial activity in the CRA-2004 PABC. The mobilization potential for microbial colloids is calculated using Equation 6.

Table 8. Parameters related to humic colloids for the CRA-2004 PABC

Material	Property	Description	CRA-2004 PABC Value	Units
PHUMOX3	PHUMCIM(b)	Multiplicative factor to calculate humic colloids for actinides in the +III oxidation state in Castile brine	(a)Cumulative Distribution 1.37E+00	NONE
PHUMOX3	PHUMSIM(b)	Multiplicative factor to calculate humic colloids for actinides in the +III oxidation state in Salado brine	1.90E-01	NONE
PHUMOX4	PHUMCIM(b)	Multiplicative factor to calculate humic colloids for actinides in the +IV oxidation state in Castile brine	6.30E+00	NONE
PHUMOX4	PHUMSIM(b)	Multiplicative factor to calculate humic colloids for actinides in the +IV oxidation state in Salado brine	6.30E+00	NONE
PHUMOX5	PHUMCIM(b)	Multiplicative factor to calculate humic colloids for actinides in the +V oxidation state in Castile brine	7.40E-03	NONE
PHUMOX5	PHUMSIM(b)	Multiplicative factor to calculate humic colloids for actinides in the +V oxidation state in Salado brine	9.10E-04	NONE
PHUMOX6	PHUMCIM(b)	Multiplicative factor to calculate humic colloids for actinides in the +VI oxidation state in Castile brine	5.10E-01	NONE
PHUMOX6	PHUMSIM(b)	Multiplicative factor to calculate humic colloids for actinides in the +VI oxidation state in Salado brine	1.20E-01	NONE
AM	CAPHUM(c)	Maximum concentration for humic colloids for Am	1.10E-05	moles/liter
NP	CAPHUM(c)	Maximum concentration for humic colloids for Np	1.10E-05	moles/liter
PU	CAPHUM(c)	Maximum concentration for humic colloids for Pu	1.10E-05	moles/liter
TH	CAPHUM(c)	Maximum concentration for humic colloids for Th	1.10E-05	moles/liter
U	CAPHUM(c)	Maximum concentration for humic colloids for U	1.10E-05	moles/liter

(a) For a cumulative distribution, the distribution is represented in the WIPP PAPDB with a single value that is the median value. The reader can reference Tierny (1996) for the conversion to the cumulative distribution.

(b)Corresponds to $\left(h_{brine}^{red/ox}\right)$ in Equation 3. (c)Corresponds to $\left(H_{elem}^{\max}\right)$ in Equation 3.

Table 9. Parameters related to mineral fragment colloids for the CRA-2004 PABC

Material	Property	Description	CRA-2004 PABC Value	Units
AM	CONCMIN[a]	Concentration for mineral colloids for Am	2.60E-08	moles/liter
NP	CONCMIN	Concentration for mineral colloids for Np	2.60E-08	moles/liter
PU	CONCMIN	Concentration for mineral colloids for Pu	2.60E-08	moles/liter
TH	CONCMIN	Concentration for mineral colloids for Th	2.60E-08	moles/liter
U	CONCMIN	Concentration for mineral colloids for U	2.60E-08	moles/liter

[a]Corresponds to $\left(mf_{brine}^{red/ox}\right)$ in Equation 4.

Table 10. Parameters related to intrinsic colloids for the CRA-2004 PABC

Material	Property	Description	CRA-2004 PABC Value	Units
AM	CONCINT[a]	Concentration for intrinsic colloids for Am	0.00E+00	moles/liter
NP	CONCINT	Concentration for intrinsic colloids for Np	0.00E+00	moles/liter
PU	CONCINT	Concentration for intrinsic colloids for Pu	1.00E-09	moles/liter
TH	CONCINT	Concentration for intrinsic colloids for Th	0.00E+00	moles/liter
U	CONCINT	Concentration for intrinsic colloids for U	0.00E+00	moles/liter

[a]Corresponds to $\left(ic_{brine}^{red/ox}\right)$ in Equation 5.

Table 11. Parameters related to microbial colloids for the CRA-2004 PABC

Material	Property	Description	CRA-2004 PABC Value	Units
AM	PROPMIC[a]	Multiplicative factor to calculate microbial colloids for Am	3.60E+00	NONE
NP	PROPMIC	Multiplicative factor to calculate microbial colloids for Np	1.20E+01	NONE
TH	PROPMIC	Multiplicative factor to calculate microbial colloids for Th	3.10E+00	NONE
PU	PROPMIC	Multiplicative factor to calculate microbial colloids for Pu	3.00E-01	NONE
U	PROPMIC	Multiplicative factor to calculate microbial colloids for U	2.10E-03	NONE
AM	CAPMIC[b]	Maximum concentration for microbial colloids for Am	1.00E+00	moles/liter
NP	CAPMIC	Maximum concentration for microbial colloids for Np	2.70E-03	moles/liter
PU	CAPMIC	Maximum concentration for microbial colloids for Pu	6.80E-05	moles/liter
TH	CAPMIC	Maximum concentration for microbial colloids for Th	1.90E-03	moles/liter
U	CAPMIC	Maximum concentration for microbial colloids for U	2.10E-03	moles/liter

[a]Corresponds to $\left(mc_{brine}^{red/ox}\right)$ in Equation 6. [b]Corresponds to $\left(MC_{elem}^{\max}\right)$ in Equation 6.

$$MC_{brine}^{red/ox} = \begin{cases} \left(S_{brine}^{red/ox}\right)\bullet\left(mc_{brine}^{red/ox}\right) & if \left(S_{brine}^{red/ox}\right)+\left(H_{brine}^{red/ox}\right)+\left(MF_{brine}^{red/ox}\right)+\left(IC_{brine}^{red/ox}\right)+\left(S_{brine}^{red/ox}\right)\bullet\left(mc_{brine}^{red/ox}\right) < \left(MC_{elem}^{\max}\right) \\ 0 & if \left(S_{brine}^{red/ox}\right)+\left(H_{brine}^{red/ox}\right)+\left(MF_{brine}^{red/ox}\right)+\left(IC_{brine}^{red/ox}\right) > \left(MC_{elem}^{\max}\right) \\ \left(MC_{elem}^{\max}\right)-\left(S_{brine}^{red/ox}\right)-\left(H_{brine}^{red/ox}\right)-\left(MF_{brine}^{red/ox}\right)-\left(IC_{brine}^{red/ox}\right) & \end{cases} \quad (6)$$

$$if \begin{cases} \left(S_{brine}^{red/ox}\right)+\left(H_{brine}^{red/ox}\right)+\left(MF_{brine}^{red/ox}\right)+\left(IC_{brine}^{red/ox}\right) < \left(MC_{elem}^{\max}\right) \\ and \\ \left(S_{brine}^{red/ox}\right)+\left(H_{brine}^{red/ox}\right)+\left(MF_{brine}^{red/ox}\right)+\left(IC_{brine}^{red/ox}\right)+\left(S_{brine}^{red/ox}\right)\bullet\left(mc_{brine}^{red/ox}\right) > \left(MC_{elem}^{\max}\right) \end{cases}$$

$MC_{brine}^{red/ox}$ is the mobilization potential for microbial colloids. $\left(S_{brine}^{red/ox}\right)$ is defined in Equation 2. $\left(H_{brine}^{red/ox}\right)$ is defined in Equation 3. $\left(MF_{brine}^{red/ox}\right)$ is defined in Equation 4. $\left(IC_{brine}^{red/ox}\right)$ is defined in Equation 5. $\left(mc_{brine}^{red/ox}\right)$ is a factor for microbial colloids that is defined for each element independent of brine type as shown in Table 11. $\left(MC_{elem}^{\max}\right)$ is a value that limits the amount of microbial colloids that can be mobilized in the presence of other mobilization processes. The values for $\left(MC_{elem}^{\max}\right)$ are shown in Table 11. None of the values in Table 11 were updated for the CRA-2004 PABC.

The total mobilization potential is the sum of the dissolution potential and the mobilization potentials for the four colloids as shown in Equation 7.

$$TC_{brine}^{red/ox} = \left(S_{brine}^{red/ox}\right)+\left(H_{brine}^{red/ox}\right)+\left(MC_{brine}^{red/ox}\right)+\left(MF_{brine}^{red/ox}\right)+\left(IC_{brine}^{red/ox}\right) \quad (7)$$

$TC_{brine}^{red/ox}$ is the total mobilization potential.

3.3 MOBILIZED RADIONUCLIDE CONCENTRATIONS

PANEL computes the concentration of radionuclides mobilized in a panel that contains a given volume of brine. This is performed in PANEL using the CONCENTRATION run type. The total mobilized concentration consists of a dissolved component and up to four colloidal components: humic, microbial, intrinsic, and mineral fragment colloids.

The dissolution part of PANEL's waste-mobilization-and-transport model is based on the following assumptions: (1) The concentration of each brine-dissolved element is uniform (i.e., constant) throughout a waste panel. (2) Mobilization is assumed to take place instantaneously and to maximum capacity, i.e., to saturation if inventory permits. (3) Supersaturation is disallowed. (4) When an element has several isotopes, the molar proportions of those isotopes dissolved in the brine are taken to be the same as the molar proportions in the total inventory contained in the waste panel, and (5) the fraction of the inventory in the panel is 0.1044. The value .1044 is the ratio of the area of one of the outside panels to the area of all ten panels (Lappin et al. 1989).

The concentration is given in Equation 8.

$$C_{brine}^{isotope} = \min\left\{\frac{\sum_i N^{isotope}}{V_{brine}}, TC_{brine}^{red/ox}\right\} \bullet \left\{\frac{N^{isotope}}{\sum_i N^{isotope}}\right\} \quad (8)$$

Where $C_{brine}^{isotope}$ is the concentration in moles/liter for the isotope. $N^{isotope}$ is the total moles of the isotope in the inventory, $\sum_i N^{isotope}$ is the sum of all isotopes of the element that contains the isotope of interest, and V_{brine} is the volume of brine in contact with the inventory. For the mobilized radionuclide concentration calculations, the brine volume, V_{brine}, is a constant value based on Stein (2005). The value derived in Stein (2005) is the minimum volume of brine required for a Direct Brine Release (DBR). The minimum volume is used because it leads to the highest value for $C_{brine}^{isotope}$. Converting to activity,

$$a_{brine}^{isotope} = C_{brine}^{isotope} \bullet MW^{isotope} \bullet SP^{isotope} \quad (9)$$

Where $a_{brine}^{isotope}$ is the activity concentration in Ci/liter for the isotope. $C_{brine}^{isotope}$ is defined in Equation 8. $MW^{isotope}$ is the molecular weight of the isotope in g/mole, and $SP^{isotope}$ is the specific activity of the isotope in Ci/g.

The EPA units are defined using Equation 10.

$$W^{isotope} = \frac{\left(a_{brine}^{isotope}\right)}{L_{isotope} \bullet f_w} \quad (10)$$

Where $W^{isotope}$ is the activity concentration in EPA Units/liter for the isotope. $L_{isotope}$ is the EPA release limit for the isotope (shown in Table 12), and f_w is the waste unit factor (shown in Table 6, defined in Leigh and Trone 2005b). None of the values in Table 12 were updated for the CRA-2004 PABC.

Table 12. Parameters related to calculation of total mobilized EPA units in PANEL.

Material	Property	CRA-2004 Value	CRA-2004 PABC Value	Units
AM241	EPAREL	1.00E+02	1.00E+02	Curies/wuf
AM243	EPAREL	1.00E+02	1.00E+02	Curies/wuf
CF252	EPAREL	0.00E+00	0.00E+00	Curies/wuf
CM243	EPAREL	1.00E+02	1.00E+02	Curies/wuf
CM244	EPAREL	0.00E+00	0.00E+00	Curies/wuf
CM245	EPAREL	1.00E+02	1.00E+02	Curies/wuf
CM248	EPAREL	1.00E+02	1.00E+02	Curies/wuf
CS137	EPAREL	1.00E+03	1.00E+03	Curies/wuf
NP237	EPAREL	1.00E+02	1.00E+02	Curies/wuf
PA231	EPAREL	1.00E+02	1.00E+02	Curies/wuf
PB210	EPAREL	1.00E+02	1.00E+02	Curies/wuf
PM147	EPAREL	0.00E+00	0.00E+00	Curies/wuf
PU238	EPAREL	1.00E+02	1.00E+02	Curies/wuf
PU239	EPAREL	1.00E+02	1.00E+02	Curies/wuf
PU240	EPAREL	1.00E+02	1.00E+02	Curies/wuf
PU241	EPAREL	0.00E+00	0.00E+00	Curies/wuf
PU242	EPAREL	1.00E+02	1.00E+02	Curies/wuf
PU244	EPAREL	1.00E+02	1.00E+02	Curies/wuf
RA226	EPAREL	1.00E+02	1.00E+02	Curies/wuf
RA228	EPAREL	0.00E+00	0.00E+00	Curies/wuf
SR90	EPAREL	1.00E+03	1.00E+03	Curies/wuf
TH229	EPAREL	1.00E+02	1.00E+02	Curies/wuf
TH230	EPAREL	1.00E+01	1.00E+01	Curies/wuf
TH232	EPAREL	1.00E+01	1.00E+01	Curies/wuf
U233	EPAREL	1.00E+02	1.00E+02	Curies/wuf
U234	EPAREL	1.00E+02	1.00E+02	Curies/wuf
U235	EPAREL	1.00E+02	1.00E+02	Curies/wuf
U236	EPAREL	1.00E+02	1.00E+02	Curies/wuf
U238	EPAREL	1.00E+02	1.00E+02	Curies/wuf

PANEL solves Equations 8 through 10 at each time step (50 year time steps). The formulation and solution for Equations 8 through 10 in PANEL are given in Section 4.3 of the PANEL User's Manual (Garner 2003b). Mobilized radionuclide concentrations are calculated for the 23 individual radionuclides and five "lumped" radionuclides shown in Table 13. The "lumped" radionuclides are defined as (Leigh and Trone 2005a):

AM241L is the amount of AM241 plus the amount of PU241.
PU238L is the same amount as PU238.
PU239L is the amount of PU239 plus the amount of PU240 plus the amount of PU242.
U234L is the amount of U234 plus the amount of U233.
TH230L is the amount of TH230 plus the amount of TH229.

"Lumped" radionuclides are used to ease the burden associated with calculation of radionuclide transport in some of the WIPP PA codes: NUTS (Leigh 2003) which calculates Salado transport and CCDFGF (Vugrin 2004) which calculates Culebra releases.

Table 13: Radionuclides Modeled in PANEL Concentration Calculations

Individual Radionuclides				
Am-241	Cm-245	Pm-147	Pu-244	Th-232
Am-243	Cm-248	Pu-238	**Ra-226**	U-233
Cf-252[a]	Cs-137	Pu-239	**Ra-228**	U-234
Cm-243	Np-237	Pu-240	Sr-90	U-235
Cm-244	**Pa-231**	Pu-241	Th-229	U-236
Sm-147	**Pb-210**	Pu-242	Th-230	U-238
Lumped Radionuclides				
AM241L	PU238L	TH230L	U234L	PU239L

[a]The isotopes shown in bold are included in the decay calculations but are not included in the mobilization calculations.

PANEL supplies information from the CONCENTRATION run to NUTS and CCDFGF. For NUTS the values supplied by PANEL are defined in Equation 11.

$$\left\{TC_{brine}^{red/ox}\right\}_{NUTS} = TC_{brine}^{red/ox} \bullet 10^{-L_{dif}^{sol}} \quad (11)$$

Where $\left\{TC_{brine}^{red/ox}\right\}_{NUTS}$ is the potential moles per liter mobilized for the lumped isotopes in Table 13. L_{dif}^{sol} is a multiplicative factor used to account for molar proportions of isotopes in the inventory. The multiplicative factors are set in MATSET through the parameters, PU238L:LSOLDIF, TH230L:LSOLDIF, U234L:LSOLDIF. Calculation of these values is discussed in Appendix A.

The total concentration in EPA units for the 23 individual radionuclides is used by CCDFGF to calculate DBR. For the calculation of DBR in CCDFGF, the values supplied by PANEL are defined in Equation 12.

$$W^{total} = \sum_{isotopes} W^{isotope} \quad (12)$$

W^{total} is the total EPA units per liter for the 23 individual isotopes in Table 13. For the calculation of Culebra releases (S1-S5) in CCDFGF, the values supplied by PANEL are defined by Equation 13.

$$W^{total}_{lumped} = \sum_{lumped} W^{isotope} \quad (13)$$

W^{total}_{lumped} is the total EPA Units per liter for the lumped isotopes in Table 13.

3.4 RADIONUCLIDES UP THE BOREHOLE TO THE CULEBRA (S6)

PANEL also computes the quantities of "lumped" radionuclides that move up the borehole to the Culebra for the S6 scenario. This is performed in PANEL using the STANDARD run type.

The PANEL calculation for S6 is similar to that discussed in Section 3.3 except that the panel brine volume and the brine flow volumes are supplied by BRAGFLO (Stein 2003a). PANEL conservatively assumes that any radionuclide that rises above the disturbed rock zone above the waste panels reaches the Culebra. The formulation and solution for this calculation in PANEL are given in Section 4.5 of the PANEL User's Manual (Garner 2003b).

4. PANEL MODELING PROCESS

Digital Command Language (DCL) scripts, referred to here as EVAL run scripts, are used to implement and document the running of all software codes for the WIPP PA. These scripts, which are the basis for the WIPP PA run control system, are stored in the CRA1BC_EVAL Configuration Management System (CMS) library. All inputs are fetched at run time by the scripts, and outputs and run logs are automatically stored by the scripts in class CRA1BC-0 of the CMS libraries (Long and Kanney 2005).

Figure 1 (left hand side) shows the run sequence for PANEL. For the CRA-2004 PABC, PANEL was run in the DECAY mode to produce decayed radionuclide inventories. This run is independent of scenario and only needs to be run once. This run is discussed further in Appendix A.

PANEL was also run in the CONCENTRATION mode for Scenarios S1 through S5. This is represented on the left-hand-side of Figure 1 where GENMESH (Stein 2003c) provides input to MATSET (Gilkey 2003b). MATSET provides input to POSTLHS (Vugrin 2005b), and POSTLHS provides input to ALGEBRACDB (Gilkey 2003a). Output from ALGEBRACDB is input to PANEL.

PANEL was also run in the STANDARD mode for Scenario S6. This is represented by the entirety of Figure 1 where the output from ALGEBRACDB on the left-hand-side of the figure is input to PANEL and the output from POSTBRAG (Stein 2003b) and ALGEBRACDB is also input to PANEL. The software version numbers used for the PANEL calculations for the CRA-2004 PABC are given in Table 14.

Table 14. Software Version Numbers Used for PANEL Calculations for the CRA-2004 PABC

Software Application	Version
GENMESH	6.08
MATSET	9.00
POSTLHS	4.07
ALGEBRACDB	2.35
SUMMARIZE	2.20
SPLAT	1.02
STEPWISE	2.21

4.1.1 GENMESH: Single-Element Grid Generation

The first step in the PANEL modeling process is the definition of a single-element grid (one block) using the GENMESH code (Stein 2003c). The analyst supplies input for GENMESH in an ASCII input file. The CRA-2004 PABC analysis uses the file: GM_PANEL_CRA1BC.INP (see Appendix B) located in CMS library: CRA1BC_PANEL.

4.1.2 MATSET: *Material Property Assignments*

Details of the functionality of MATSET are discussed in the users manual (Gilkey 2003b). MATSET assigns the material property values needed by PANEL. The GENMESH binary output file (GM_PANEL_CRA1BC.CDB), which is required as input for the MATSET code, provides the initial material map. All materials and properties that are used in PANEL modeling should be specified in this modeling step, although the values may be changed in subsequent steps. For example, the parameters that are assigned sampled values by the LHS code (Vugrin 2005a), must be assigned initial values by MATSET in order that they can be reassigned in later steps.

Each property assignment requires specification of both the material (e.g. Pu) and the property (e.g. maximum concentration for microbial colloids for Pu) to be associated with that material. For PA analyses, MATSET extracts the information from the WIPP PAPDB according to instructions in the user-supplied input control file. If the database contains information defining a distribution of values for a material/property pair, MATSET retrieves the median value. The MATSET input file used for the CRA-2004 PABC is MS_PANEL_CRA1BC.INP (see Appendix B) and is located in the CMS library: CRA1BC_PANEL.

4.1.3 POSTLHS: Uncertain Parameter Values

The third step in the run sequence employs the POSTLHS code, which takes the binary output from MATSET (MS_PANEL_CRA1BC.CDB) and creates 100 copies of this file replacing median values with the sampled values for every sampled parameter in each vector. The sampled parameters for PANEL are: GLOBAL:OXSTAT, PHUMOX3:PHUMCIM, SOLMOD3:SOLVAR, SOLMOD4:SOLVAR, and WAS_AREA:PROBDEG. POSTLHS requires that a dummy ASCII file be specified, which is not used in the calculations. The dummy file used for the CRA-2004 PABC is LHS3_DUMMY.INP (see Appendix B) and is located in CMS library: LIBCRA1BC_LHS. Output from LHS (LHS2_PANEL_CRA1BC_R1.TRN, LHS2_PANEL_CRA1BC_R2.TRN, LHS2_PANEL_CRA1BC_R3.TRN for the three replicates) are also used by POSTLHS in this step. These files are stored in CMS library: CRA1BC_LHS.

4.1.4 ALGEBRACDB: Data Modification

The next modeling step employs the ALGEBRACDB code which is used to manipulate data from the binary output files from POSTLHS. ALGEBRACDB is capable of performing most common algebraic manipulations and evaluating most common transcendental functions (trigonometric, logarithmic, exponential, etc.). Its functionality is discussed in the users manual (Gilkey 2003a).

ALGEBRACDB reads its instructions from a user-supplied ASCII input file that employs an algebraic syntax that is similar in appearance to FORTRAN syntax. The ALGEBRACDB input file used for this step in the CRA-2004 PABC is ALG_PANEL_CRA1BC.INP (see Appendix B) and is located in CMS library: LIBCRA1BC_PANEL. It executes the mathematical instructions to modify the output data from POSTLHS:

- LHS3_PANEL_CRA1BC_R1_V001.CDB - LHS3_PANEL_CRA1BC_R1_V100.CDB;
- LHS3_PANEL_CRA1BC_R2_V001.CDB - LHS3_PANEL_CRA1BC_R2_V100.CDB; and
- LHS3_PANEL_CRA1BC_R3_V001.CDB - LHS3_PANEL_CRA1BC_R3_V100.CDB

which are stored in the CMS library: CRA1BC_PANEL.

The results are written to new binary (.CDB) output files:

- ALG_PANEL_CRA1BC_R1_V001.CDB - ALG_PANEL_CRA1BC_R1_V100.CDB;
- ALG_PANEL_CRA1BC_R2_V001.CDB - ALG_PANEL_CRA1BC_R2_V100.CDB; and
- ALG_PANEL_CRA1BC_R3_V001.CDB - ALG_PANEL_CRA1BC_R3_V100.CDB

Which are stored in the CMS library: CRA1BC_PANEL.

4.1.5 BRAGFLO Output to PANEL

As mentioned above, for the S6 scenario, PANEL requires BRAGFLO results (right-hand-side of Figure 1). The required PANEL input for the S6 scenario is generated by the BRAGFLO run and is stored in the files ALG2_BF_CRA1BC_R1_S6_V001.CDB through ALB2_BF_CRA1BC_R3_S6_V100.CDB which are stored in the CMS library: CRA1BC_BF.

4.1.6 SUMMARIZE and SPLAT

The SUMMARIZE code (Baker 2003c) is used to extract data from the binary output files (.CDB) from PANEL 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. In this case, SUMMARIZE will linearly interpolate output values at specific times from the nearest times included in the binary file. SUMMARIZE can take input from many vectors and combine it into a single table file.

Tables from SUMMARIZE are used to make horsetail 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). These plots are generated using the SPLAT code (Baker 2003b).

Output from SUMMARIZE is also entered into the WIPP Parameter Output Database (WIPP POD) (Tisinger 2002) where it is accessible to perform queries and analysis. Data from SUMMARIZE and from the WIPP POD is also exported to external "off the shelf" graphical software on the Personal Computer (PC) to generate figures that demonstrate various analytical observations and conclusions.

4.1.7 Sensitivity Analysis

Several approaches are used in this analysis to evaluate the effects of sampled input parameters on BRAGFLO results. The simplest method is to use scatter plots to visually evaluate relationships of an output variable with a single input parameter (or another output variable).

The other sensitivity tool used in this analysis is the STEPWISE code (Baker 2003a). STEPWISE performs a stepwise linear regression analysis. The linear regression analysis is looking to identify which uncertain input variables are most responsible for producing uncertainty in the output.

Used for DECAY and CONCENTRATION runs.

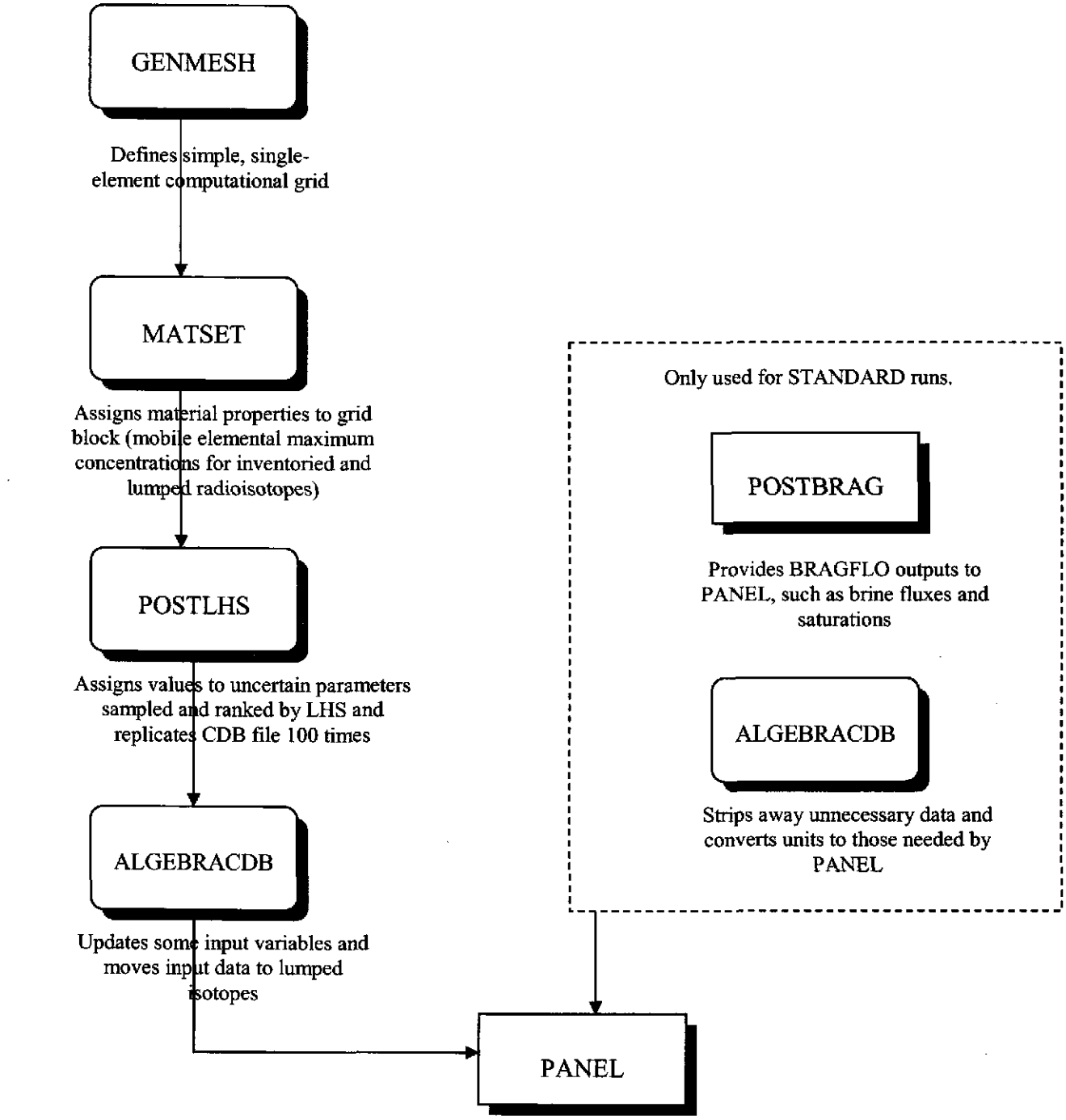


Figure 1. The run sequence for PANEL in the CRA-2004 PABC. Process codes are square and support codes are rounded.

5. PANEL RESULTS

PANEL is unique in the performance assessment 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. In addition, PANEL is frequently used in a stand-alone mode to calculate radionuclide decay.

NUTS needs information for the "lumped" radionuclides AM241L, PU238L, PU239L, U234L, and TH230L. CCDFGF (for DBR releases) needs the mobilized radionuclide concentrations in brine (Salado and/or Castile brine) reported as the sum of the EPA units for the 23 isotopes listed in Table 13 (the non-bold isotopes in Table 13). CCDFGF (for Culebra releases in the S6 scenario) needs the EPA units of the "lumped" radionuclides AM241L, PU238L, PU239L, U234L, and TH230L up the borehole to the Culebra.

PANEL is run in the CONCENTRATION mode for Scenarios S1, S2, S3, S4, and S5. The concentrations for S1, S4, and S5 are all equivalent (as they all involve Salado brine), as are the concentrations for S2 and S3 (Castile brine). The concentration data for S1 (Salado brine) and S2 (Castile brine) are used together with DBR volumes to obtain radionuclide releases through the DBR pathway in CCDFGF. PANEL is run in the STANDARD mode for S6.

Calculation of the mobilized concentration is basically a three step process that starts with calculation of the potential for a particular brine to contain both dissolved and mobilized colloidal components of an element. If colloidal components were not involved (an element with only a dissolved component), this potential would be the solubility of the element in the brine. When colloidal components are involved, the potential has been referred to in previous PANEL documents as the "source term" for an element. The "source term" corresponds to the moles of an element that can be mobilized in a liter of brine (either through dissolution and/or colloidal suspension) if the inventory of the element is unlimited. It loosely corresponds to what is known in other chemical applications as the saturation state.

Once the potential that a particular brine has to contain dissolved and mobilized colloidal components of an element has been established, then the inventory of the element that is available for mobilization is required. If there is more material available for mobilization than the brine can hold, the concentration in the brine will be equivalent to "saturation." If there is less material available for mobilization than the brine can hold, the concentration in the brine will be equivalent to the inventory value divided by the brine volume.

The inventory value is a function of time because of radioactive decay and production. Isotopes (of which an element is comprised) decay and produce other isotopes as discussed in Section 3.1. At any given time, the isotopic mix in the inventory and thus the elemental mix in the inventory will change. Plus, material can leave the panel in S6 scenario. Thus, the second step in the calculation of mobilized concentrations is determining the remaining inventory as a function of time.

Once the available inventory is determined, the volume of brine in contact with the inventory is required. PANEL computes mobilized radionuclide concentrations in a panel that contains a given volume of brine. The volume of brine for the CONCENTRATION run is an assumed

quantity based on Stein (2005) for the CRA-2004 PABC. Stein (2005) gives an estimate of the volume of brine in the repository that would lead to a brine release. This value is 10,011 cubic meters. To determine the fraction of that volume that would be in a panel, the 10,011 cubic meter value is multiplied by 0.1044.

$$10{,}111 \bullet 0.1044 = 1045 m^3$$

The value .1044 is the ratio of the area of one of the outside panels to the area of all ten panels (Lappin et al. 1989). The inventory is also multiplied by 0.1044 to determine how much would reside in one panel if the inventory is distributed evenly among panels. The volume of brine in the STANDARD run is determined by BRAGFLO.

Results from each of these process steps are shown in this section. Comparisons are made between the CRA-2004 results and the CRA-2004 PABC results. Section 5.1 presents "source term" results for Am and Pu. These results show how much Am or how much Pu could be mobilized in a liter of brine (either Salado or Castile brine) if there is adequate inventory present. PANEL calculates these values for the isotopes not shown in bold in Table 13. However, only Am and Pu are shown here. Am was chosen for discussion because it has a single oxidation state (+III), and it is important in WIPP PA results. Pu was chosen for discussion because it has two oxidation states (+III and +IV) and it is important in WIPP PA results.

Section 5.2 shows changes in the radionuclide inventory over time due to radioactive decay and production for isotopes of Am, Pu, U, Sr, Cs and other minor isotopes. PANEL calculates decayed activities for all of the isotopes in Table 14. However, these isotopes were chosen for discussion because they are important in WIPP PA, and they demonstrate most of the decay/production trends that one sees in the WIPP PA decay chains.

Section 5.3 presents calculated concentrations for the "lumped" isotopes (needed by CCDFGF for Culebra releases in S1-S5) and for the total EPA units (needed for CCDFGF DBR calculations).

Section 5.4 presents results for quantities of radionuclides up the borehole to the Culebra in the S6 scenario.

5.1 PANEL SOURCE TERM

PANEL source term results for Am and Pu are presented in Figures 2 through 23. Figures 2 through 23 are scatter plots with both the CRA-2004 results (Part b in each figure) and the CRA-2004 PABC results (Part a in each figure) presented. Each scatter plot shows the mobilization potential (either dissolved, humic colloid, microbial colloid, mineral fragment, intrinsic colloid or total) as the dependent variable (ordinate) in moles/liter and the sampled solubility value as the independent variable (abscissa). Table 15 provides definitions for the variables plotted in Figures 2 through 23.

Table 15. Definitions of Variables Plotted in Figures 2 through 23

Name	Type/Units	Description
AM_DIS	Moles/liter	The dissolution potential for Am
AM_HUM	Moles/liter	The mobilization potential for Am in humic colloids
AM_MIC	Moles/liter	The mobilization potential for Am in microbial colloids
AM_MIN	Moles/liter	The mobilization potential for Am in mineral fragment colloids
AM_TMOB	Moles/liter	The total mobilization potential for Am
PU_DIS	Moles/liter	The dissolution potential for Pu
PU_HUM	Moles/liter	The mobilization potential for Pu in humic colloids
PU_MIC	Moles/liter	The mobilization potential for Pu in microbial colloids
PU_INT	Moles/liter	The mobilization potential for Pu in intrinsic colloids
PU_MIN	Moles/liter	The mobilization potential for Pu in mineral fragment colloids
PU_TMOB	dimensionless	The total mobilization potential for Pu
WSOLVAR3	dimensionless	This variable is the sampled value of the solubility variability for oxidation state III (used in CRA-2004 PABC)
WSOLVAR4	dimensionless	This variable is the sampled value of the solubility variability for oxidation state IV (used in CRA-2004 PABC)
WSOLPUC	dimensionless	This variable is the sampled value of the solubility variability for Pu in Castile brine (used in CRA-2004 PABC) depending on the oxidation state of Pu[(a)]
WSOLPUS	dimensionless	This variable is the sampled value of the solubility variability for Pu in Salado brine (used in CRA-2004 PABC) depending on the oxidation state of Pu[(a)]
WSOLAM3S	dimensionless	This variable is the sampled value of the solubility variability for Am in Salado brine (used in CRA-2004)
WSOLAM3C	dimensionless	This variable is the sampled value of the solubility variability for Am in Castile brine (used in CRA-2004)

[(a)]WSOLPUC and WSOLPUS were also used in the CCA. In the CCA, WSOLPUC and WSOLPUS were constructed from different distribution sets than the ones used to construct them in the CRA-2004 PABC.

Scatter plots illustrate the range of uncertainty in each radionuclide's potential mobilized concentration. For Am, which has only one oxidation state (+III), the independent variable (the sampled value of the solubility variability for oxidation state +III) varies from –2.85 to 2.85 in log units (Xiong et. al. 2005) in the case of the CRA-2004 PABC. This solubility variability range is larger than the solubility variability range in the case of CRA-2004 which varied from -2.0 to 1.4 in log units.

Figures 2 to 6 are for Am in Salado brine. Figure 2 indicates that the potential dissolved component for Am in Salado brine ranged in value from 3.51E-09 to 6.05E-06 moles/liter in the CRA-2004. Due to changes in the solubility values for Am, the potential dissolved component for Americium in Salado brine ranges from 5.22E-10 to 1.32E-04 moles/liter in the CRA-2004 PABC.

Figure 3 indicates that the range of values for the potential humic component of mobilized Am in Salado brine is larger in the CRA-2004 PABC (from 9.92E-11 to 1.10E-05 moles/liter) than it was in CRA-2004 (from 6.67E-10 to 1.24E-06 moles/liter). This is to be expected since, even though the multiplier $\left(h_{brine}^{red/ox}\right)$ in Equation 3 was not updated for the CRA-2004 PABC, the dissolved component (which is part of Equation 3) did change (see Figure 2). It is also interesting to note in Figure 3 that the humic colloid component did not reach the maximum

value [$\left(H_{elem}^{max}\right)$ in Equation 3] in CRA-2004. It did reach the maximum value in CRA-2004 PABC. This is apparent on the far right-hand-side of Figure 3 Part a where the two vectors have values equivalent to the maximum, 1.10E-05 moles/liter.

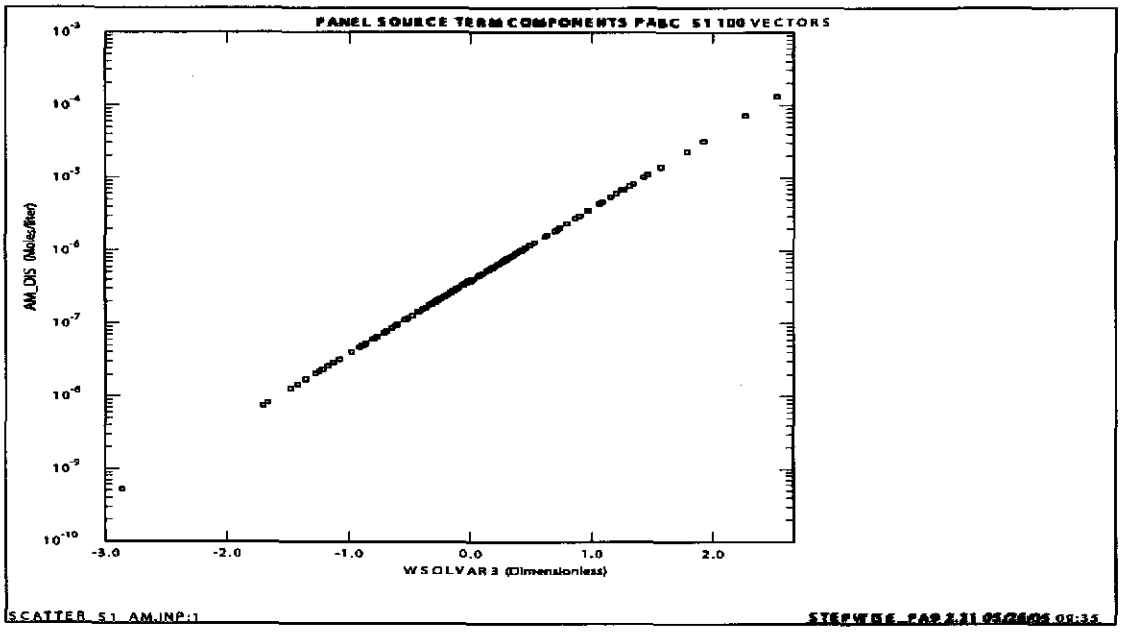
Figure 4 shows the effect of changing the probability of microbial degradation in the CRA-2004 PABC. The potential microbial component of mobilized Am in CRA-2004 (Part b of Figure 4) shows two sets of data. The set of higher values corresponds to the 50% of the vectors assumed to have microbial degradation. The set of lower values corresponds to the 50% of the vectors assumed to be free of microbial degradation (microbial colloids are zero). Part a of Figure 4 shows that since all vectors are assumed to have microbial degradation in the CRA-2004 PABC, the mobilization potential for microbial colloids for Am is more of a continuous distribution with a range of 1.88E-09 to 4.75E-04 moles/liter.

Figure 5 indicates that the mobilization potential for mineral fragments for Am did not change from CRA-2004 to CRA-2004 PABC. It has a constant value of 2.60E-08 moles/liter.

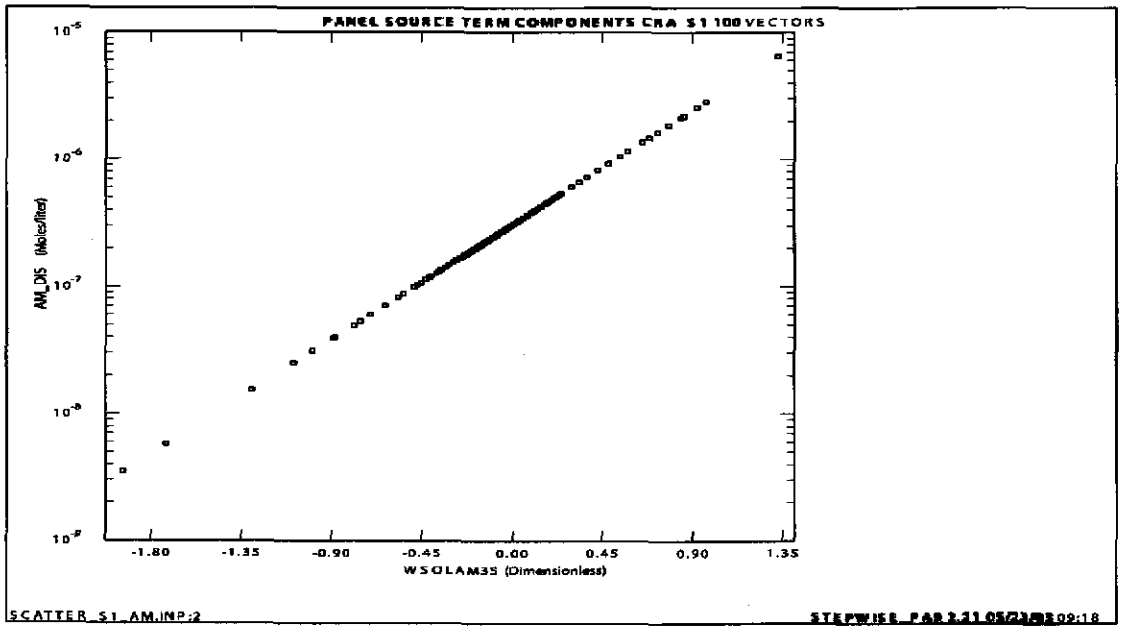
Figure 6 shows the total mobilization potential for Am in Salado brine. Part a shows the CRA-2004 PABC results and Part b shows the CRA-2004 results. As expected Part a shows a fairly continous curve while Part b shows two curves because 50% of the vectors have microbial degradation and 50% of the vectors do not have microbial degradation. The trend in lower values (left-hand-side of the plots) for both CRA-2004 and CRA-2004 PABC is toward a constant low value set by the mobilization potential for mineral fragments shown in Figure 5.

Figures 7 to 11 are for Am in Castile brine. Most of the same conclusions that were drawn above for Am in Salado brine can be drawn as well for Am in Castile brine. The same trends are apparent. The most notable exception is shown in Figures 8 and 11. Figure 8 shows the mobilization potential for humic colloids for Am in Castile brine. In this particular case, the value of $\left(h_{brine}^{red/ox}\right)$ in Equation 3 is not a constant but is instead a sampled variable (see Table 8). The result is more "scatter" in the figure. Figure 8 also shows that humic colloids can reach the maximum value of 1.1 x 10-5 moles/liter in the CRA-2004 PABC (see the right-hand-side of Part a of Figure 8). Four vectors reach the maximum value in this case. In Figure 11, Part a shows a fairly continous curve while Part b shows two curves because 50% of the vectors have microbial degradation and 50% of the vectors do not have microbial degradation.

The scatter seen in Figure 8 for the Am humic colloid component in Castile brine causes some scatter in Figure 11 which is the total mobilization potential for Am in Castile brine.



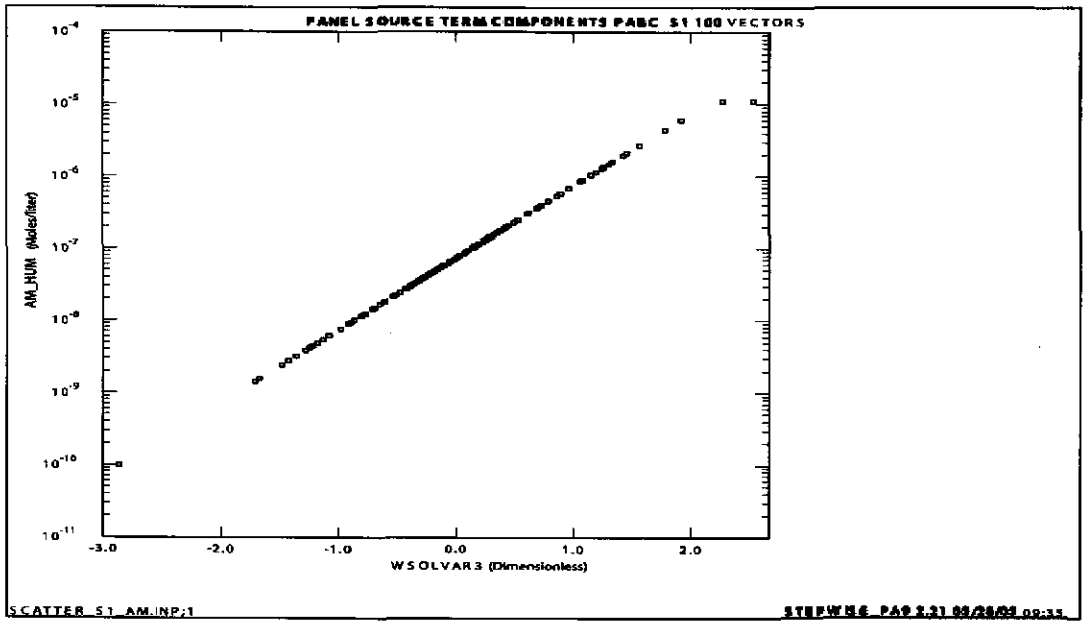
a) PABC



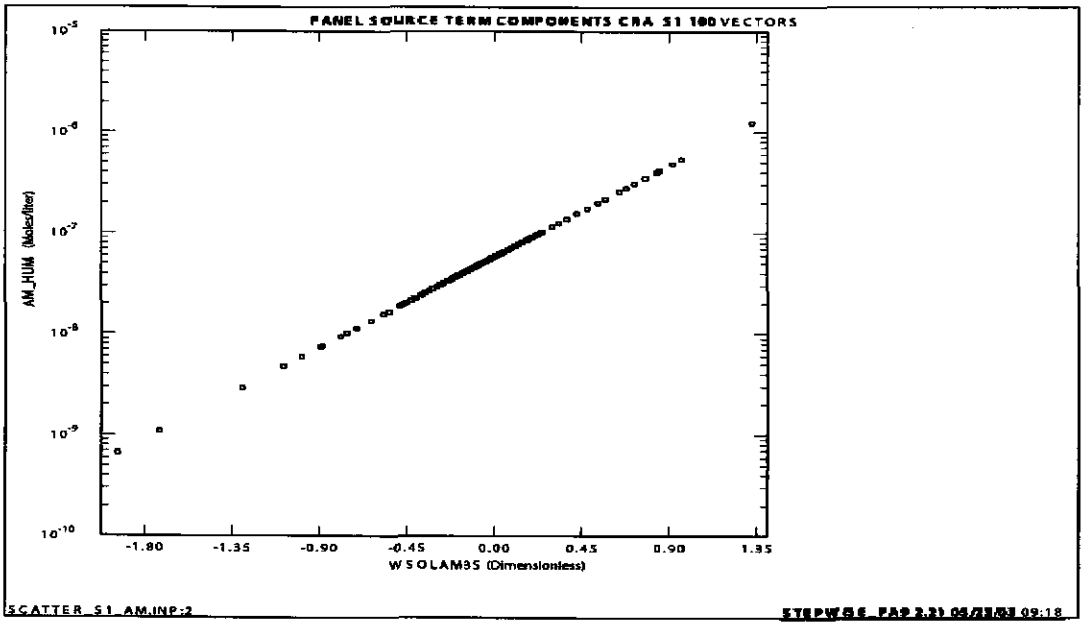
b) CRA1

Figure 2: Scatter Plot of Dissolution Potential for Am in Salado Brine for all 100 Vectors in Scenario S1, Replicate 1.

Part a) shows results from the CRA-2004 PABC. Part b) shows results from the CRA-2004.



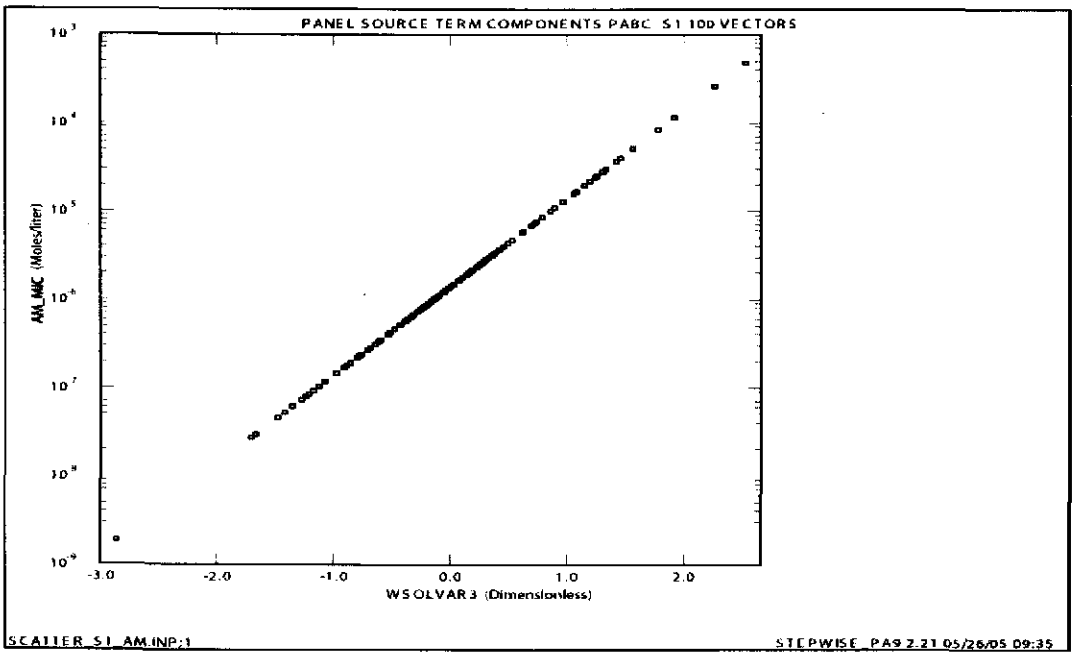
a) PABC



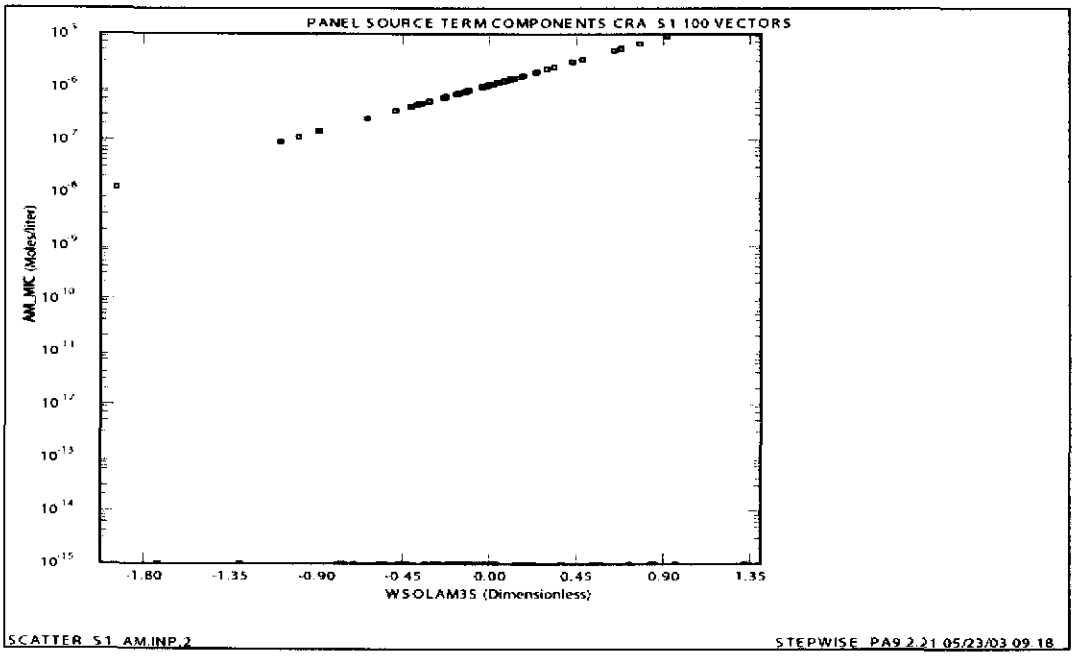
b) CRA1

Figure 3: Scatter Plot of Potential Humic Colloid Component for Am in Salado Brine for all 100 Vectors in Scenario S1, Replicate 1.

Part a) shows results from the CRA-2004 PABC. Part b) shows results from the CRA-2004.



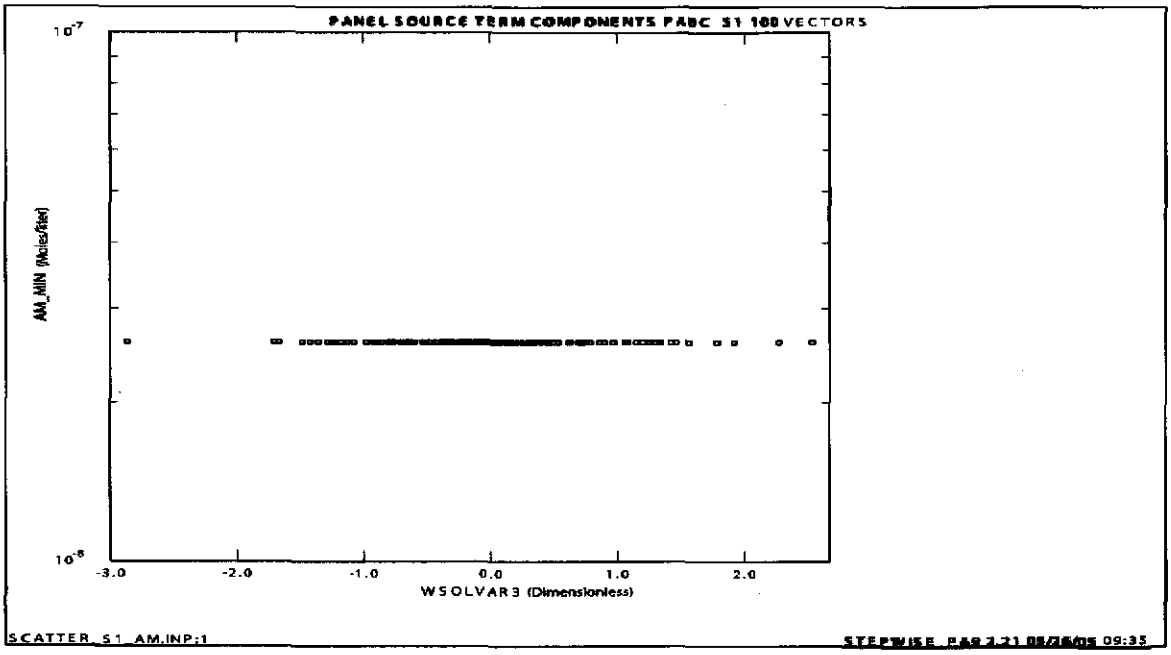
a) PABC



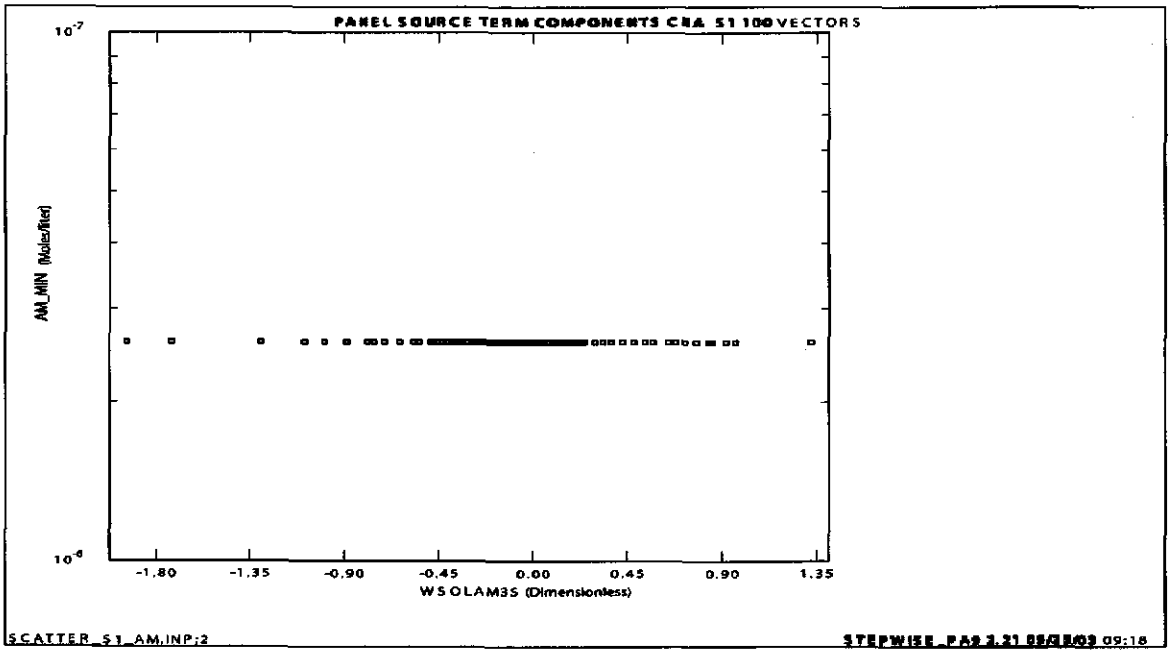
b) CRA1

Figure 4: Scatter Plot of Mobilization Potential for Microbial Colloids for Am in Salado Brine for all 100 Vectors in Scenario S1, Replicate 1.

Part a) shows results from the CRA-2004 PABC. Part b) shows results from the CRA-2004.



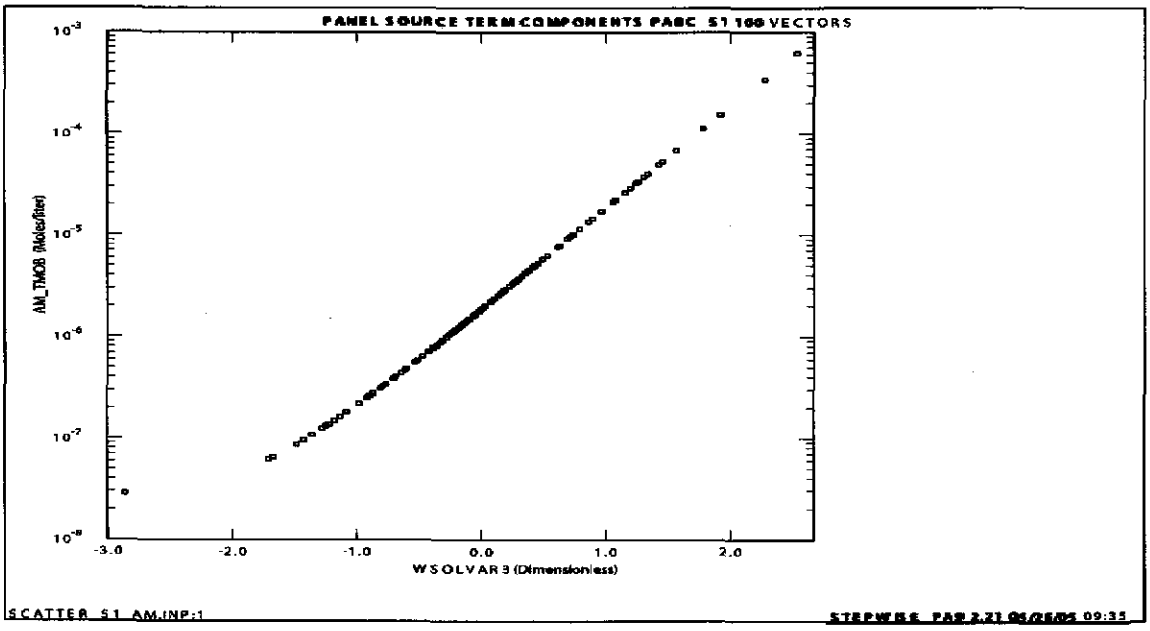
a) PABC



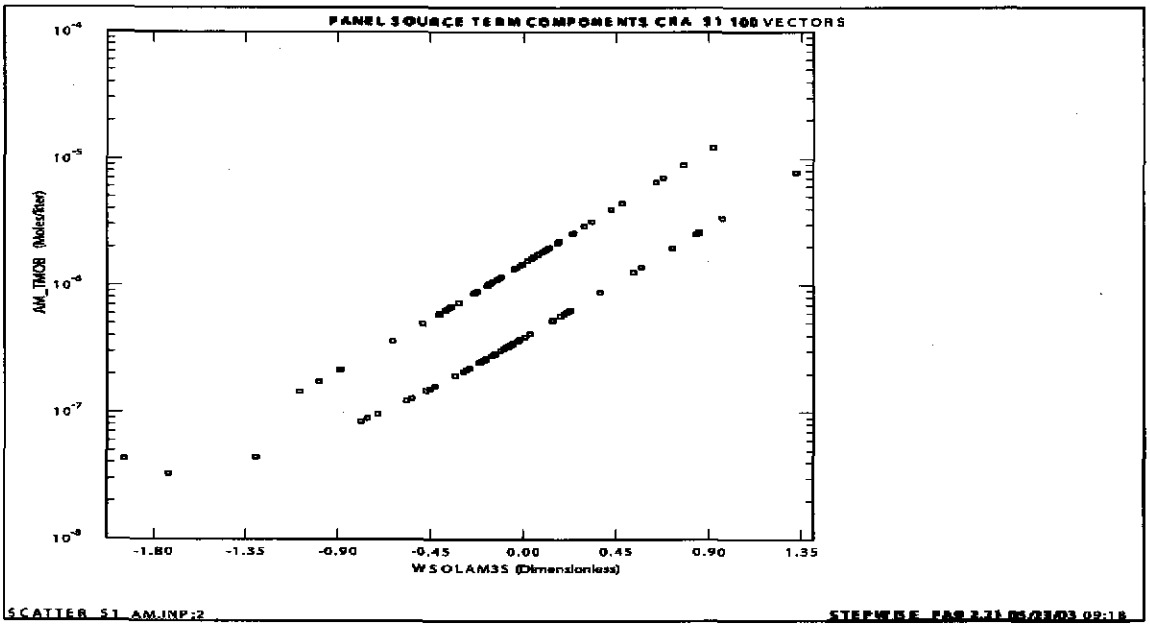
b) CRA1

Figure 5: Scatter Plot of Mobilization Potential for Mineral Fragments for Am in Salado Brine for all 100 Vectors in Scenario S1, Replicate 1.

Part a) shows results from the CRA-2004 PABC. Part b) shows results from the CRA-2004.



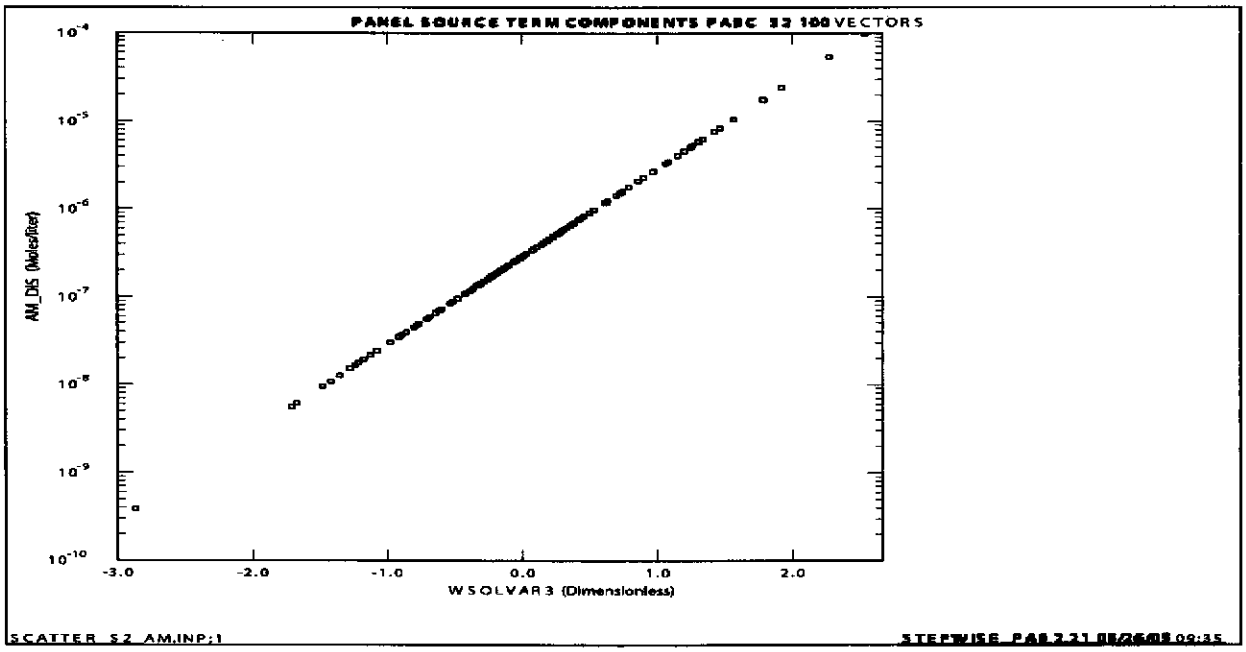
a) PABC



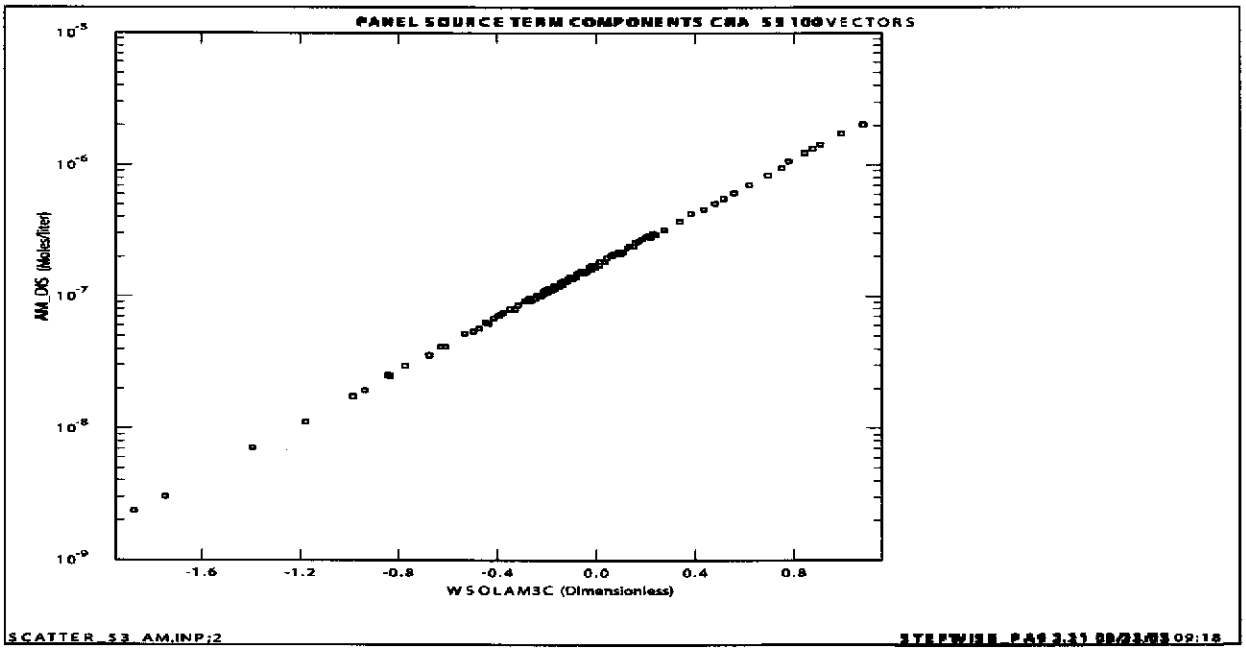
b) CRA1

Figure 6: Scatter Plot of Total Mobilization Potential for Am in Salado Brine.

Part a) shows results from the CRA-2004 PABC. Part b) shows results from the CRA-2004.



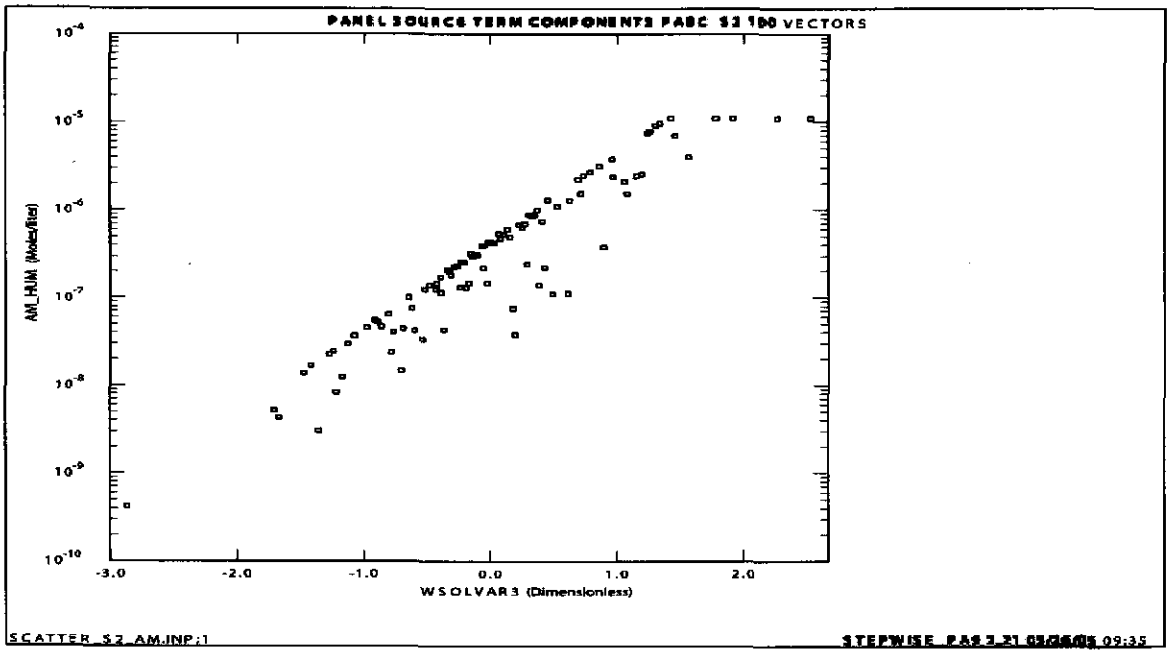
a) PABC



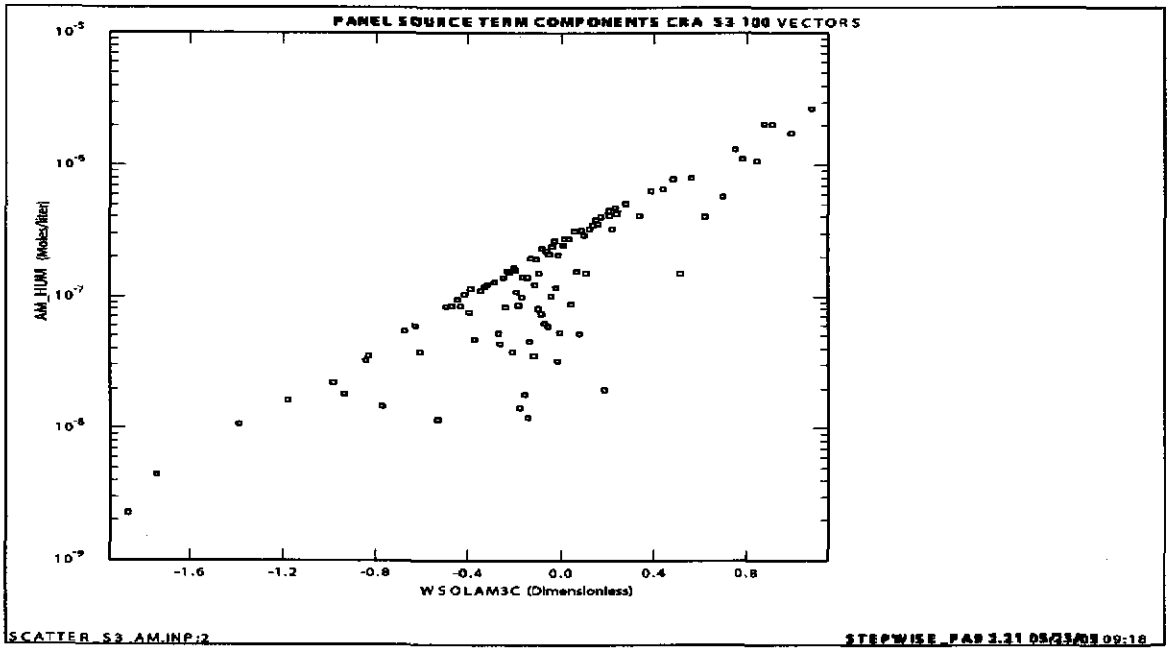
b) CRA1

Figure 7: Scatter Plot of Dissolution Potential for Am in Castile Brine for all 100 Vectors in Scenario S1, Replicate 1.

Part a) shows results from the CRA-2004 PABC. Part b) shows results from the CRA-2004.



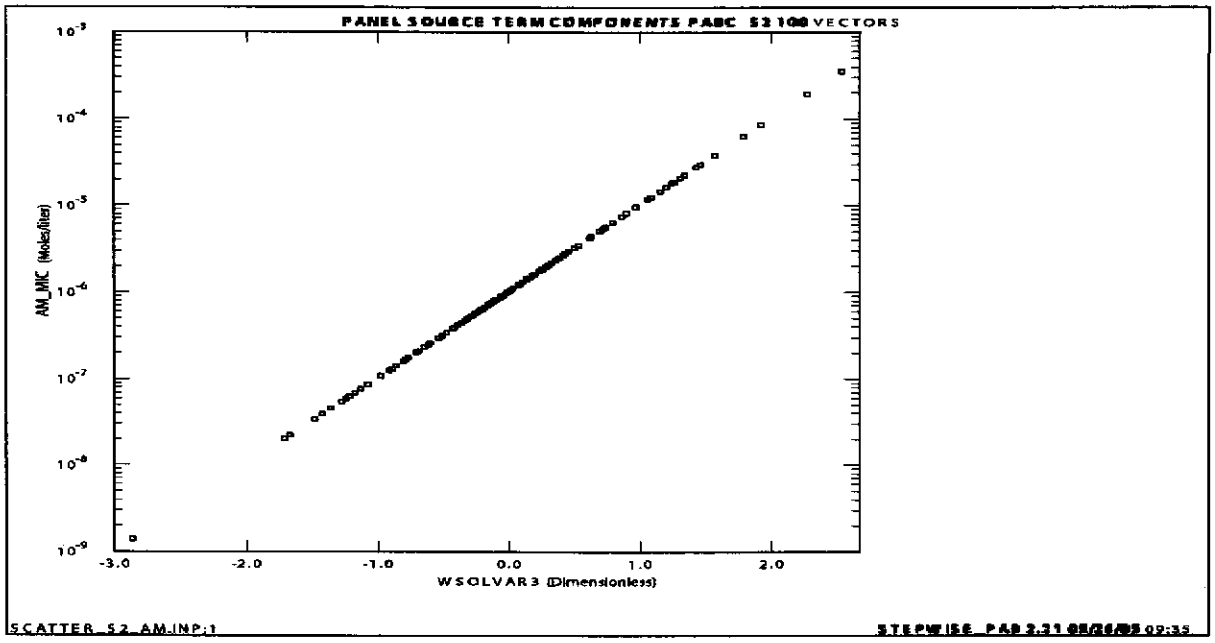
a) PABC



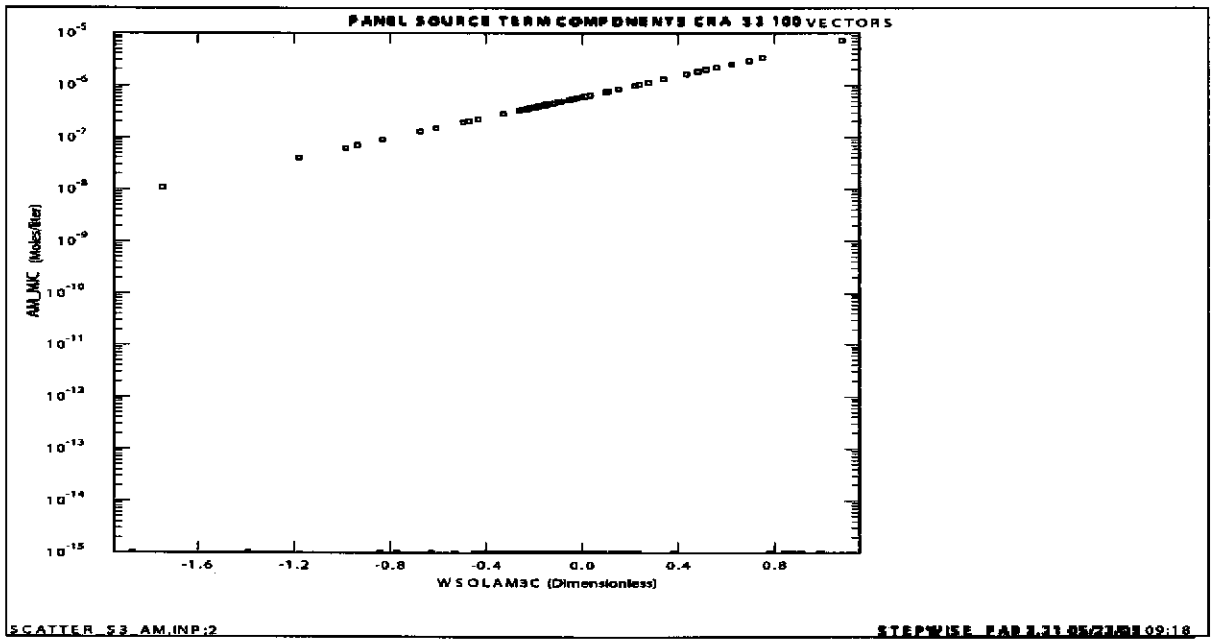
b) CRA1

Figure 8: Scatter Plot of Mobilization Potential for Humic Colloids for Am in Castile Brine for all 100 Vectors in Scenario S1, Replicate 1.

Part a) shows results from the CRA-2004 PABC. Part b) shows results from the CRA-2004.



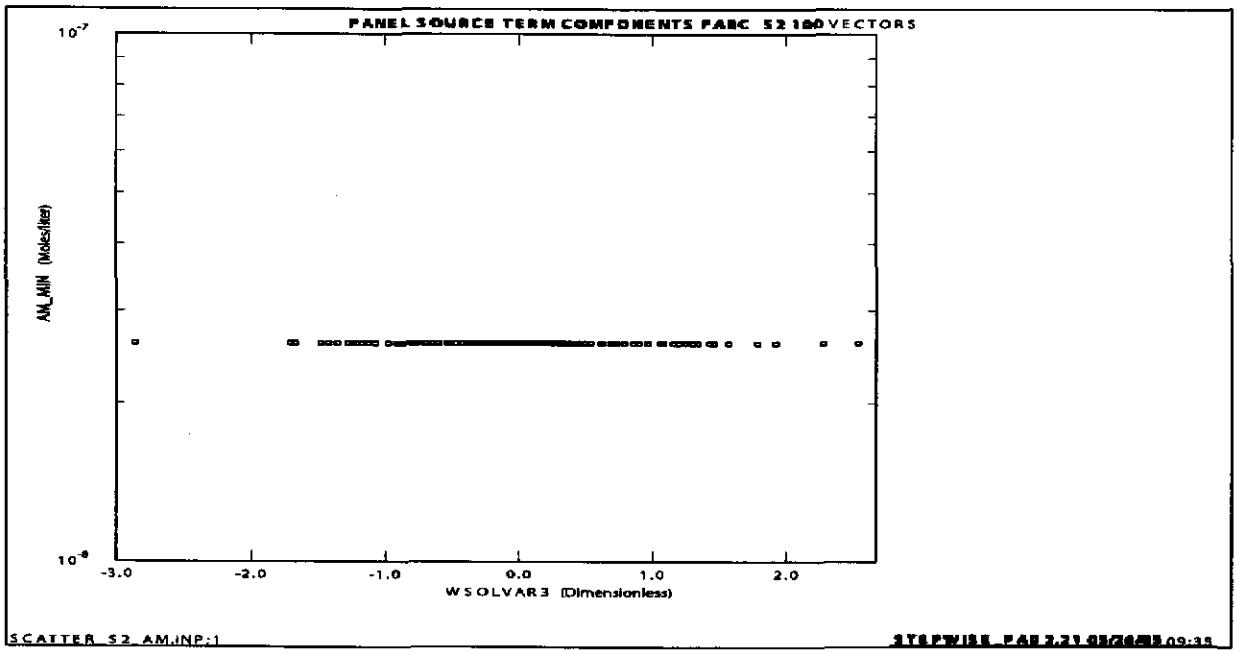
a) PABC



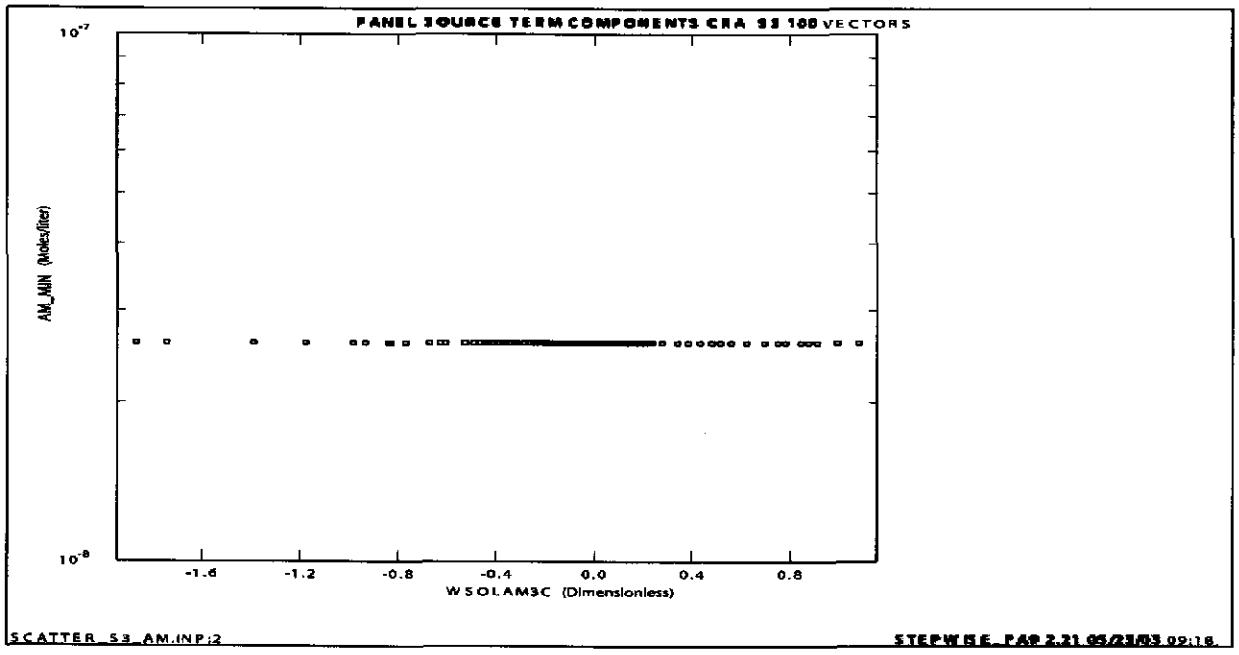
b) CRA1

Figure 9: Scatter Plot of Mobilization Potential for Microbial Colloids for Am in Castile Brine for all 100 Vectors in Scenario S1, Replicate 1.

Part a) shows results from the CRA-2004 PABC. Part b) shows results from the CRA-2004.



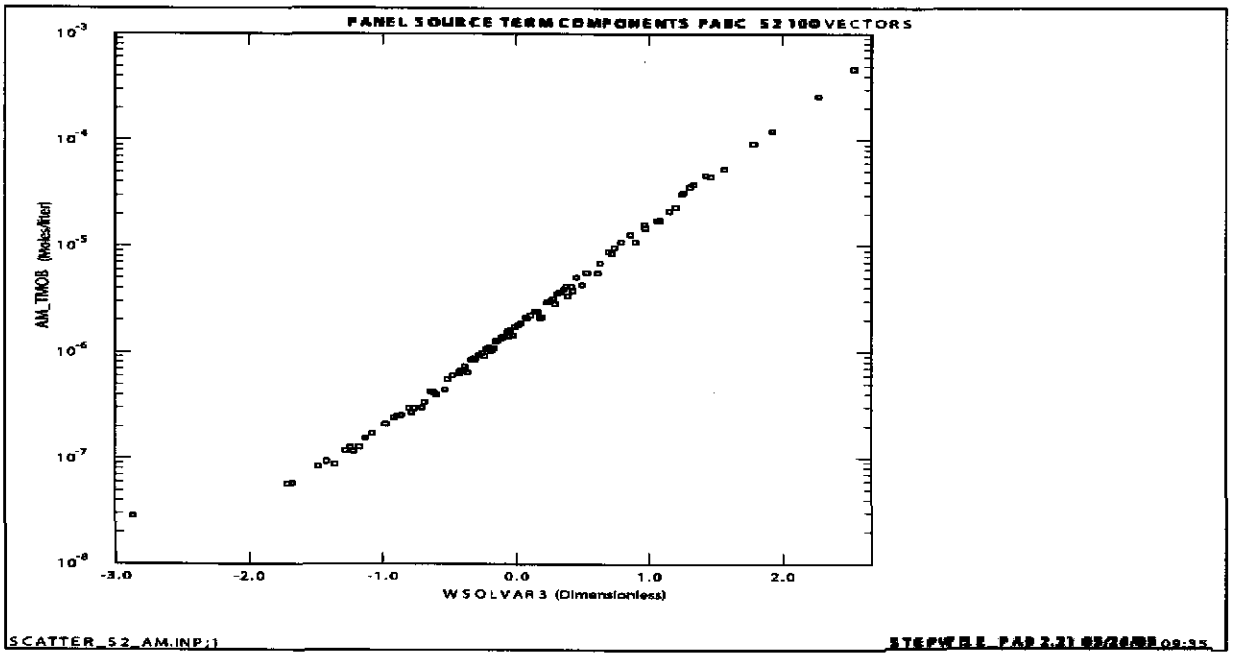
a) PABC



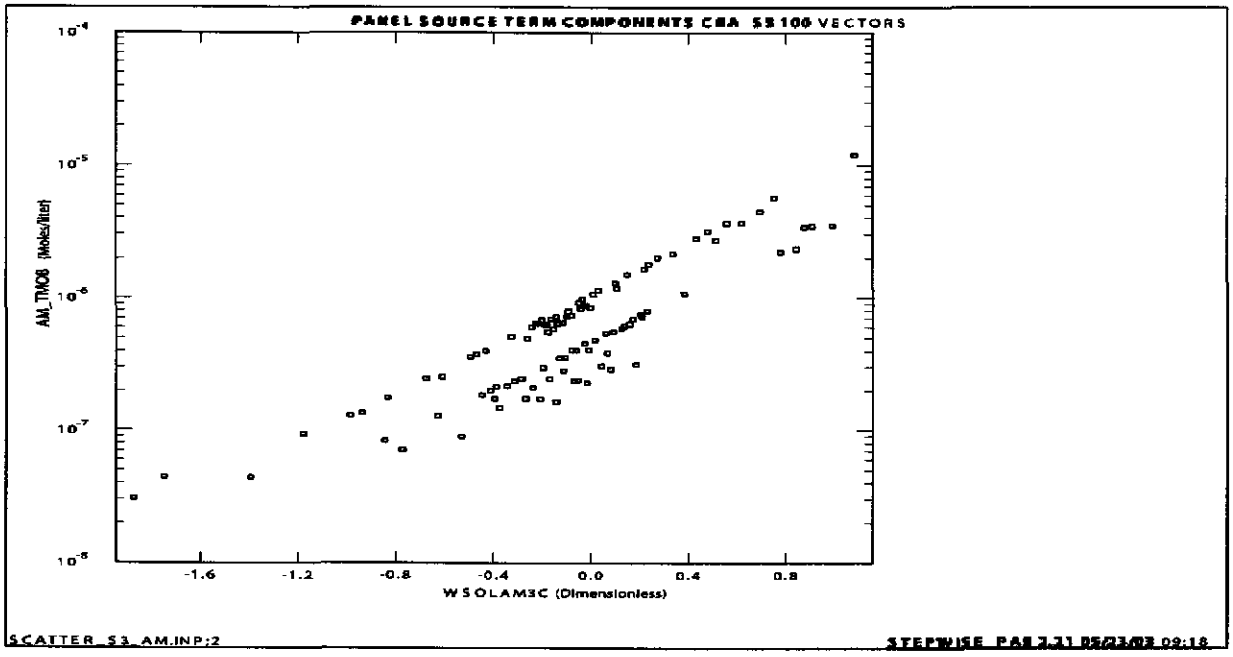
b) CRA1

Figure 10: Scatter Plot of Mobilization Potential for Mineral Fragments for Am in Salado Brine for all 100 Vectors in Scenario S1, Replicate 1

Part a) shows results from the CRA-2004 PABC. Part b) shows results from the CRA-2004.



a) PABC



b) CRA1

Figure 11 : Scatter Plot of Total Mobilization Potential for Am in Castile Brine.

Part a) shows results from the CRA-2004 PABC. Part b) shows results from the CRA-2004.

In WIPP PA, Pu can occur in either oxidation state +III or +IV, depending on the value of GLOBAL:OXSTAT (see Table 3) which is sampled from a uniform distribution between 0 and 1. If GLOBAL:OXSTAT is less than or equal to .5, Pu will be in oxidation state +III. If it is greater than .5, the oxidation state for Pu will be +IV.

PANEL source term results for Pu are presented in Figures 12 through 23. Figures 12 to 17 are for Pu in Salado brine. Figures 18 to 23 are for Pu in Castile brine. Most of these figures show at least two distinct sets of data, one that corresponds to Pu in the +III oxidation state and one that corresponds to Pu in the +IV oxidation state. The exceptions are Figures 15, 16, 21, and 22 showing the mobilization potential for mineral fragments and intrinsic colloids which are constant values (see Equations 4 and 5) and independent of oxidation state.

In the figures where two sets of data are shown (Figures 12-14, 17-23), the upper set of data corresponds to Pu in the +III oxidation state. These results are essentially identical to those for Am in the +III oxidation state. The lower set of data corresponds to Pu in the +IV oxidation state.

Figure 12 indicates that the dissolution potential for Pu in Salado brine ranged from 2.19E-10 to 2.20E-06 moles/liter in the CRA-2004. Due to changes in the solubility values and solubility variability for Pu, the dissolution potential for Pu in Salado brine ranges from 5.22E-10 to 1.32E-04 moles/liter in the CRA-2004 PABC.

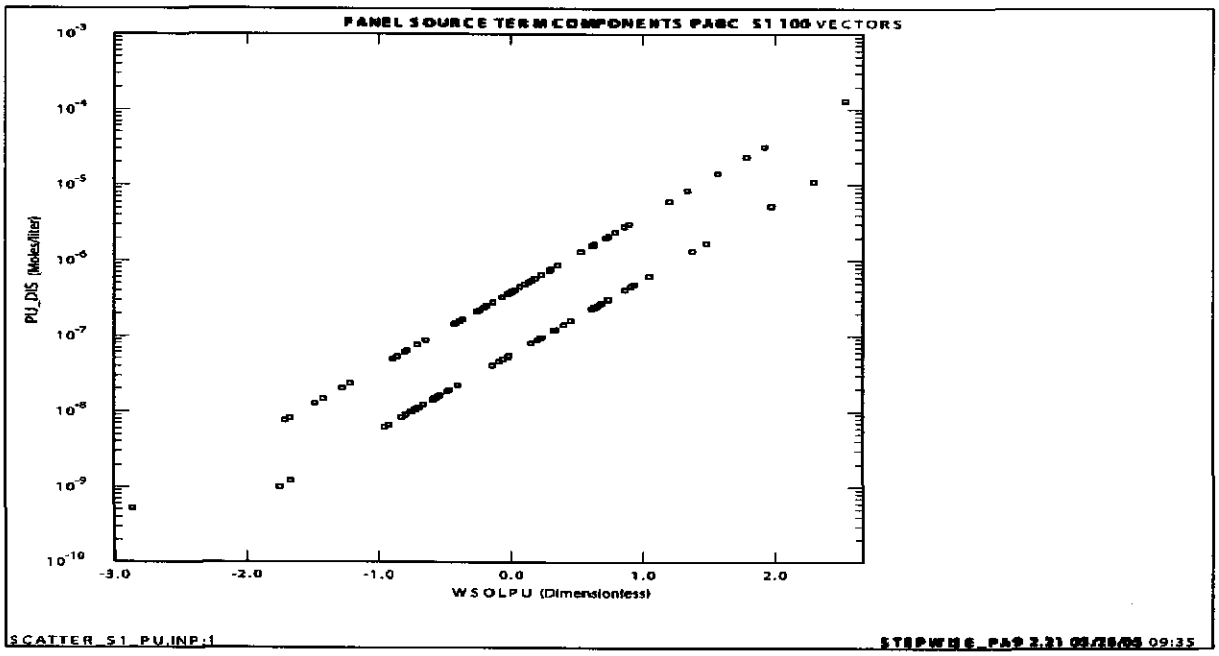
Figure 18 indicates that the dissolution potential for Pu in Castille brine ranged from 6.77E-11 to 1.31E-06 moles/liter in the CRA-2004. Due to changes in the solubility values and solubility variability for Pu, the dissolution potential for Pu in Castille brine ranges from 3.89E-10 to 9.83E-05 moles/liter in the CRA-2004 PABC.

Figure 13 indicates that the range of values for the mobilization potential for humic colloids for Pu in Salado brine is larger in the CRA-2004 PABC (from 9.92E-11 to 1.10E-05 moles/liter) than it was in CRA-2004 (from 1.38E-09 to 7.67E-07 moles/liter). It is also interesting to note in Figure 13 that the mobilization potential for humic colloids for Pu did not reach the maximum value in CRA-2004. It did reach the maximum value in CRA-2004 PABC. Similarly, Figure 19 shows that the range of values for humic colloids for Pu in Castile brine is larger in the CRA-2004 PABC (from 4.24E-10 to 1.10E-05 moles/liter) than it was in CRA-2004 (from 3.21E-10 to 1.96E-06 moles/liter).

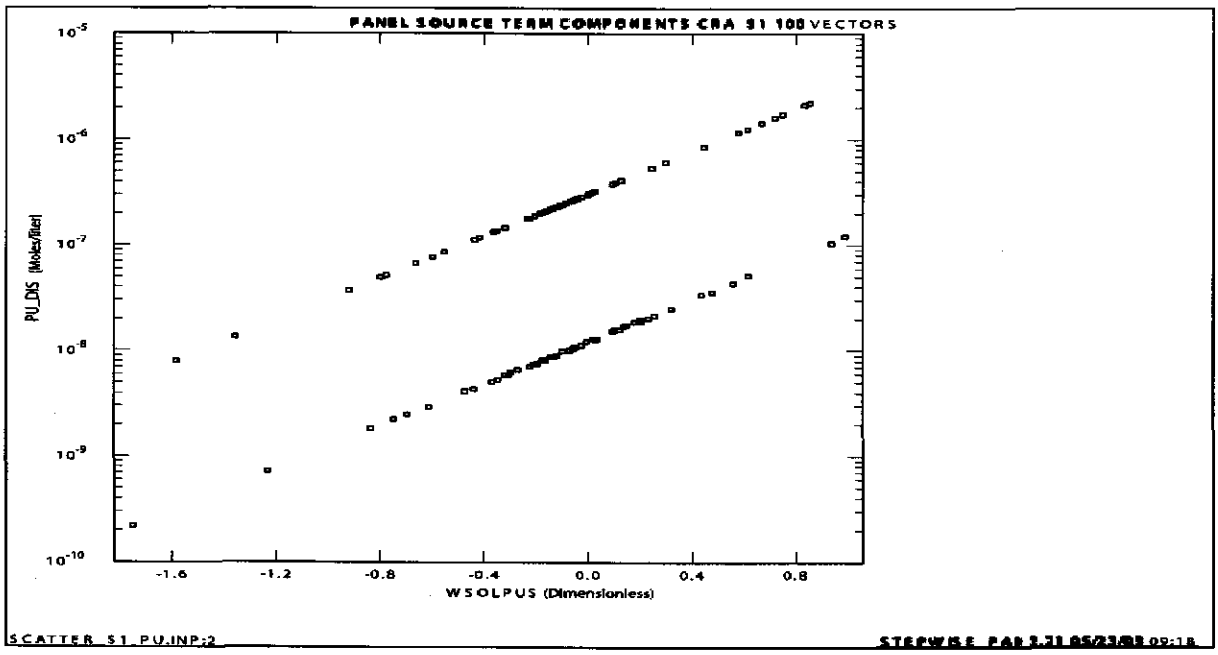
Figure 14 shows two sets of data in Part a (CRA-2004 PABC results) and three sets of data in Part b (the CRA-2004 results). The two sets of data in Part a correspond to Pu in the two different oxidation states. The third set of data (lowest data set shown) in Part b of Figure 14 corresponds to the non-microbial vectors for both the +III and +IV Pu.

Figure 17 shows the total mobilization potential for Pu in Salado brine. Part a shows the CRA-2004 PABC results and Part b shows the CRA-2004 results. Part a shows two sets of data corresponding to the two oxidation states for Pu. Part b shows a third set of data which corresponds to Pu in both oxidation states for the non-microbial vectors (the lower data set in Figure 17). Figure 23 shows the same trend in the total mobilization potential for Pu in Castille brine.

Figure 18 shows another interesting affect of changing the probability of microbial degradation in the CRA-2004 PABC. Figure 18 shows the dissolution potential for Pu in Castile brine. The solubility is given by Equation 2. In Equation 2, the base solubility value $\left(s_{brine}^{red/ox}\right)$ is a function of the oxidation state, the brine type, and the assumed buffering reaction. For the CRA-2004 PABC, all vectors are microbial vectors and the assumed buffer for all vectors is brucite/hydromagnesite. In the CRA-2004, the assumed buffer for microbial vectors is brucite/hydromagnesite and the assumed buffer for non-microbial vectors is brucite/calcite. Therefore, there is a third set of data shown in Figure 18 Part b corresponding to a different base solubility value for non-microbial vectors (the lower data set in Figure 18).



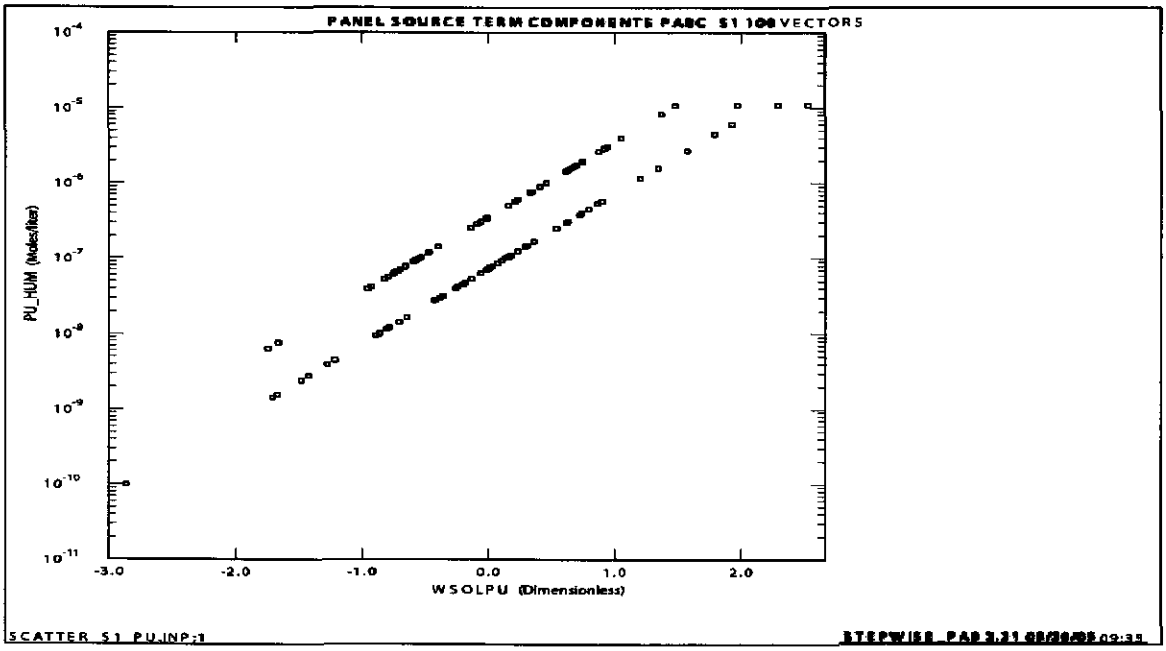
a) PABC



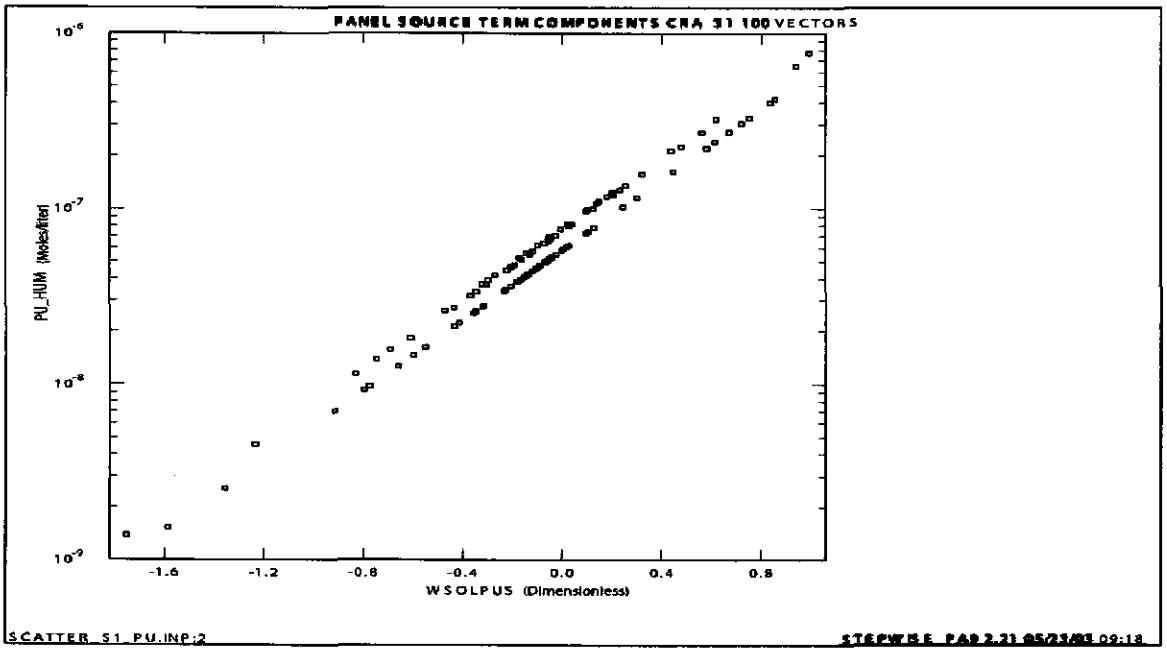
b) CRA1

Figure 12: Scatter Plot of Dissolution Potential for Pu in Salado Brine for all 100 Vectors in Scenario S1, Replicate 1.

Part a) shows results from the CRA-2004 PABC. Part b) shows results from the CRA-2004.



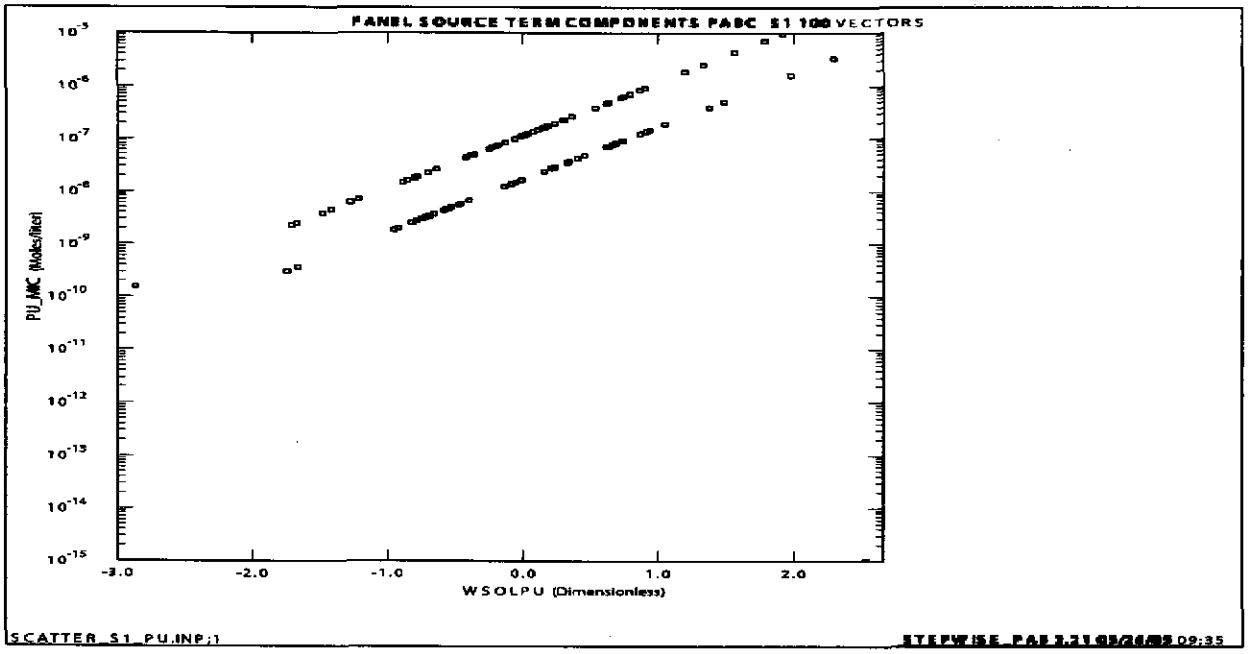
a) PABC



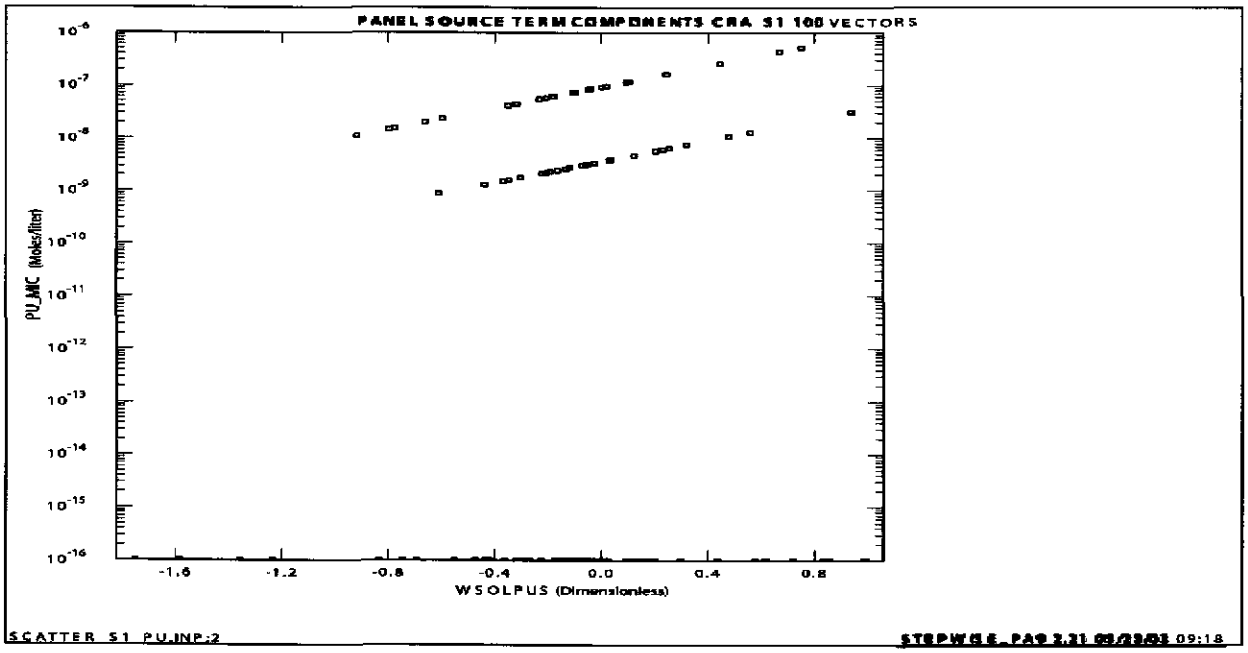
b) CRA1

Figure 13: Scatter Plot of Mobilization Potential for Humic Colloids for Plutonium in Salado Brine for all 100 Vectors in Scenario S1, Replicate 1.

Part a) shows results from the CRA-2004 PABC. Part b) shows results from the CRA-2004.



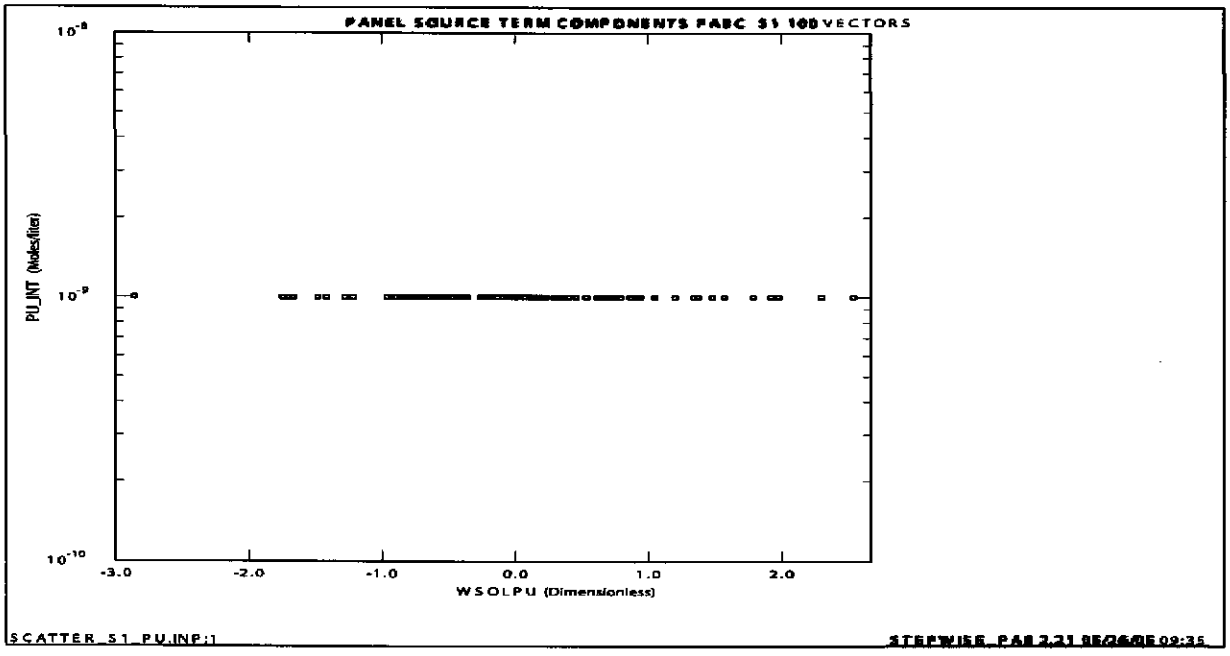
a) PABC



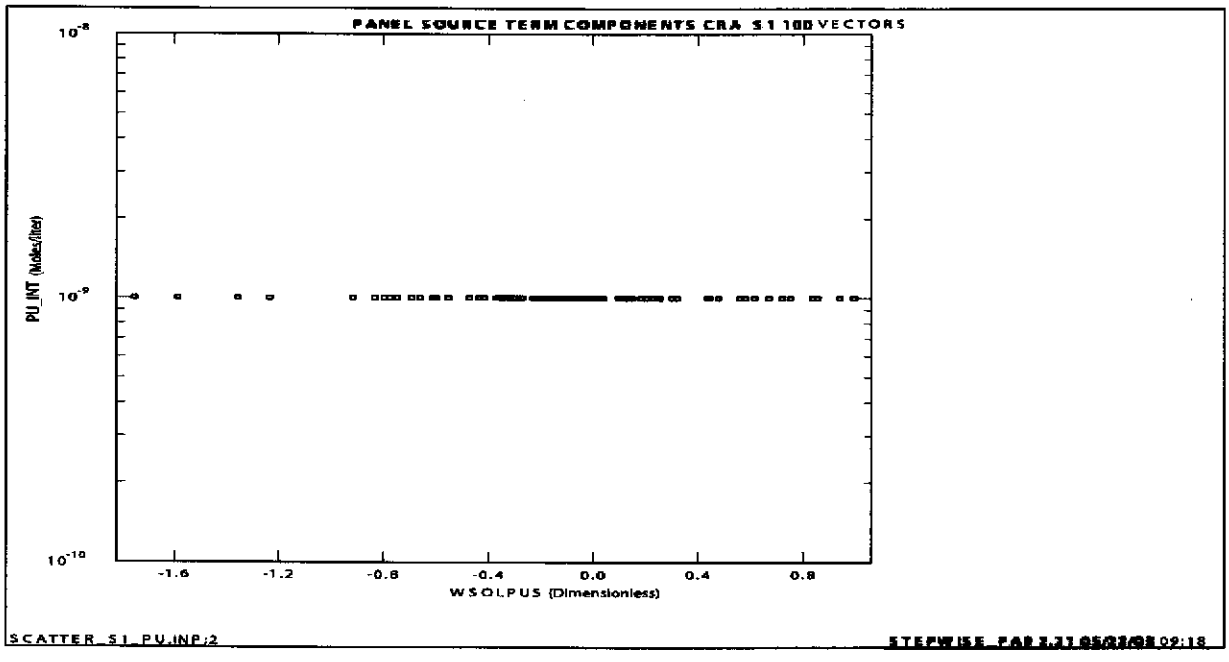
b) CRA1

Figure 14: Scatter Plot of Mobilization Potential for Microbial Colloids for Pu in Salado Brine for all 100 Vectors in Scenario S1, Replicate 1.

Part a) shows results from the CRA-2004 PABC. Part b) shows results from the CRA-2004.



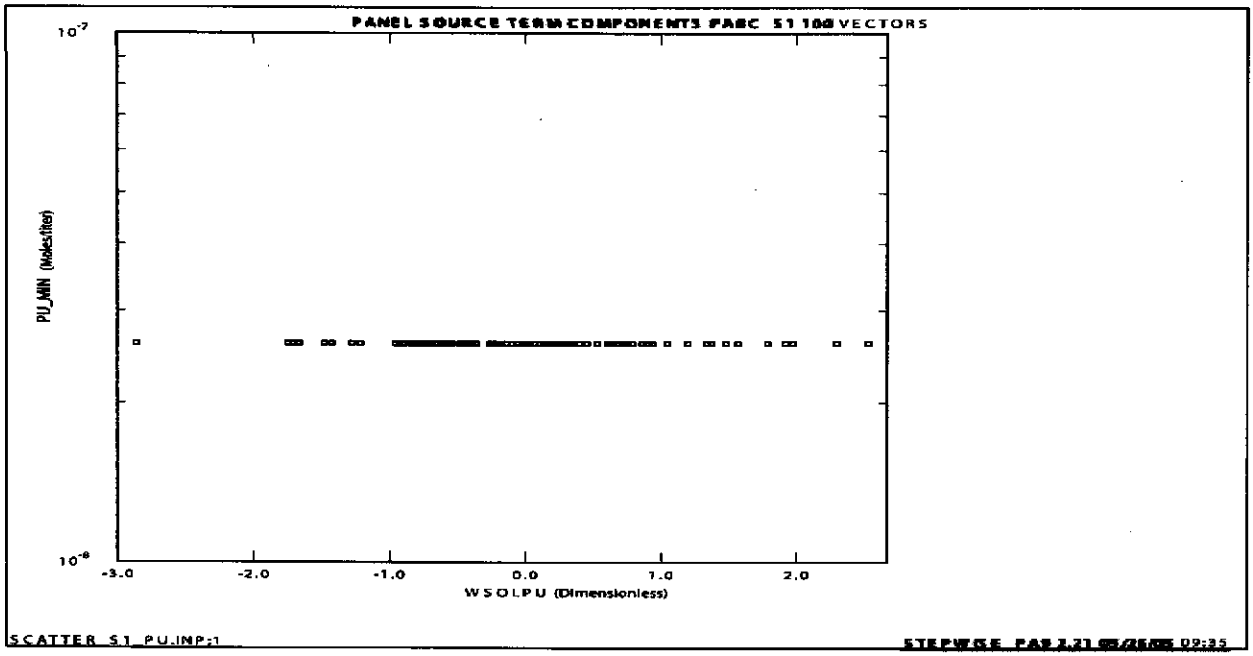
a) PABC



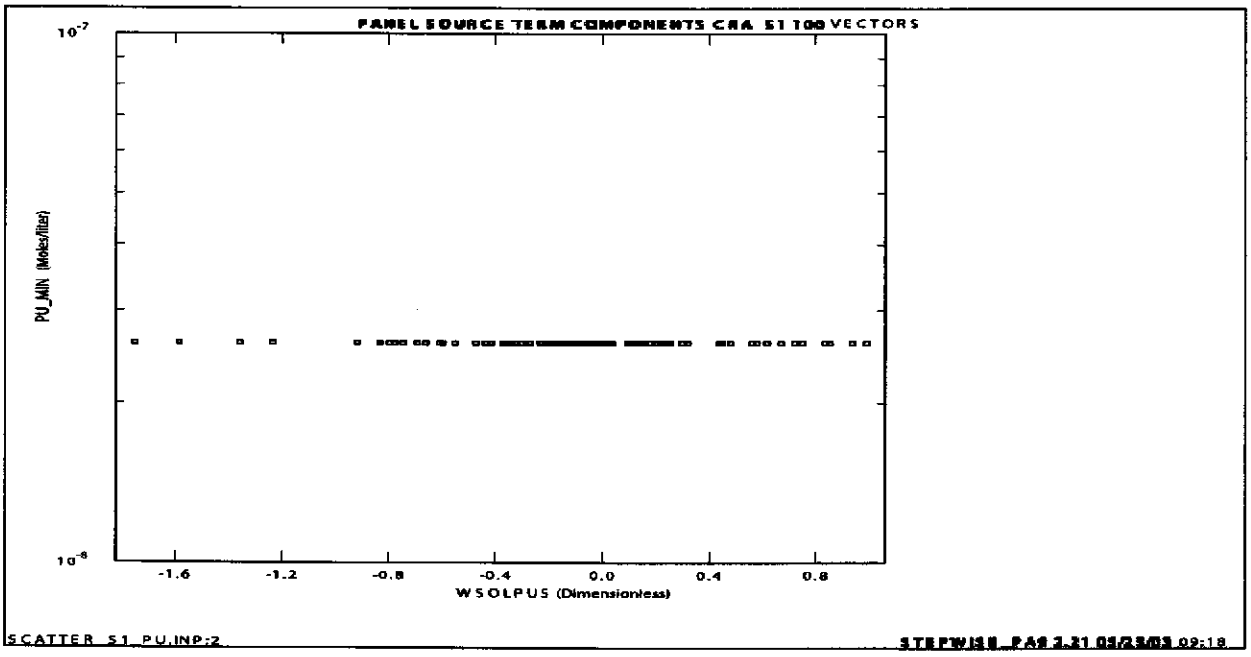
b) CRA1

Figure 15: Scatter Plot of Mobilization Potential for Intrinsic Colloids for Pu in Salado Brine for all 100 Vectors in Scenario S1, Replicate 1.

Part a) shows results from the CRA-2004 PABC. Part b) shows results from the CRA-2004 PA.



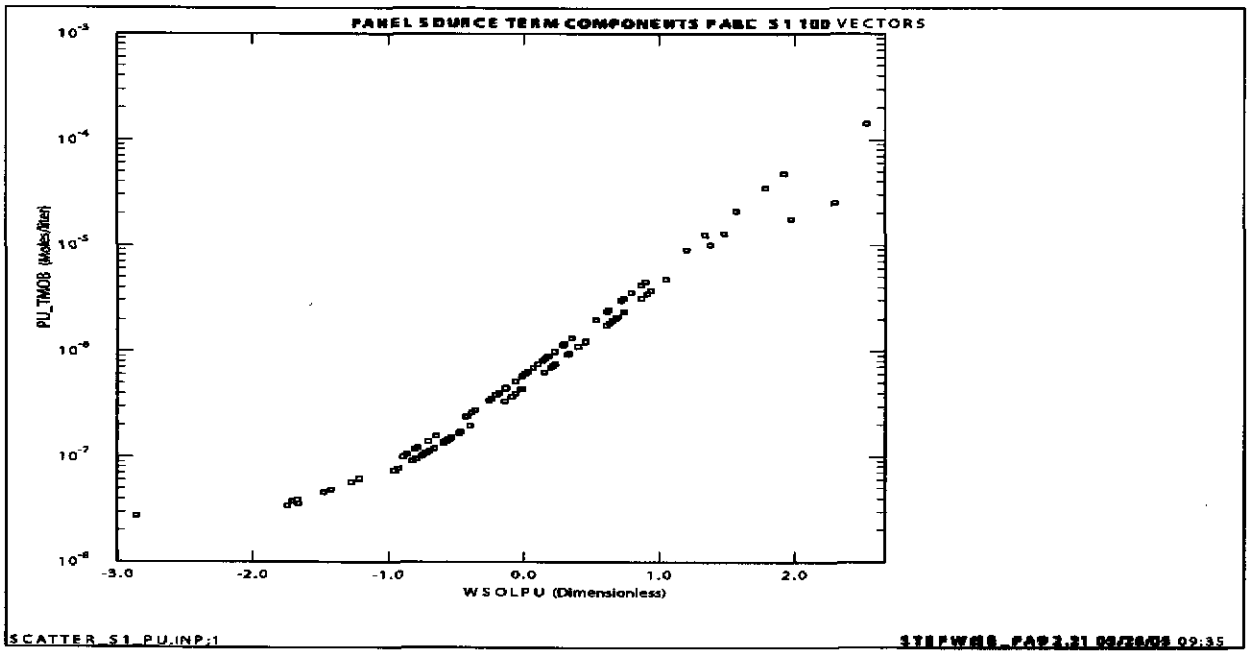
a) PABC



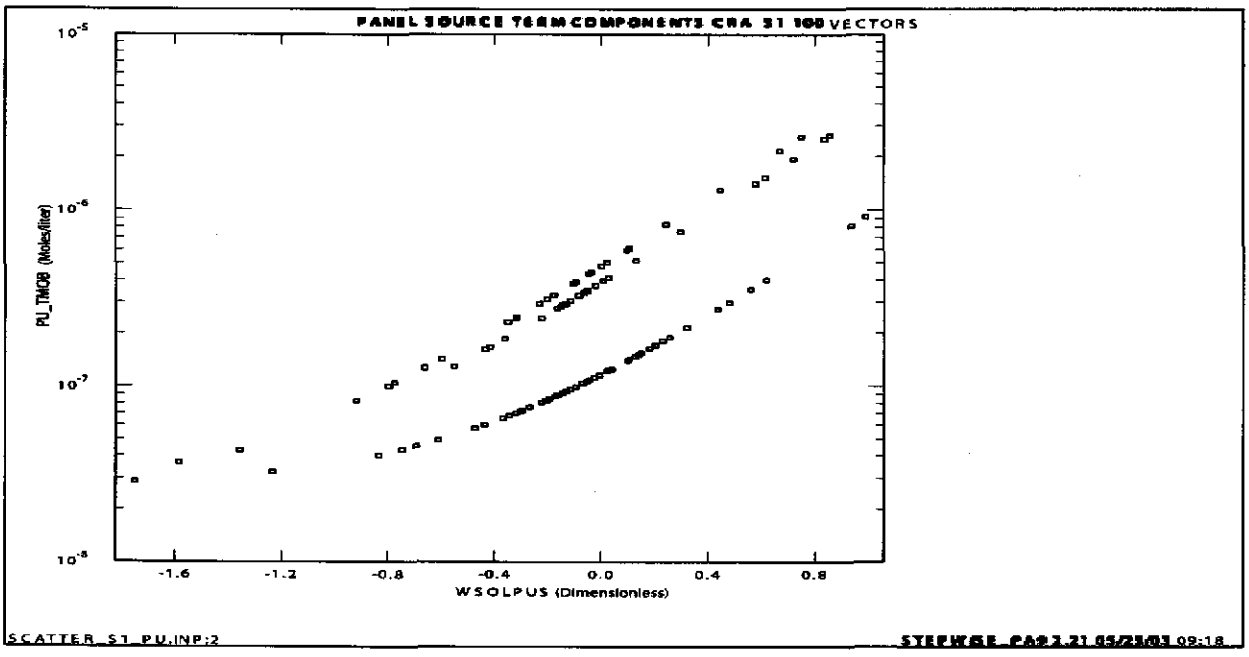
b) CRA1

Figure 16: Scatter Plot of Mobilization Potential for Mineral Fragments for Pu in Salado Brine for all 100 Vectors in Scenario S1, Replicate 1.

Part a) shows results from the CRA-2004 PABC. Part b) shows results from the CRA-2004 PA



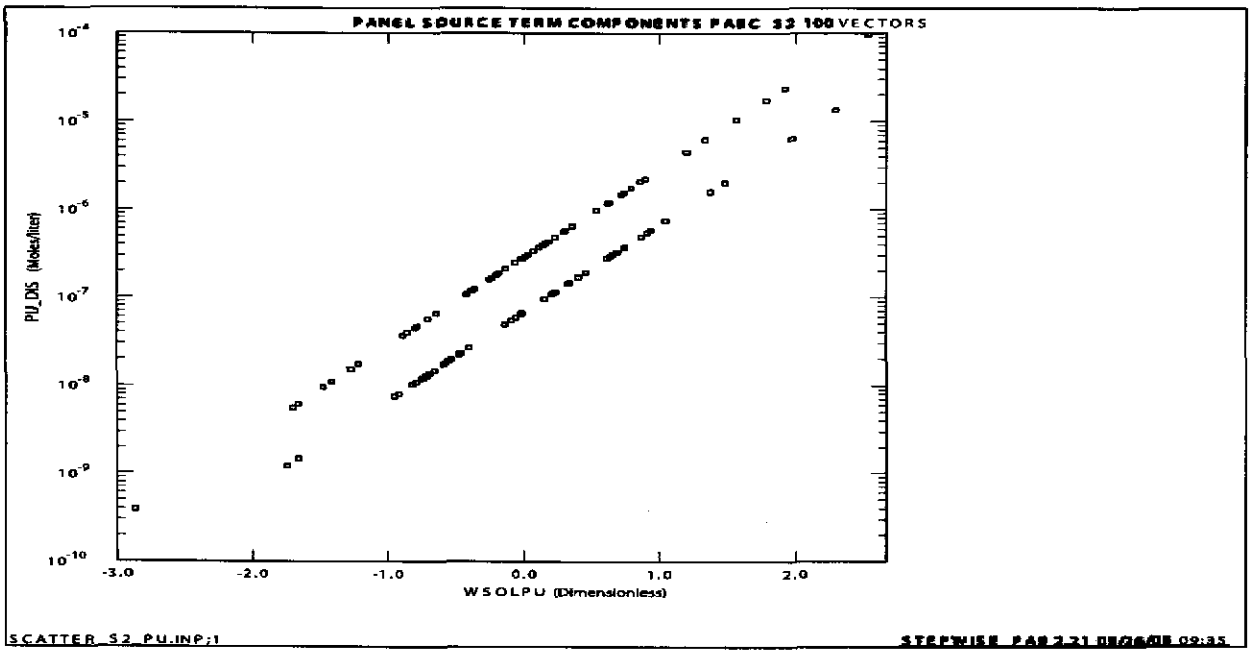
a) PABC



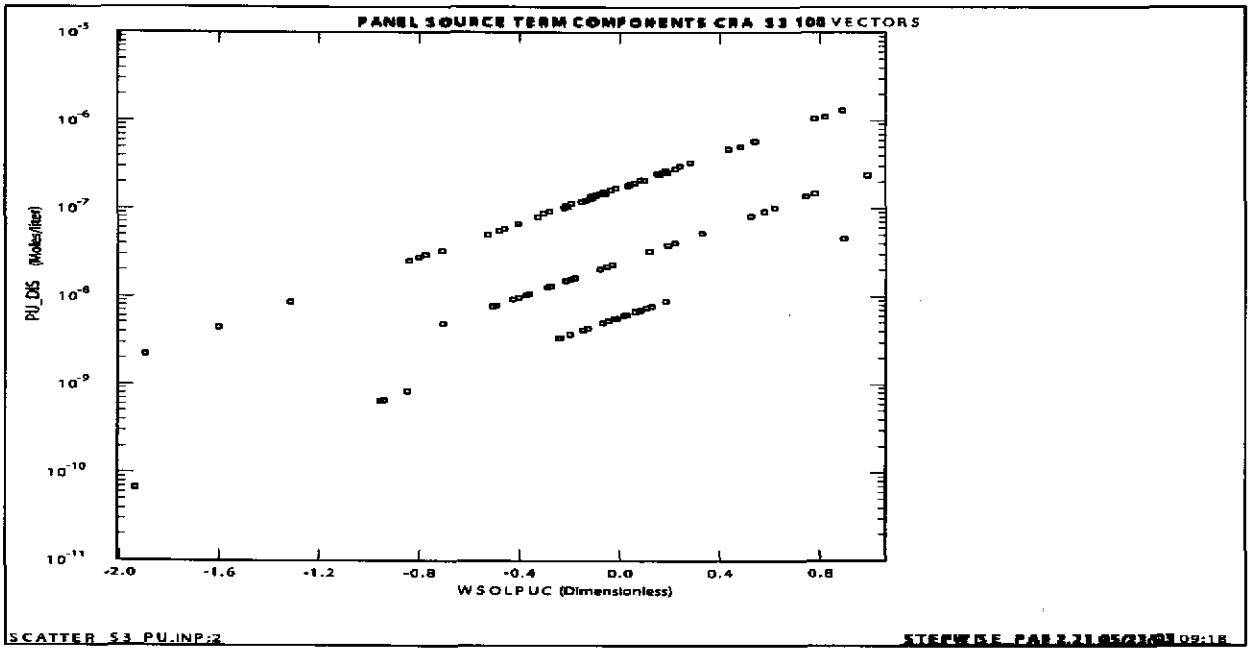
b) CRA1

Figure 17: Scatter Plot of Total Mobilization Potential for Pu in Salado Brine.

Part a) shows results from the CRA-2004 PABC. Part b) shows results from the CRA-2004.



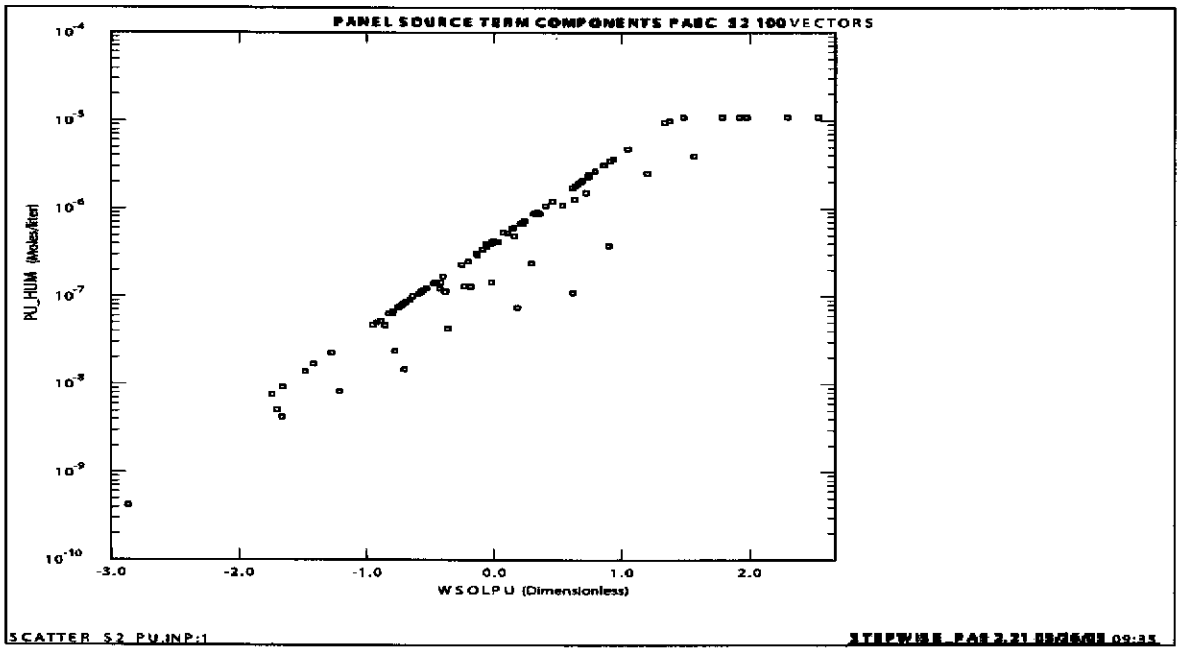
a) PABC



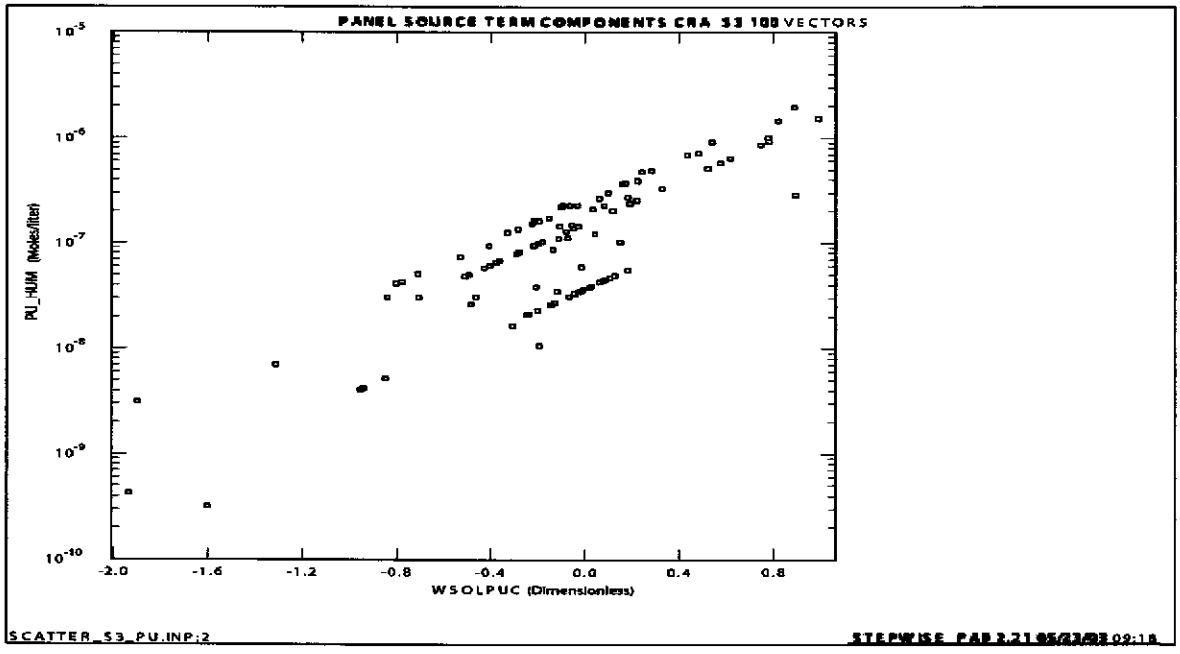
b) CRA1

Figure 18: Scatter Plot of Dissolution Potential for Pu in Castile Brine for all 100 Vectors in Scenario S1, Replicate 1.

Part a) shows results from the CRA-2004 PABC. Part b) shows results from the CRA-2004.



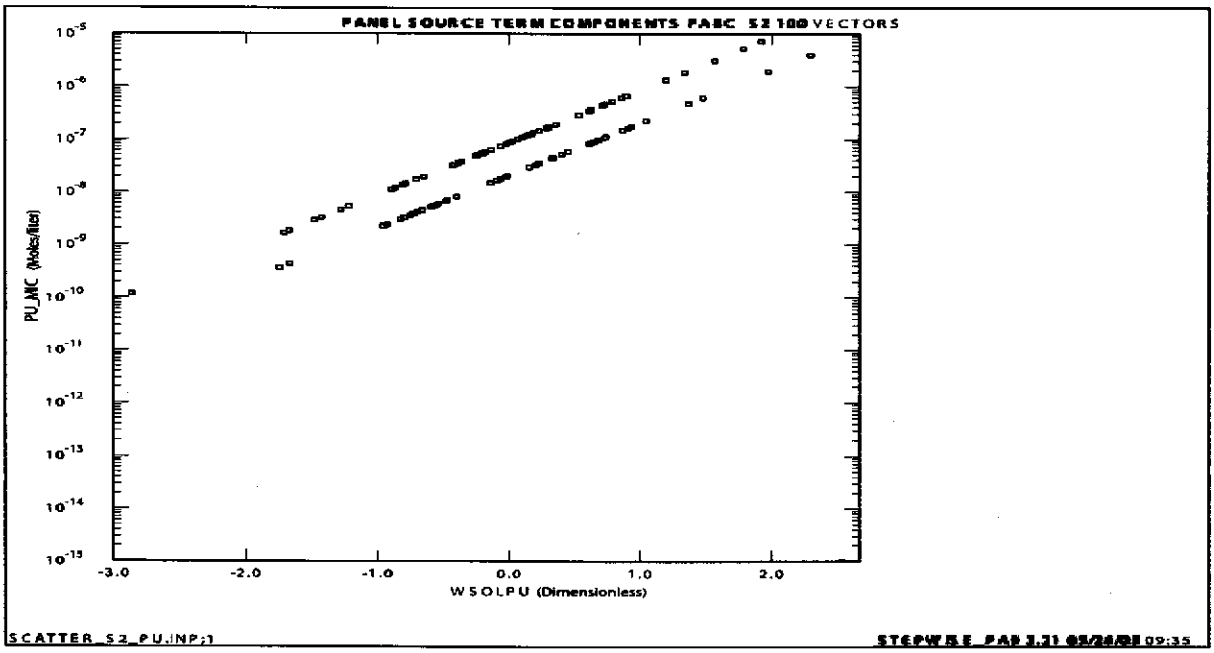
a) PABC



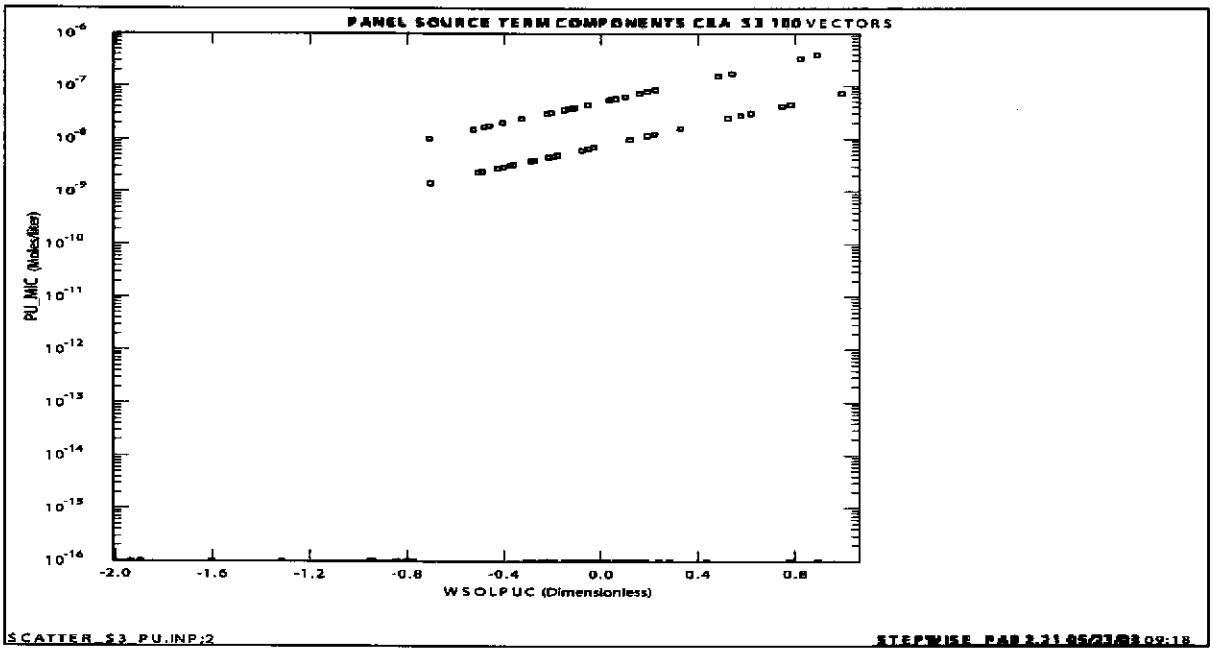
b) CRA1

Figure 19: Scatter Plot of Mobilization Potential for Humic Colloids for Pu in Castile Brine for all 100 Vectors in Scenario S1, Replicate 1.

Part a) shows results from the CRA-2004 PABC. Part b) shows results from the CRA-2004.



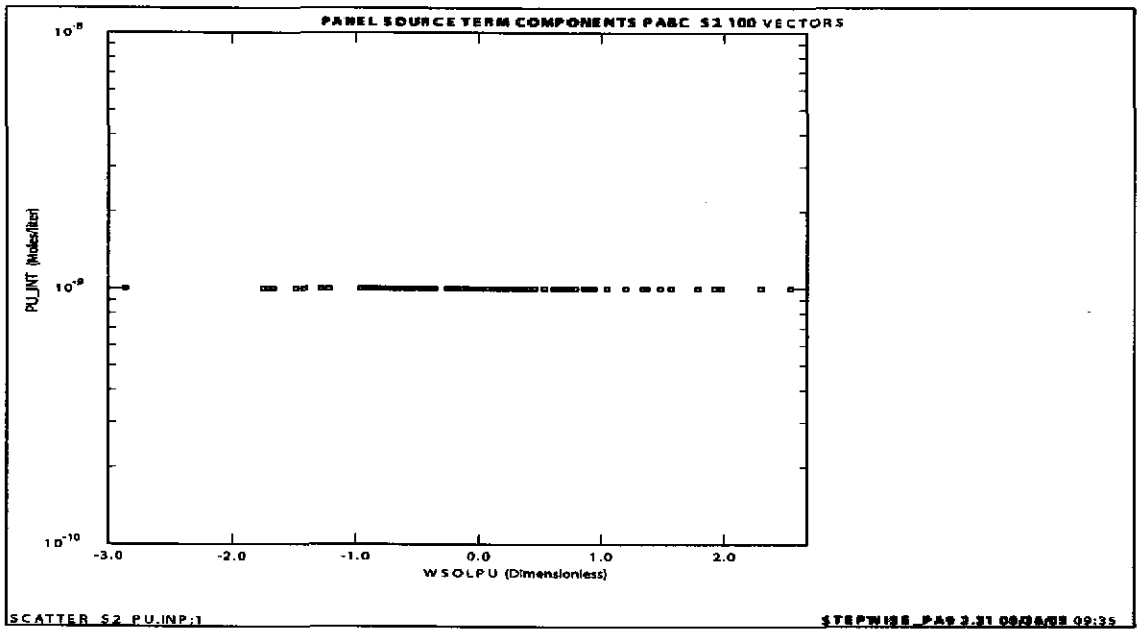
a) PABC



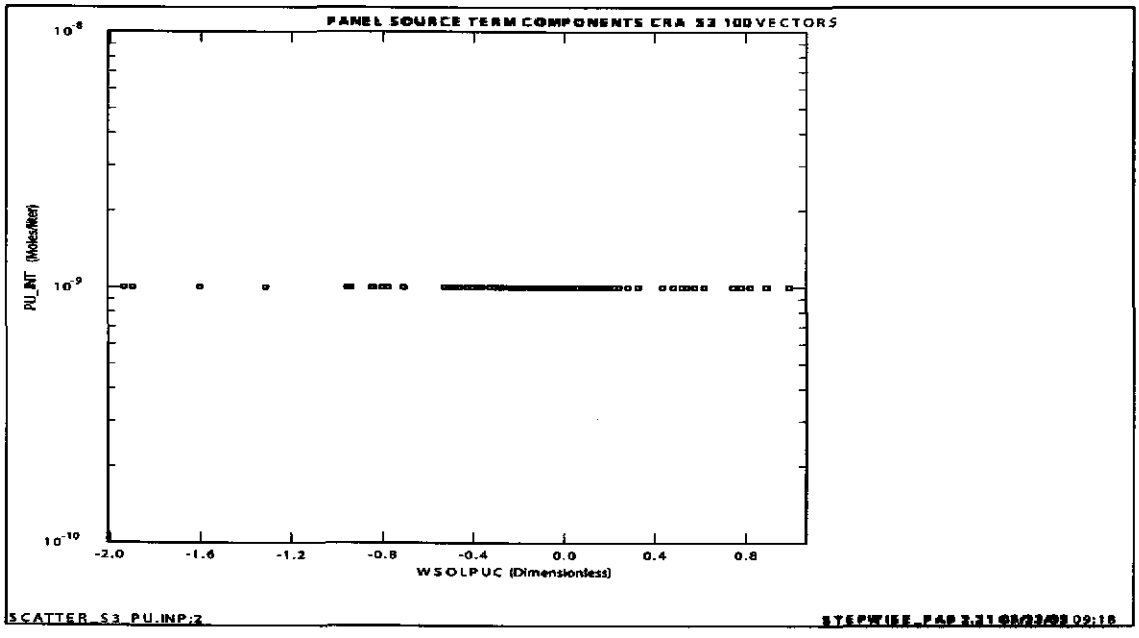
b) CRA1

Figure 20: Scatter Plot of Mobilization Potential for Microbial Colloids for Pu in Castile Brine for all 100 Vectors in Scenario S1, Replicate 1.

Part a) shows results from the CRA-2004 PABC. Part b) shows results from the CRA-2004.



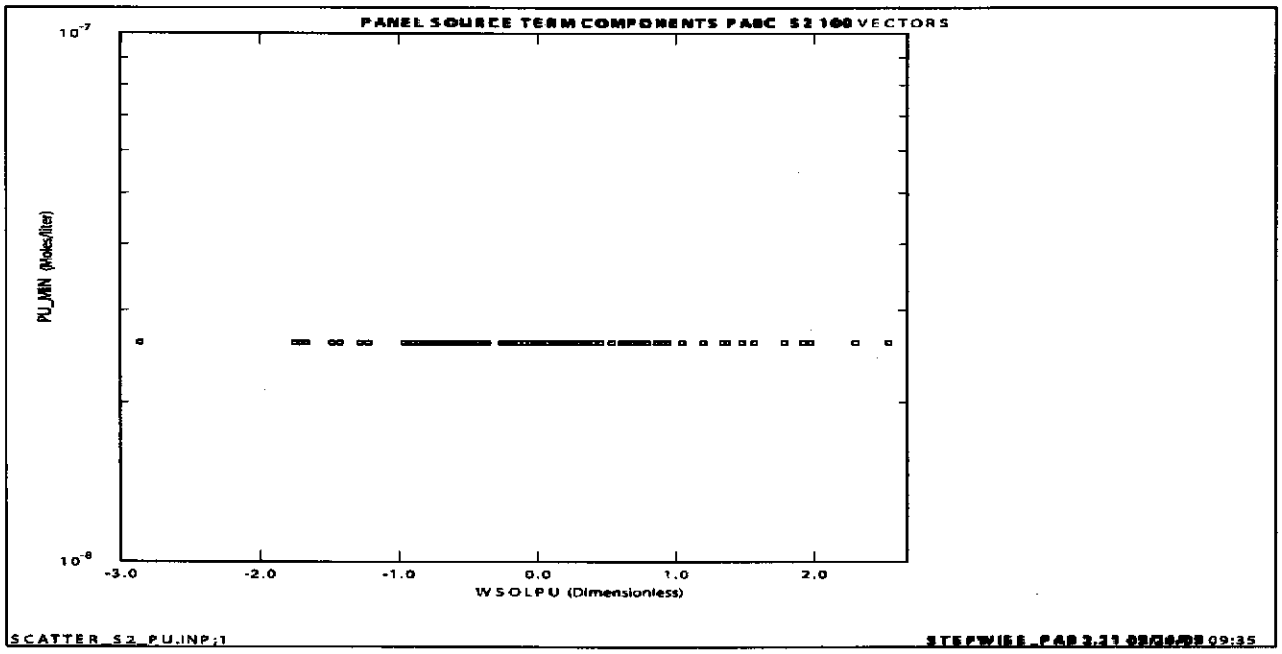
a) PABC



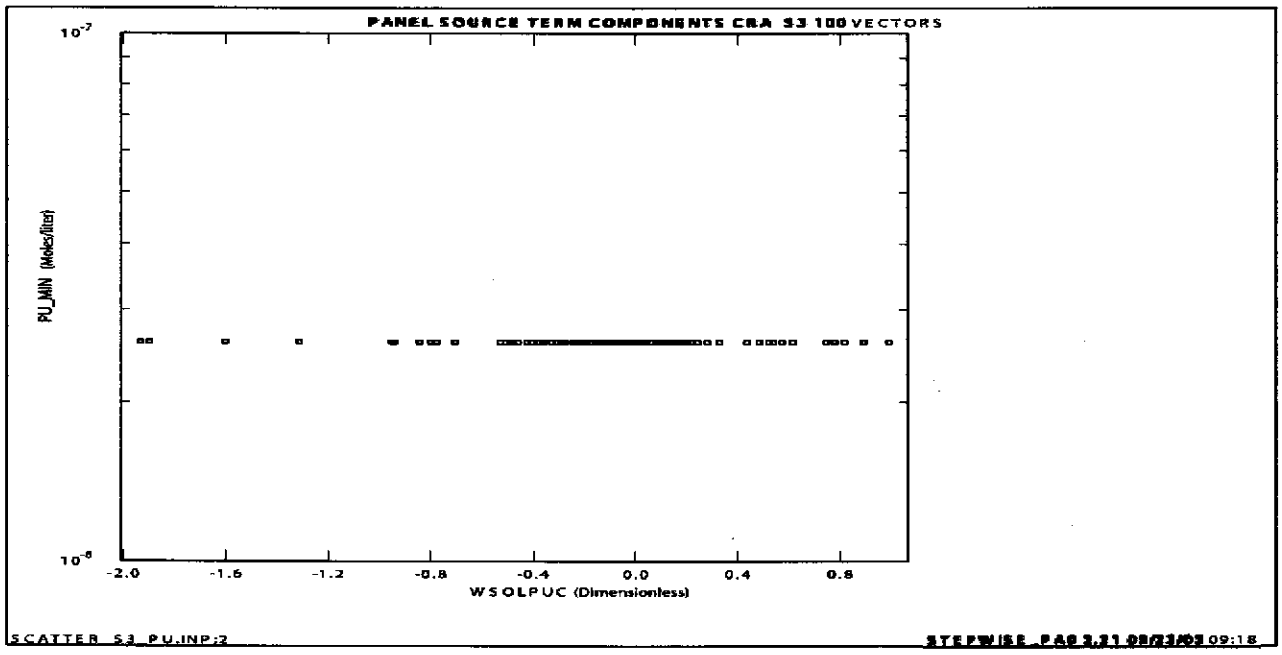
b) CRA1

Figure 21: Scatter Plot of Mobilization Potential for Intrinsic Colloids for Pu in Castile Brine for all 100 Vectors in Scenario S1, Replicate 1.

Part a) shows results from the CRA-2004 PABC. Part b) shows results from the CRA-2004.



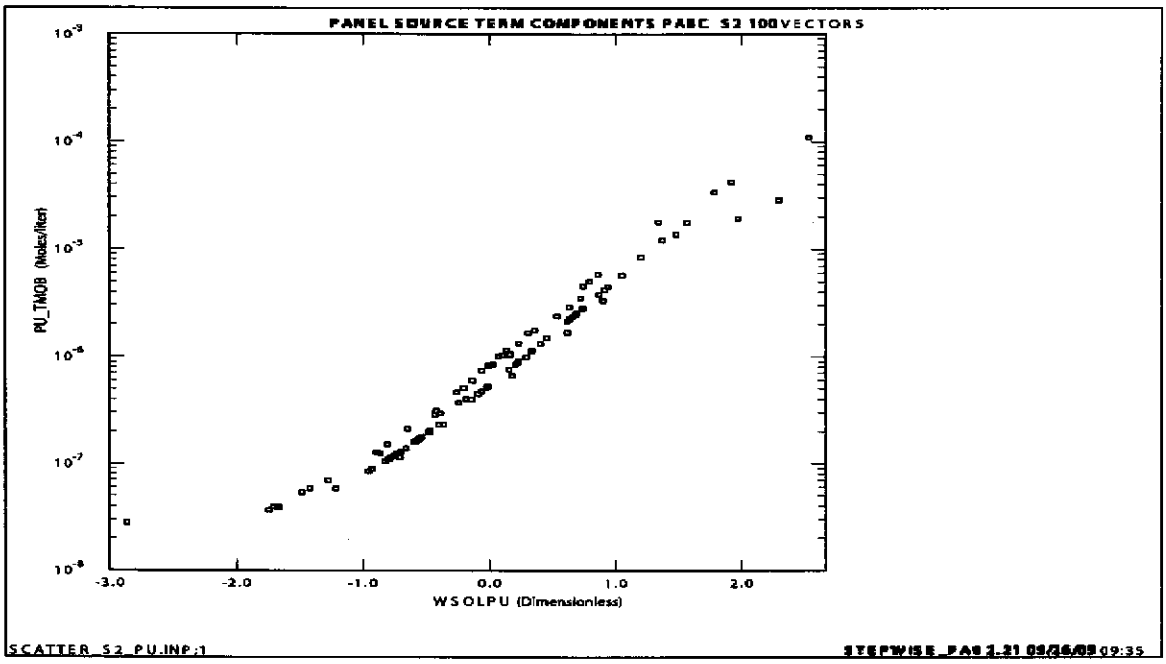
a) PABC



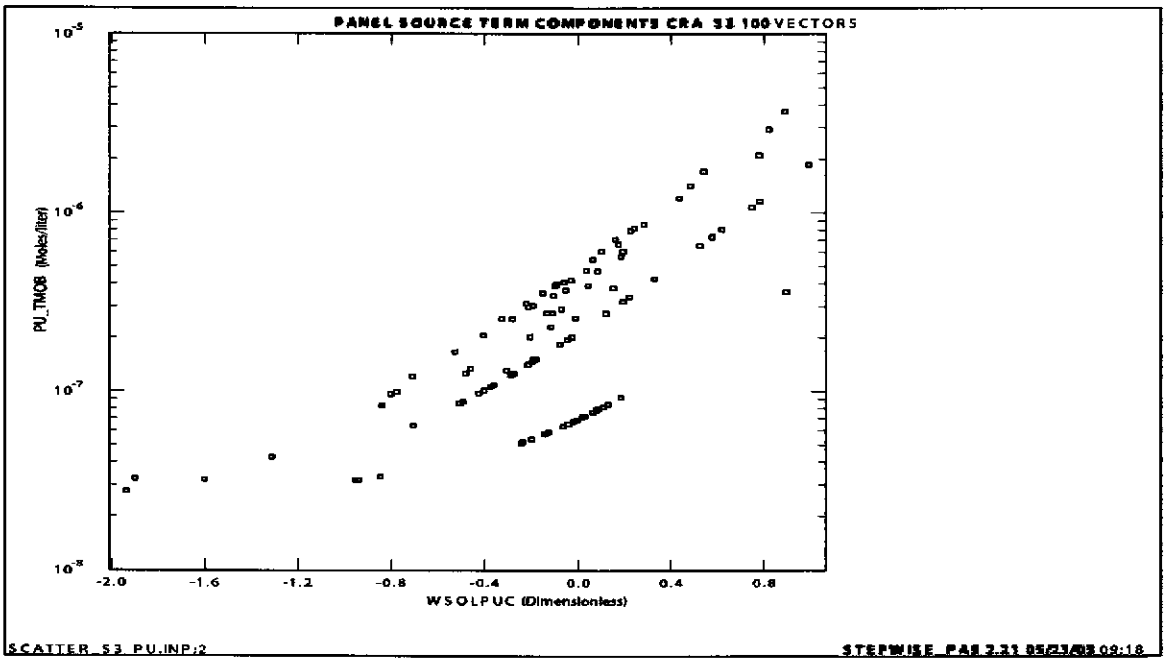
b) CRA1

Figure 22: Scatter Plot of Mobilization Potential for Mineral Fragments for Pu in Castile Brine for all 100 Vectors in Scenario S1, Replicate 1.

Part a) shows results from the CRA-2004 PABC. Part b) shows results from the CRA-2004.



a) PABC



b) CRA1

Figure 23: Scatter Plot of Total Potential Mobilized Pu in Castile Brine.

Part a) shows results from the CRA-2004 PABC. Part b) shows results from the CRA-2004.

5.2 RADIONUCLIDE DECAY

PANEL was run in the DECAY mode with the entire WIPP inventory so that plots can be generated to show how the radionuclide inventory changes over the 10,000-year regulatory period. Figures 24 to 29 show the results of these decay calculations. Figures 24 through 29 are simple x-y plots with both the CRA-2004 results (Part b in each figure) and the CRA-2004 PABC results (Part a in each figure) presented. Each x-y plot shows an isotopic component as the dependent variable (ordinate) in EPA Units and the time as the independent variable (abscissa). Table 16 provides definitions for the variables plotted in Figures 24 through 29.

Table 16. Definitions of Variables Plotted in Figures 24 through 29

Name	Type/Units	Description
SDETOTAL	EPA Units	Total Activity
SDEPU239	EPA Units	Activity of PU239
SDEPU240	EPA Units	Activity of PU240
SDEPU242	EPA Units	Activity of PU242
SDEAM241	EPA Units	Activity of AM241
SDEPU238	EPA Units	Activity of PU238
SDEU233	EPA Units	Activity of U233
SDEU234	EPA Units	Activity of U234
SDEU238	EPA Units	Activity of U238
SDEU236	EPA Units	Activity of U236
SDEU235	EPA Units	Activity of U235
SDETH229	EPA Units	Activity of TH229
SDETH230	EPA Units	Activity of TH230
SDENP237	EPA Units	Activity of NP237
SDERA226	EPA Units	Activity of RA226
SDETH232	EPA Units	Activity of TH232
SDEAM243	EPA Units	Activity of AM243
SDECM245	EPA Units	Activity of CM245
SDECS137	EPA Units	Activity of CS137
SDESR90	EPA Units	Activity of SR90
SDEPB210	EPA Units	Activity of PB210
SDEPA231	EPA Units	Activity of PA231
SDECM248	EPA Units	Activity of CM248
SDEPU244	EPA Units	Activity of PU244
SDECM243	EPA Units	Activity of CM243
SDERA228	EPA Units	Activity of RA228
SDEPU241	EPA Units	Activity of PU241
SDECM244	EPA Units	Activity of CM244
SDECF252	EPA Units	Activity of CF252
LDETOTAL	EPA Units	Lumped Activity of TOTAL
LDEPU239	EPA Units	Lumped Activity of PU239
LDETH230	EPA Units	Lumped Activity of TH230
LDEU234	EPA Units	Lumped Activity of U234
LDEAM241	EPA Units	Lumped Activity of AM241
LDEPU238	EPA Units	Lumped Activity of PU238

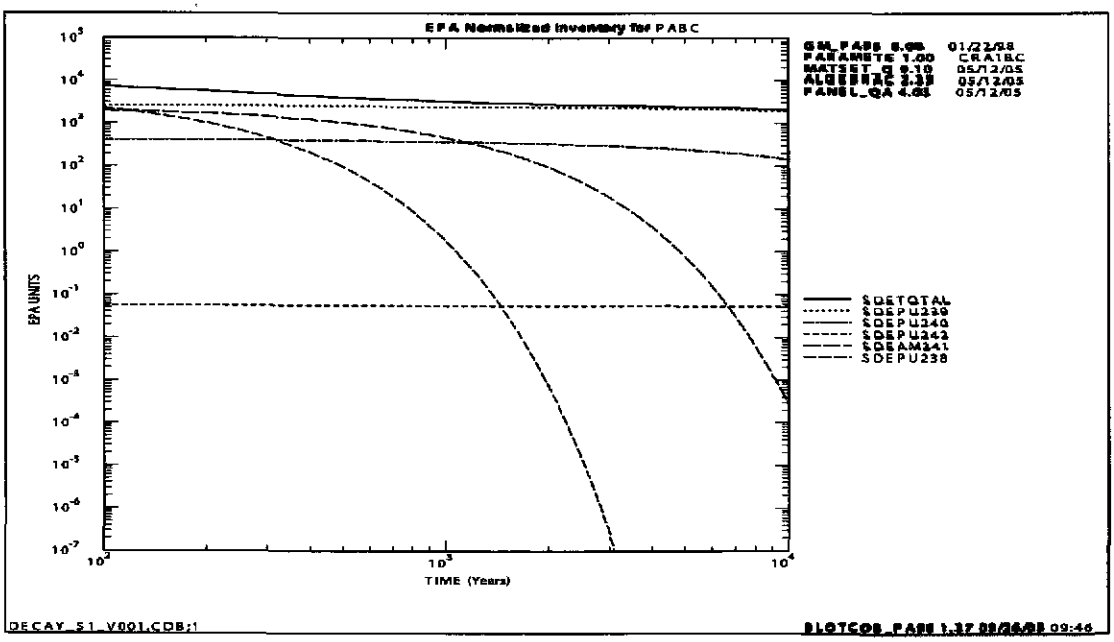
The total radionuclide inventory for CRA-2004 was 2.98E+06 Ci. The total radionuclide inventory for CRA-2004 PABC is 2.32E+06 Ci. Figures 24 through 29 indicate that while the

radionuclide inventory decreased in CRA-2004 PABC, the overall differences were minor since EPA Units are normalized by f_w.

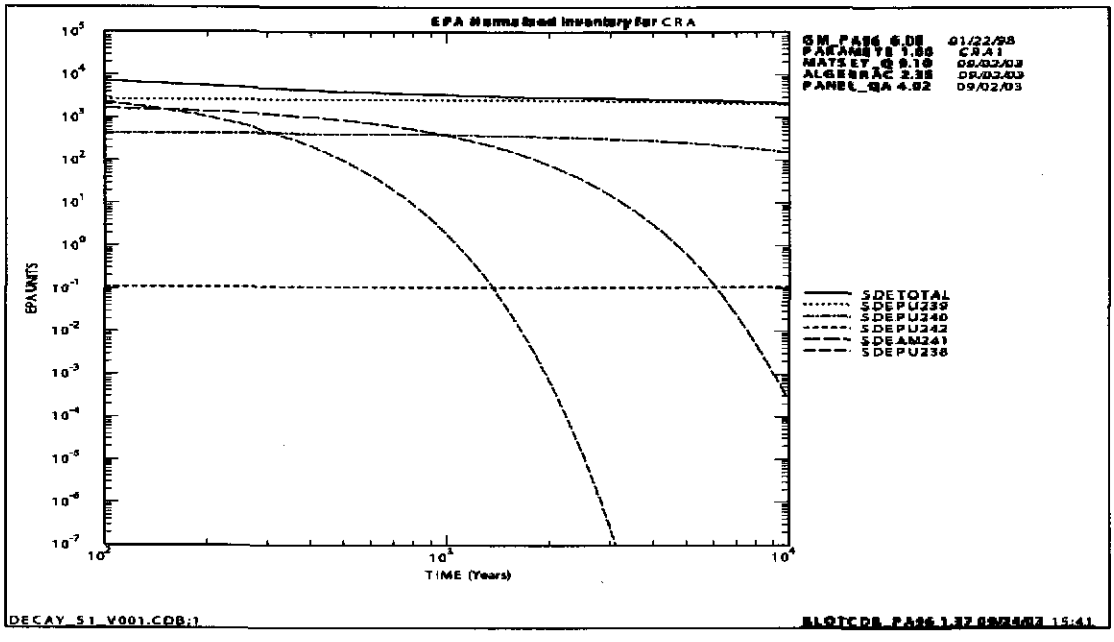
Figure 24 shows the decay behavior for the Am and Pu isotopes over time. In general, the Pu isotopic inventory is steady over time with the exception of Pu238 which decays away by about 2000 years. In addition, Am241 decays away over time with the final inventory of Am241 at 10,000 years about 10^{-7} of the initial inventory.

Figure 25 shows the decay behavior of the U isotopes over time. The U isotopes are fairly steady over time with U234 and U235 isotopes increasing slightly over time. Figure 27 shows the decay behavior for the fission products: Sr90 and Cs137. Both of these isotopes decay away before 2000 years. The time dependent behavior of various minor isotopes is shown in Figure 28.

The time dependent behavior of the lumped radionuclides (Figure 29) is directly attributable to the component radionuclides in the lumped radionuclides. Therefore, the AM241L behavior is like that of Am241 (Figure 24). The PU239L behavior is like that of Pu239 (Figure 24). The U234L behavior is like that of U234 (Figure 25). The PU238L behavior is like that of Pu238 (Figure 24). The TH230L behavior is like that of TH230 (Figure 26).



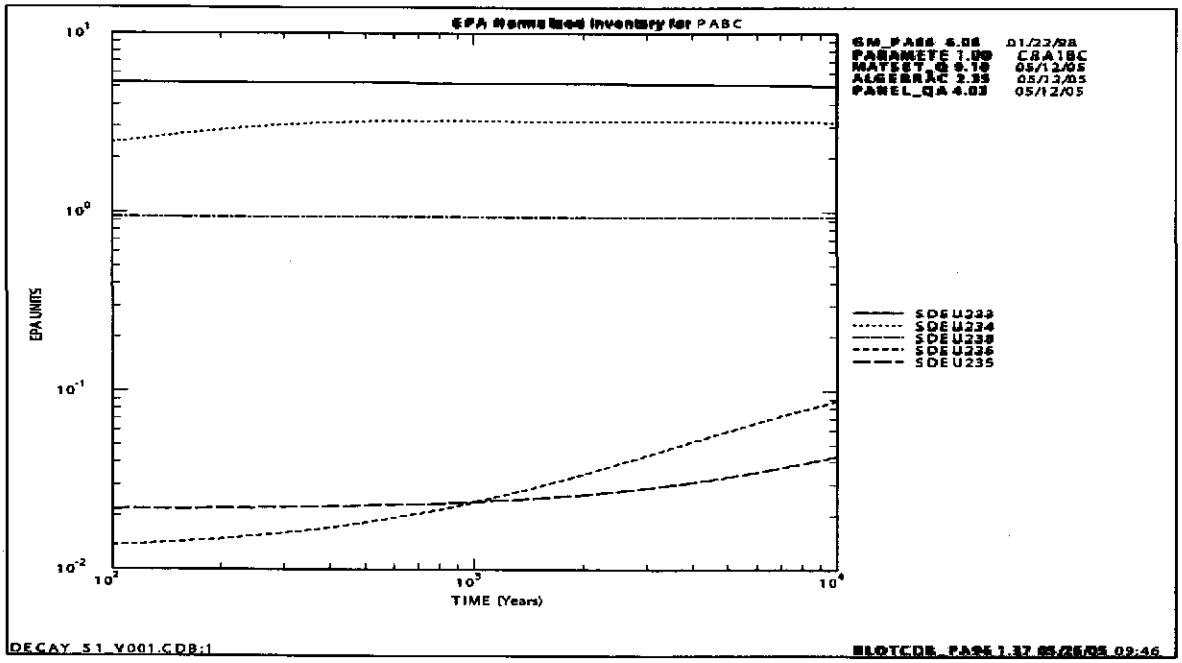
a) PABC



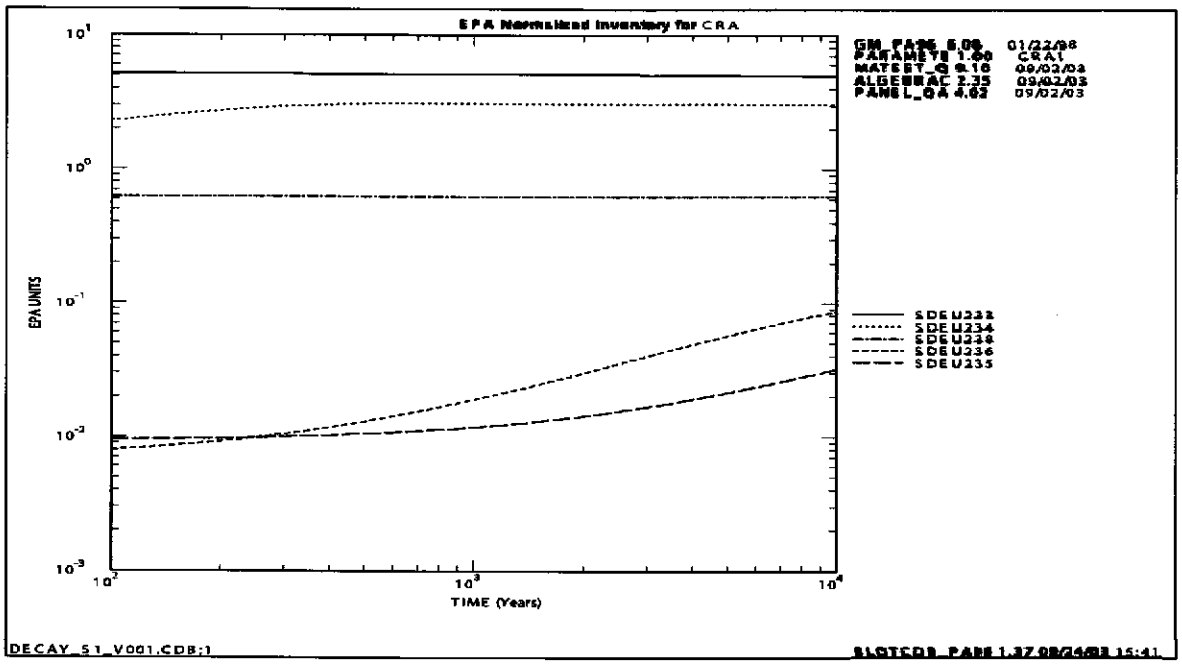
b) CRA1

Figure 24: Time dependent inventories of Am and Pu isotopes.

Part a) shows results from the CRA-2004 PABC. Part b) shows results from the CRA-2004.



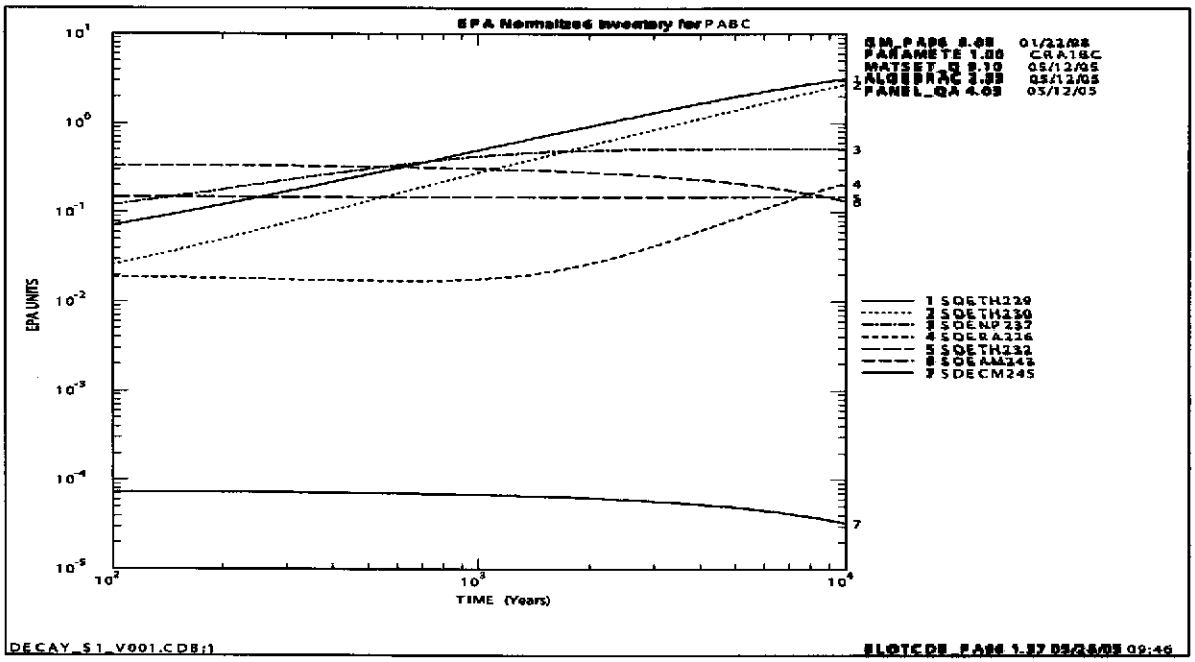
a) PABC



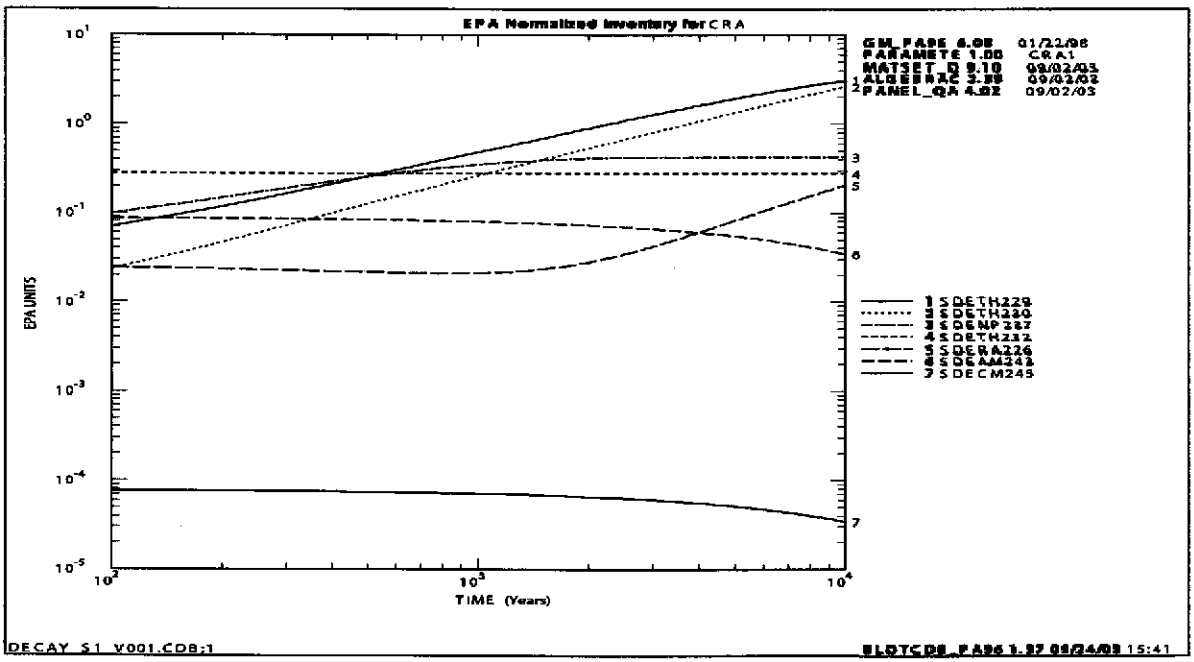
b) CRA1

Figure 25: Time dependent inventories of U isotopes.

Part a) shows results from the CRA-2004 PABC. Part b) shows results from the CRA-2004 PA.



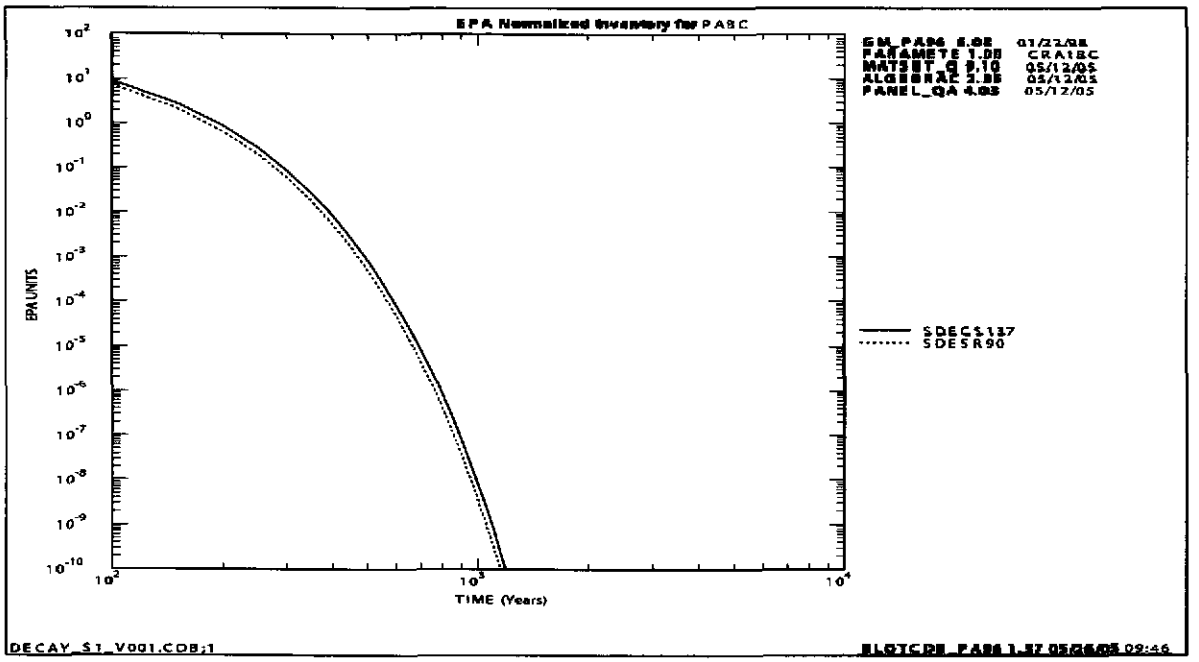
a) PABC



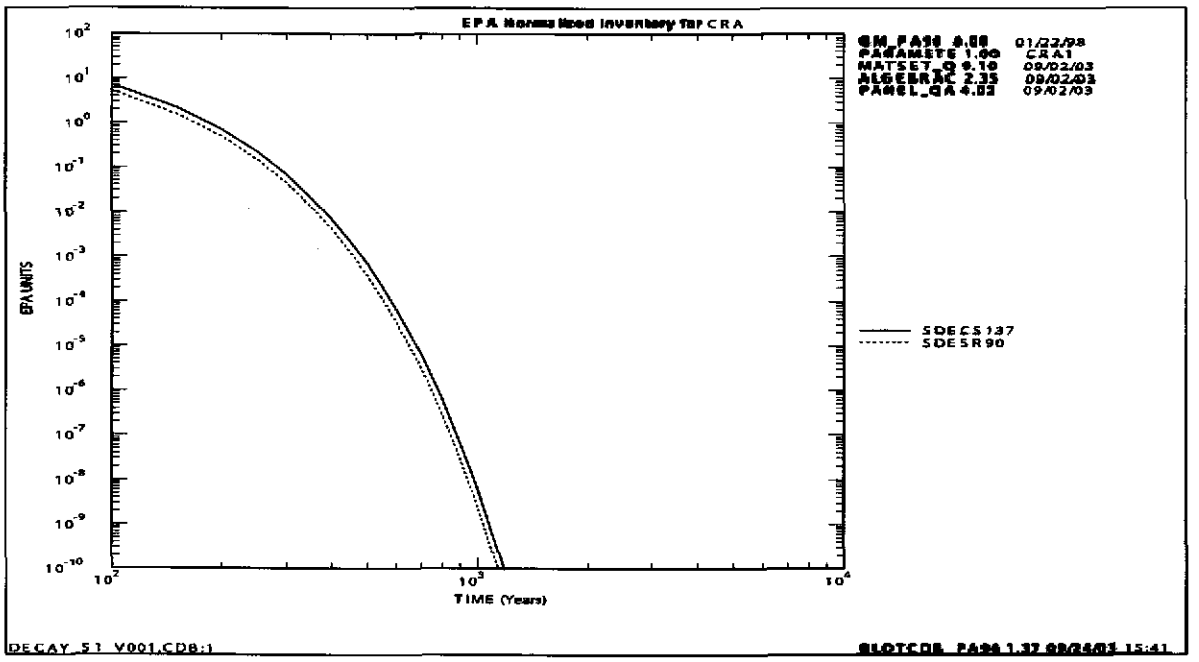
b) CRA1

Figure 26: Time dependent inventories of various isotopes.

Part a) shows results from the CRA-2004 PABC. Part b) shows results from the CRA-2004.



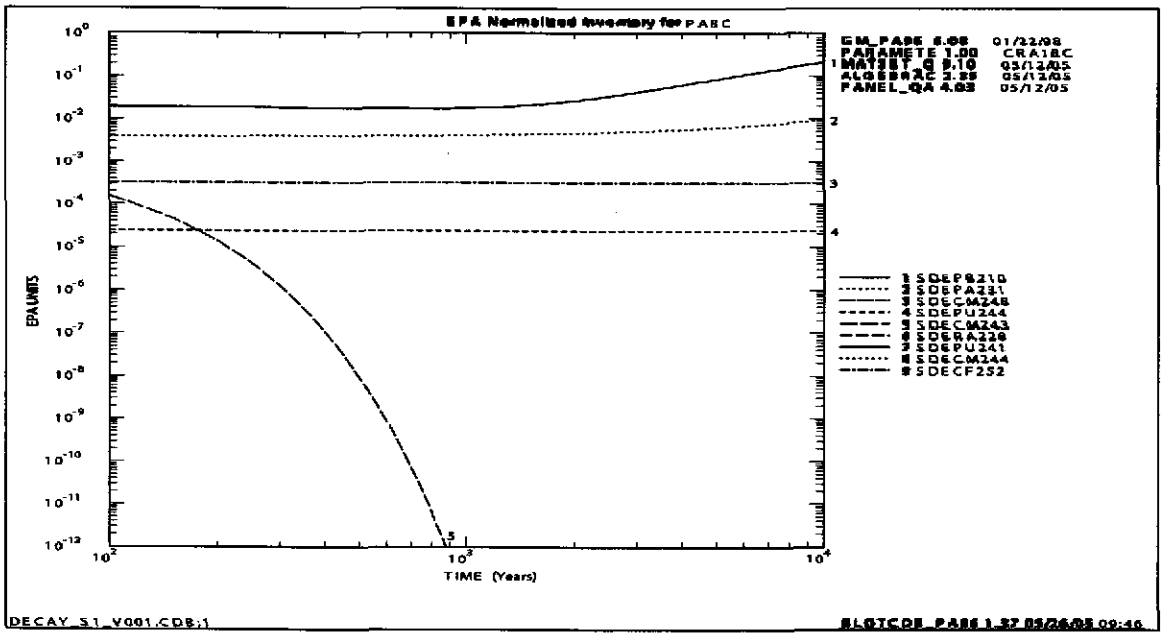
a) PABC



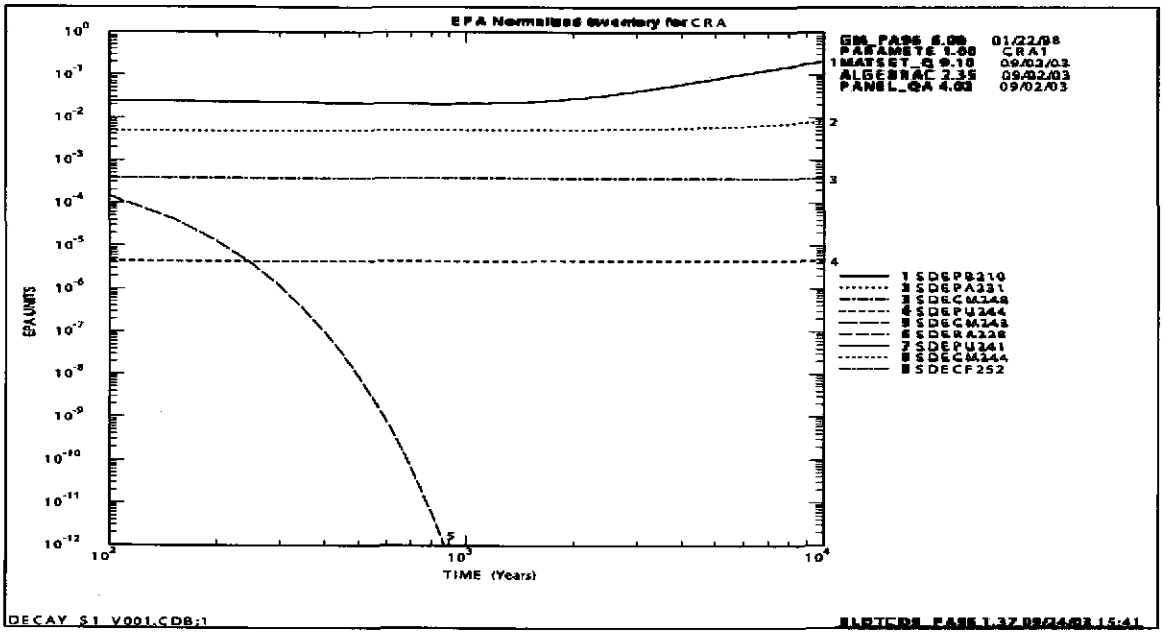
b) CRA1

Figure 27: Time dependent inventories of Sr and Cs isotopes.

Part a) shows results from the CRA-2004 PABC. Part b) shows results from the CRA-2004.



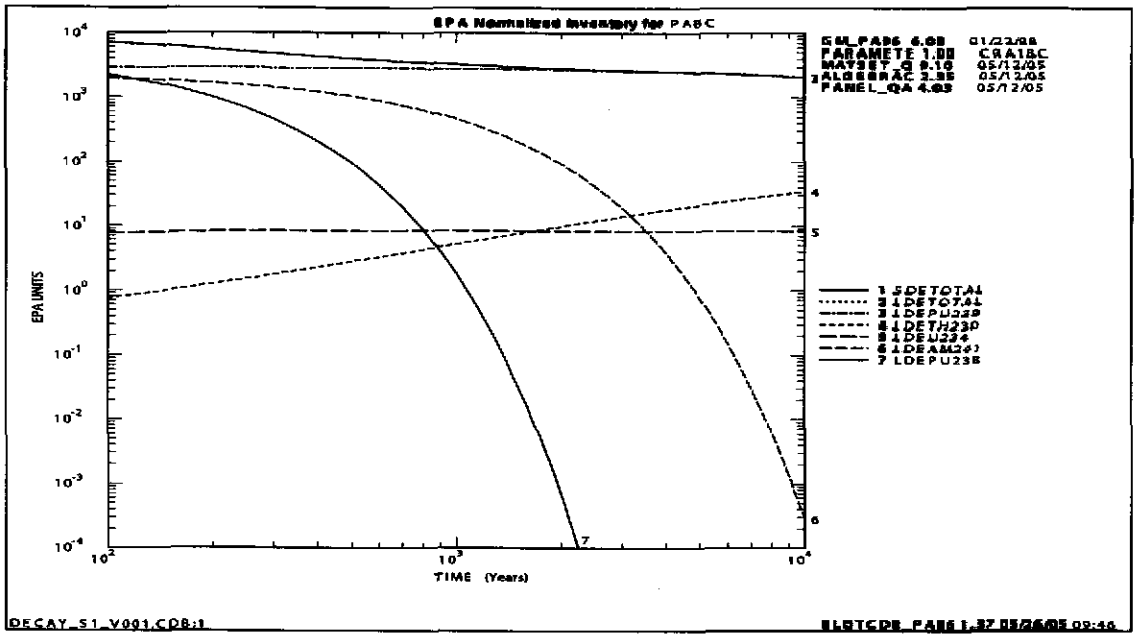
a) PABC



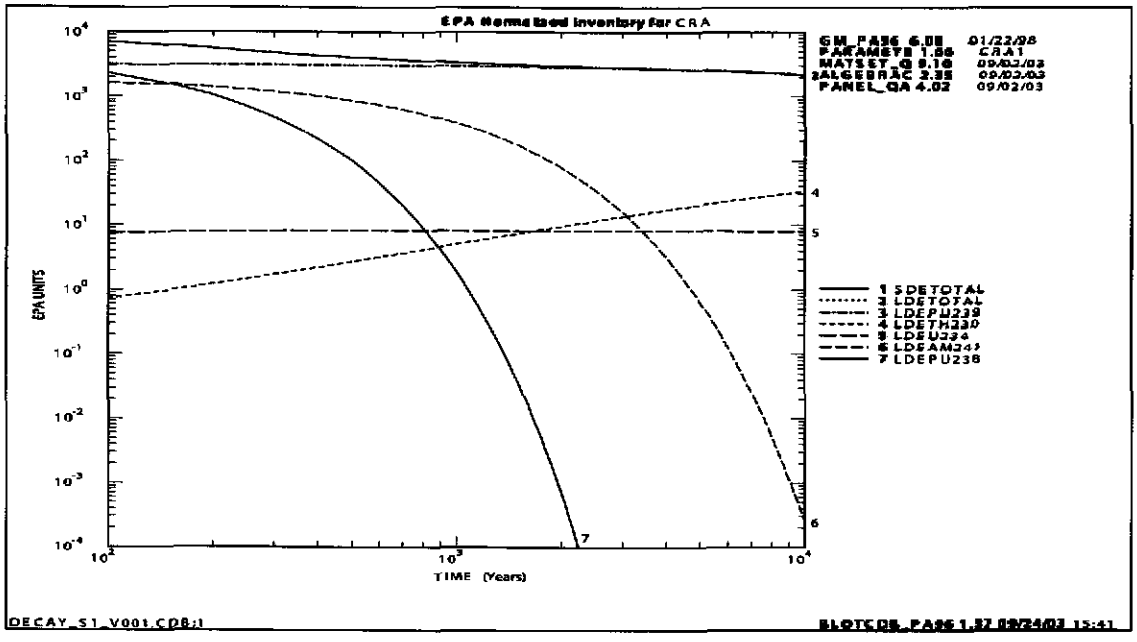
b) CRA1

Figure 28: Time dependent inventories of various minor isotopes.

Part a) shows results from the CRA-2004 PABC. Part b) shows results from the CRA-2004.



a) PABC



b) CRA1

Figure 29: Time dependent inventories of lumped isotopes.

Part a) shows results from the CRA-2004 PABC. Part b) shows results from the CRA-2004 PA.

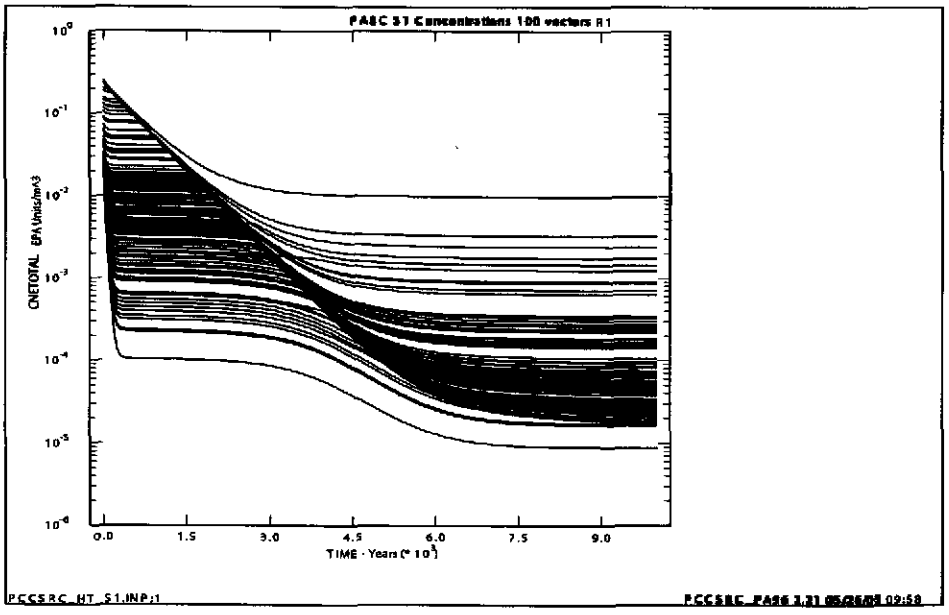
5.3 PANEL CONCENTRATIONS

PANEL concentration results are presented in Figures 30 through 39. Figures 30 through 39 are horsetail plots. "Horsetail" plots show values of individual variables for all vectors in a scenario as a function of time for the entire 10,000-year regulatory compliance period. These plots are an effective method for demonstrating the potential range and behavior of results. Thus, the independent variable (abscissa) in Figures 30 through 39 is time in years. The dependent variable (ordinate) in Figures 30 through 39 is concentration in EPA units per cubic meter.

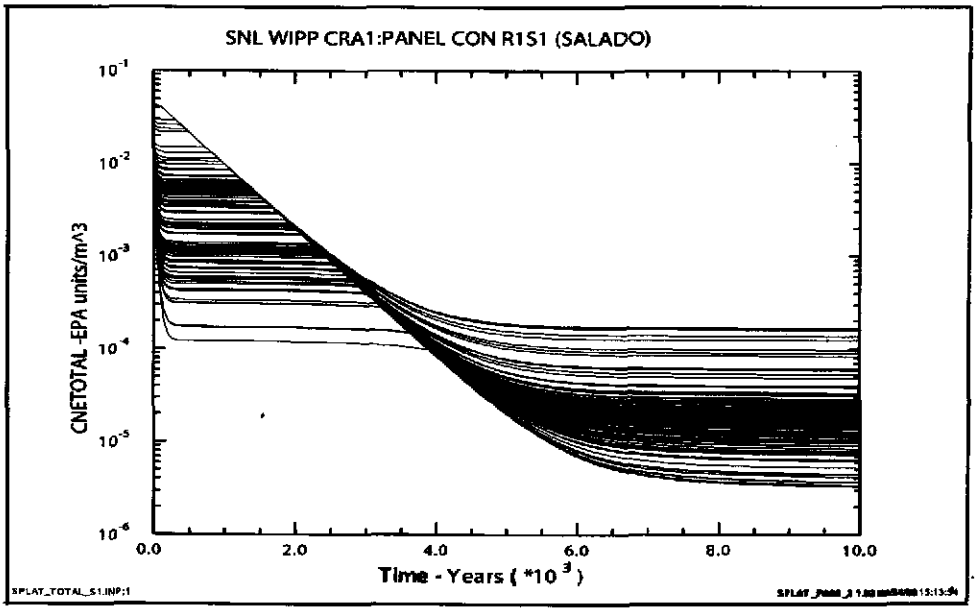
Figure 30 shows the total mobilized concentration (summed for the individual radionuclides from Table 13) in Salado brine in EPA units per cubic meter. Figure 35 shows the total mobilized concentration in Castile brine in EPA units per cubic meter. These concentration values are supplied to CCDFGF to calculate DBR releases. Figures 31, 32, 33, and 34 show the mobilized concentrations for the lumped radionuclides in Salado brine. Figures 36, 37, 38, and 39 show the mobilized concentrations for the lumped radionuclides in Castile brine.

At early times (before 4000 years), the total mobilized concentrations (in both Salado and Castile brines) have their highest values because of the contribution of Am (see Figures 31 and 36). After about 4000 years, the contribution from Am decreases because of the decay of Am241. After about 4000 years, the total mobilized concentrations are dominated by Pu (see Figures 32 and 37). U and Th contributions are orders of magnitudes lower than Pu (see Figures 33, 34, 38 and 39).

CRA-2004 PABC results for total mobilized concentrations show more variability (more spread in the curves) than seen in the CRA-2004 results. More variability in the CRA-2004 PABC results is understandable because in general the variability in solubility was increased for the CRA-2004 PABC.



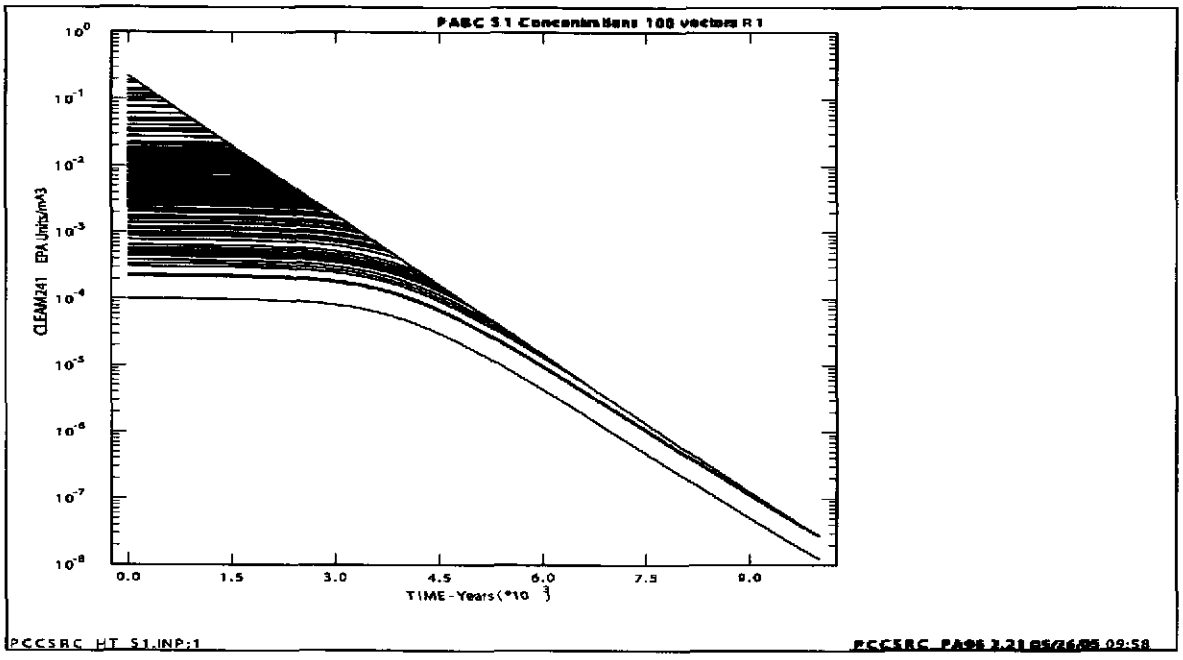
a) PABC



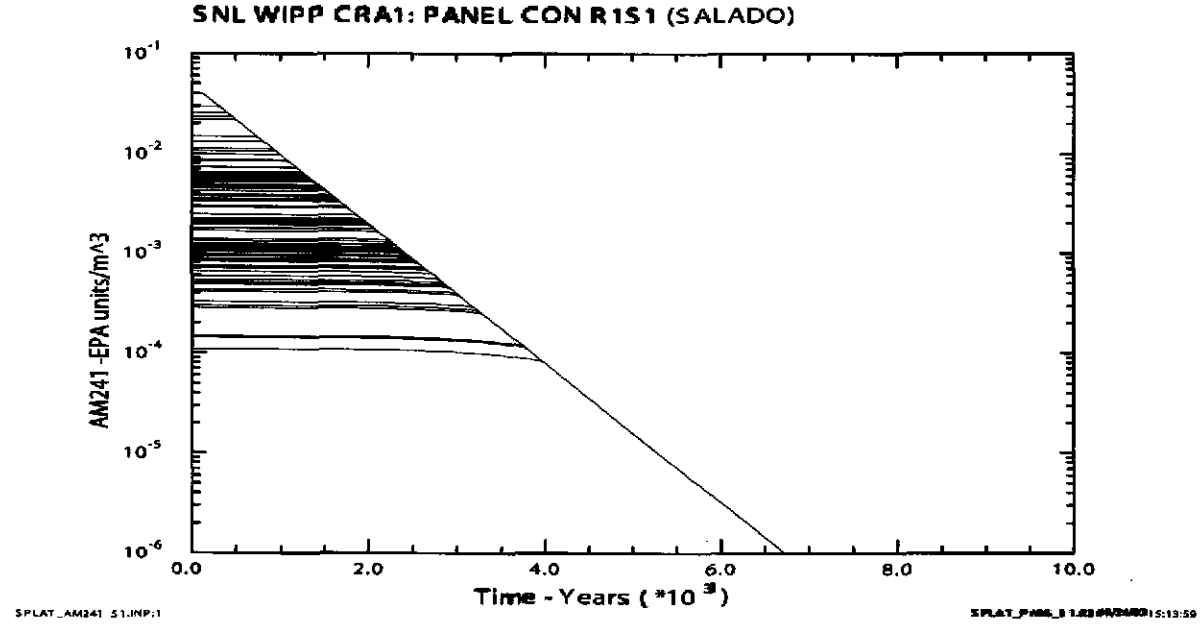
b) CRA1

Figure 30: Time dependent total concentrations in Salado brine.

Part a) shows results from the CRA-2004 PABC. Part b) shows results from the CRA-2004.



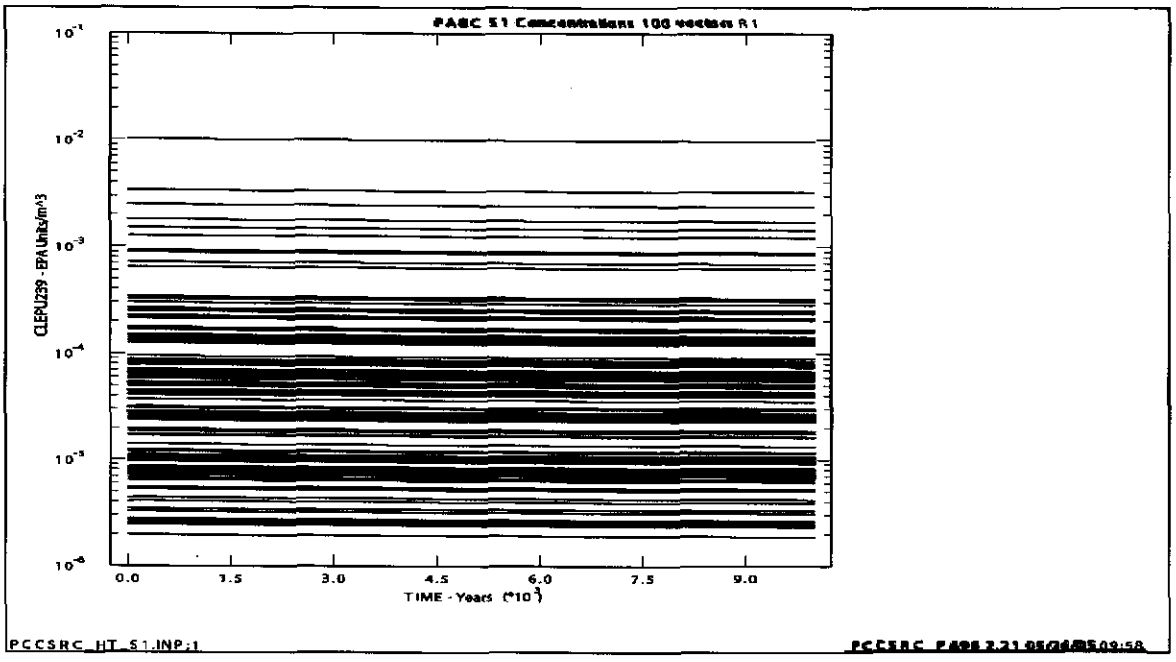
a) PABC



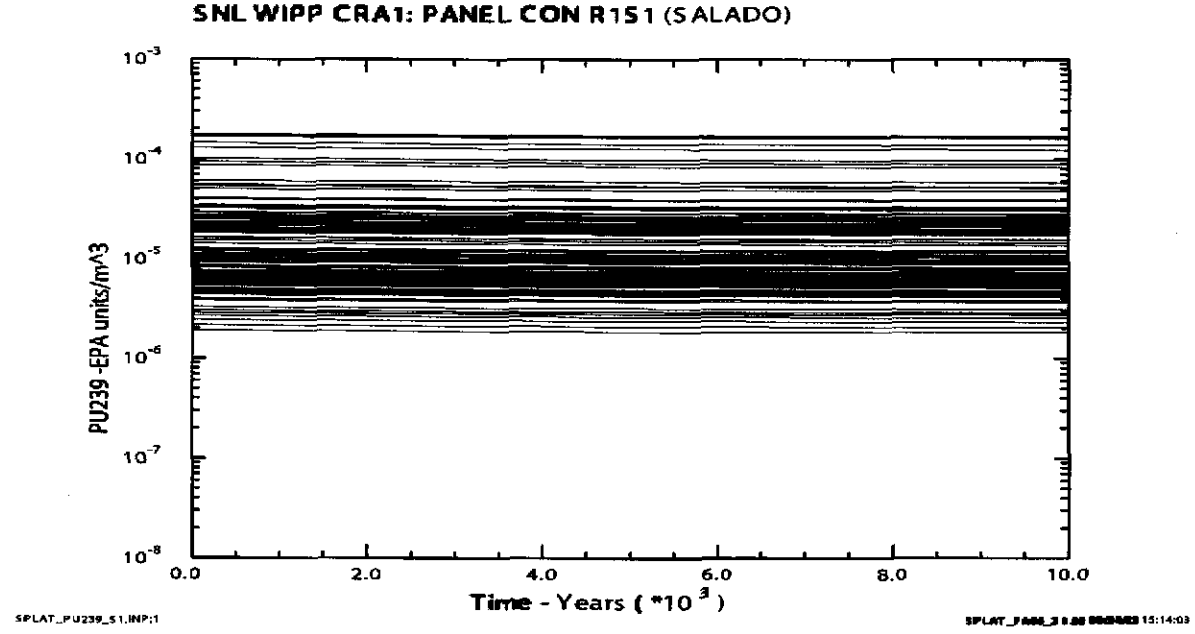
b) CRA1

Figure 31: Time dependent AM241L concentration in Salado brine.

Part a) shows results from the CRA-2004 PABC. Part b) shows results from the CRA-2004.



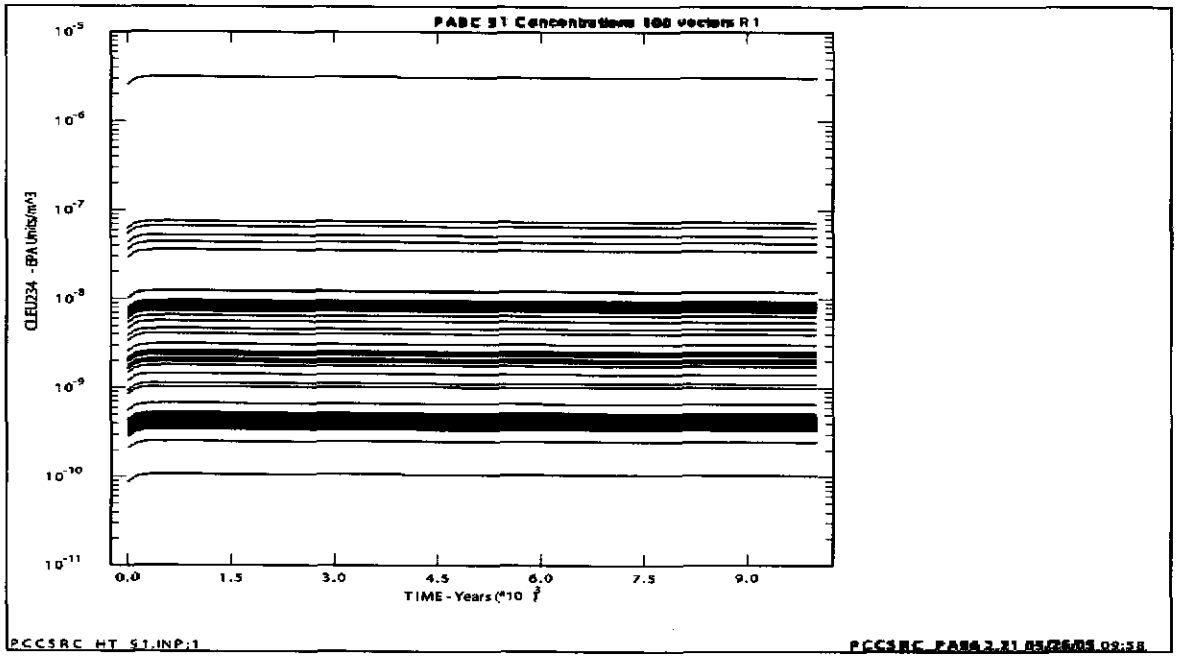
a) PABC



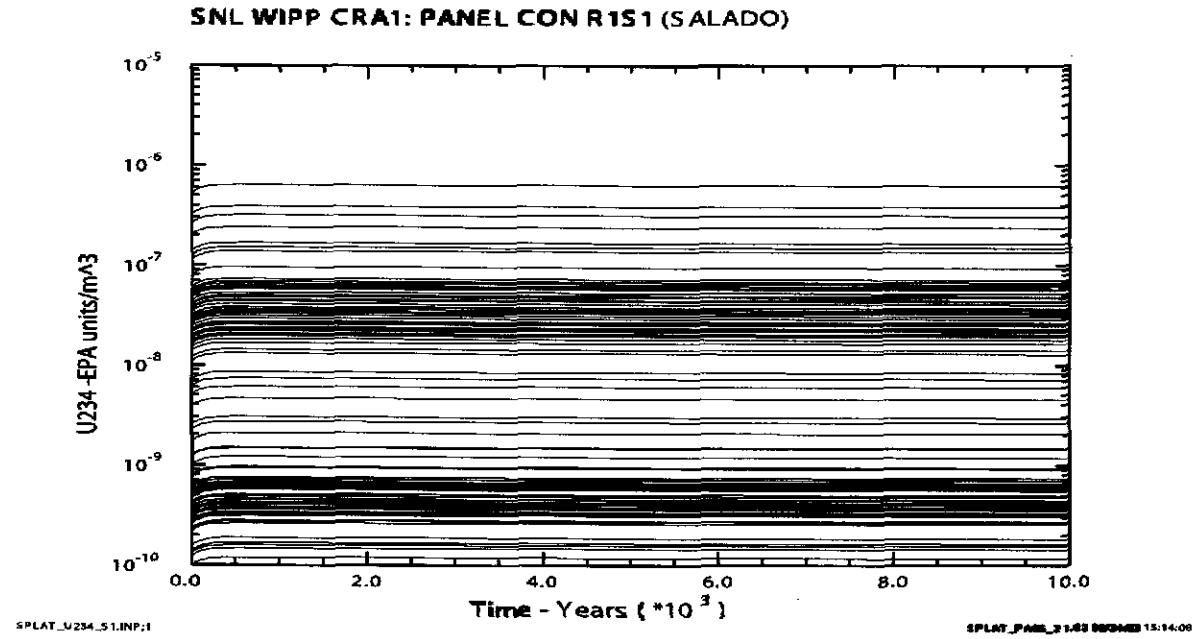
b) CRA1

Figure 32: Time dependent PU239L concentration in Salado brine.

Part a) shows results from the CRA-2004 PABC. Part b) shows results from the CRA-2004.



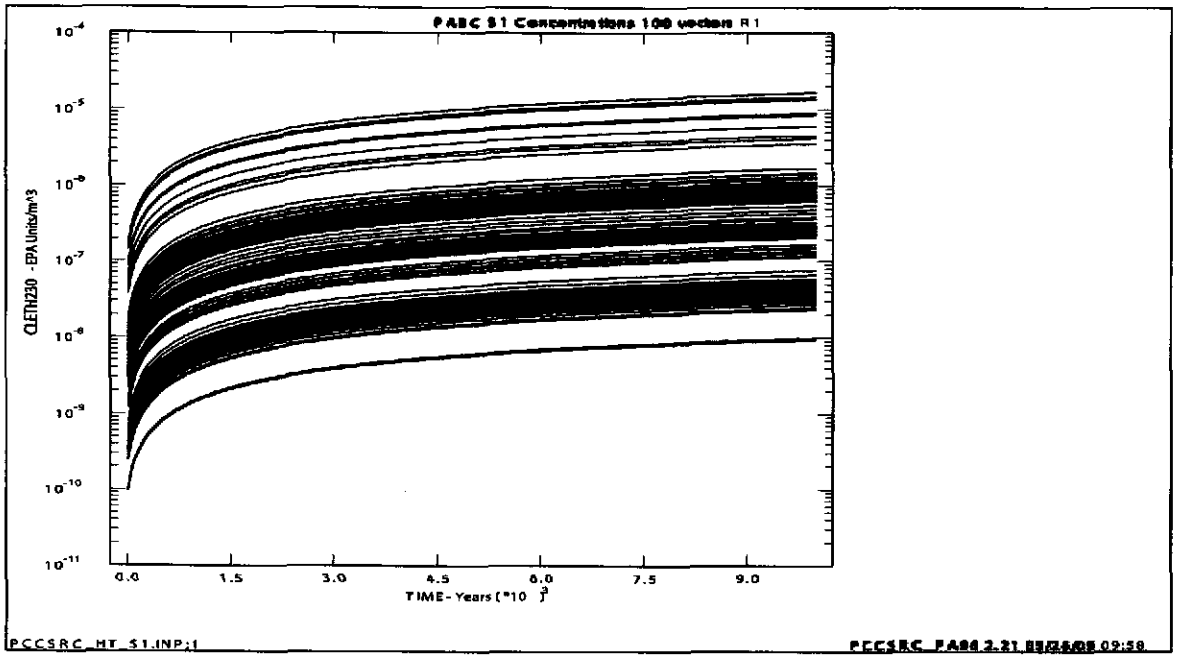
a) PABC



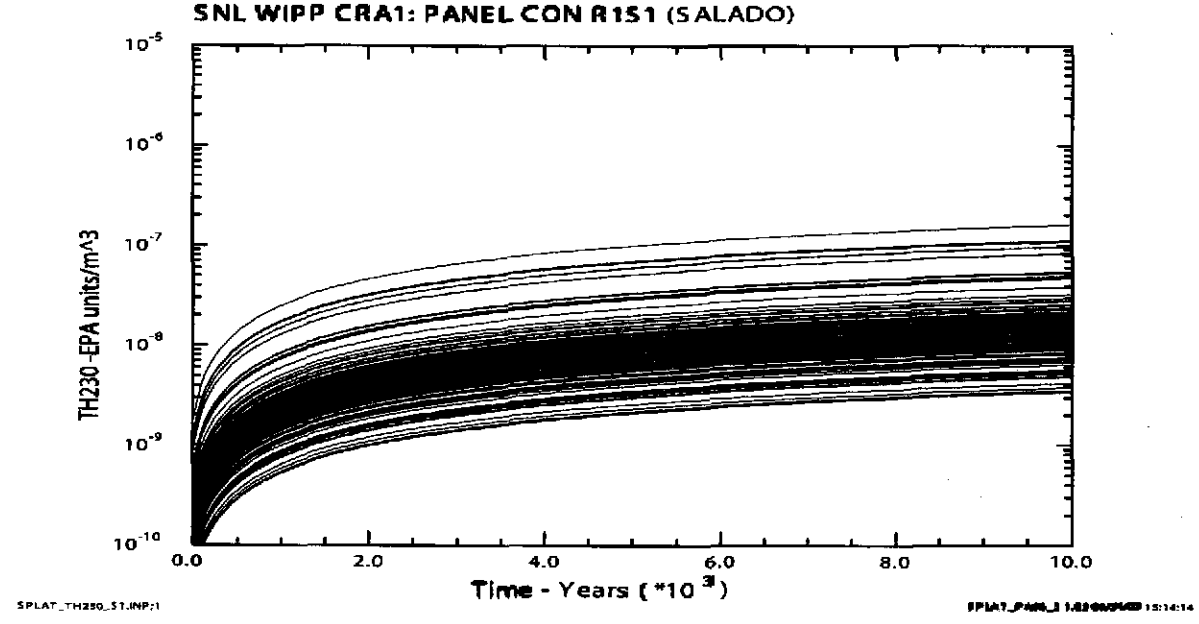
b) CRA1

Figure 33: Time dependent U234L concentration in Salado brine.

Part a) shows results from the CRA-2004 PABC. Part b) shows results from the CRA-2004.



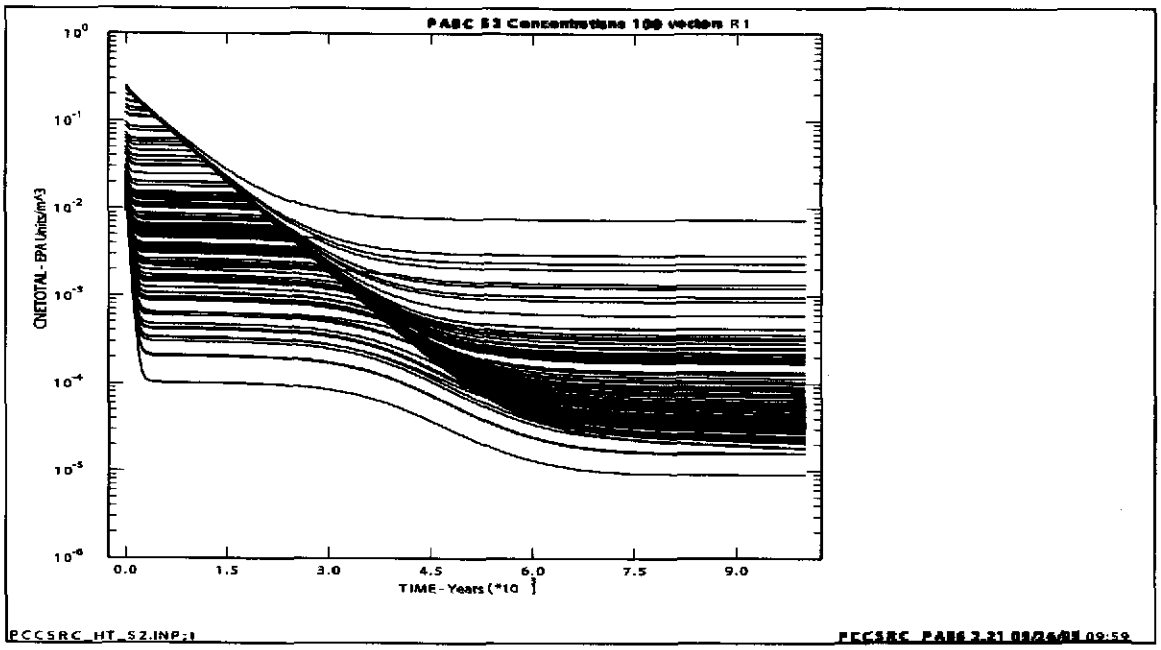
a) PABC



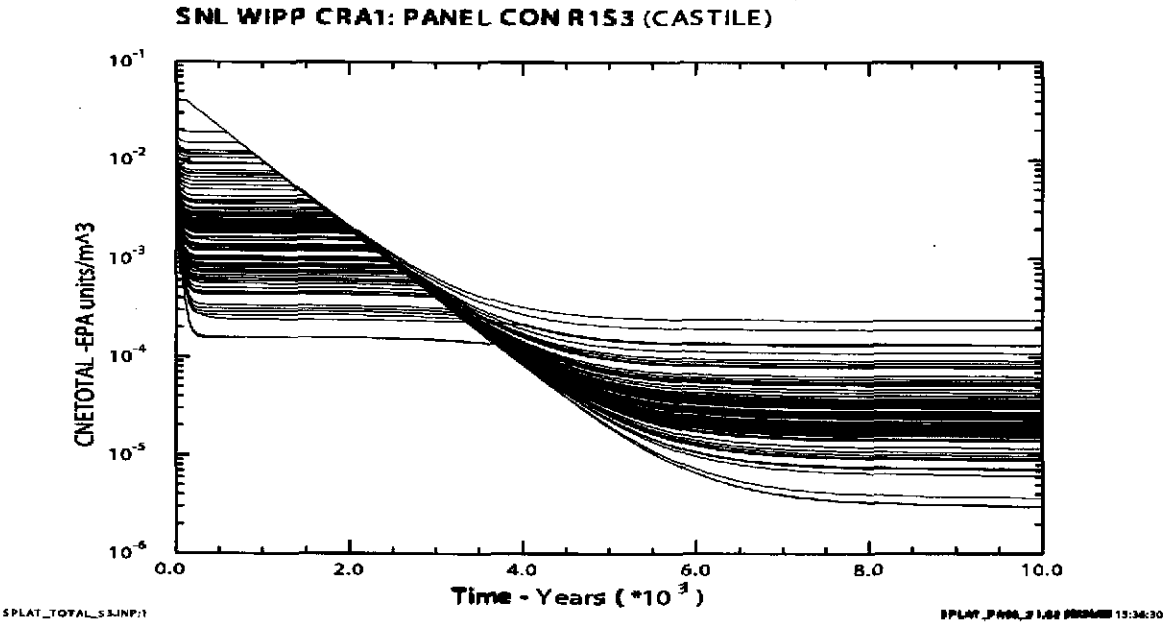
b) CRA1

Figure 34: Time dependent TH230L concentration in Salado brine.

Part a) shows results from the CRA-2004 PABC. Part b) shows results from the CRA-2004.



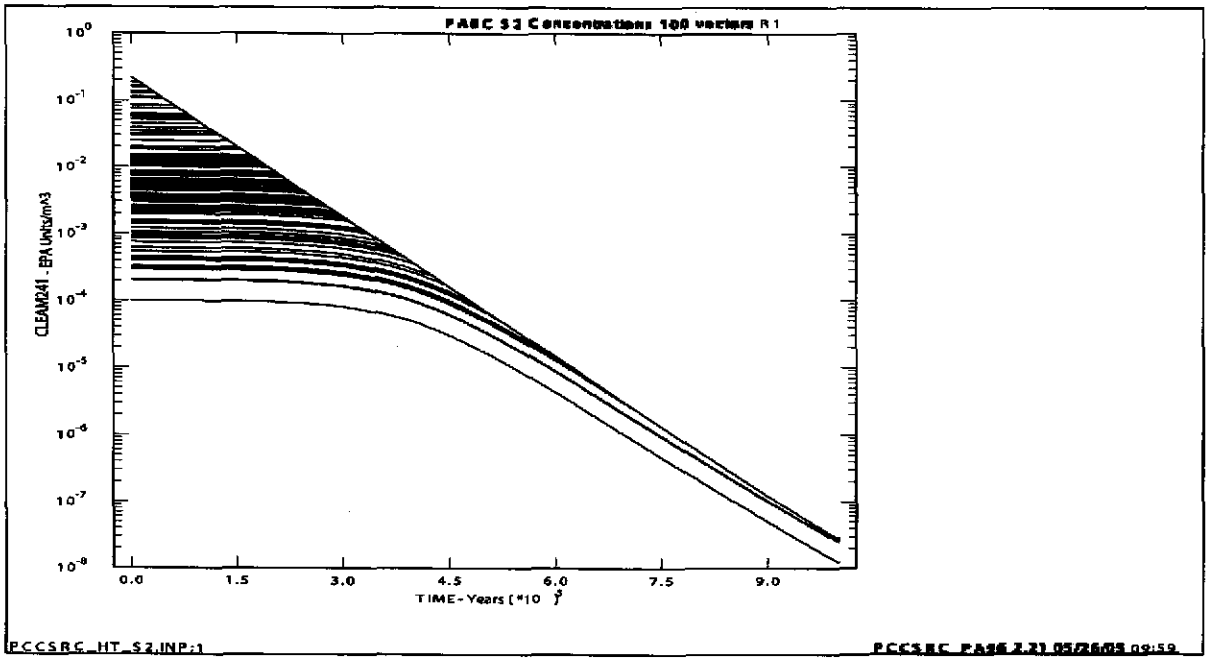
a) PABC



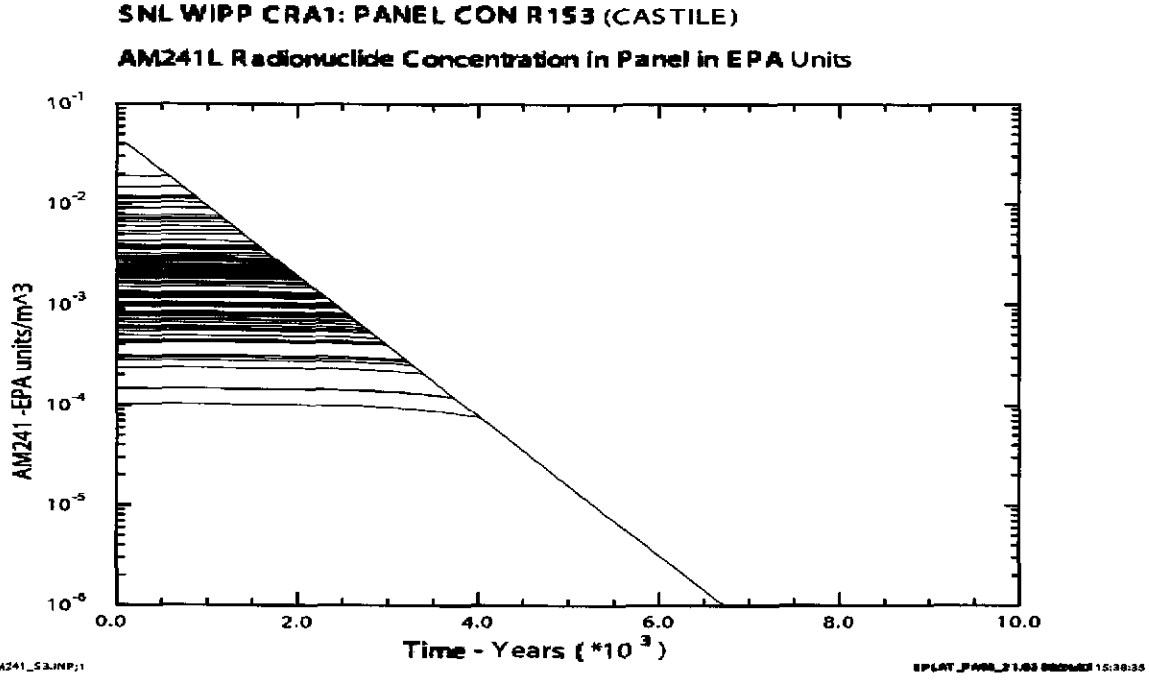
b) CRA1

Figure 35: Time dependent total concentrations in Castile brine.

Part a) shows results from the CRA-2004 PABC. Part b) shows results from the CRA-2004.



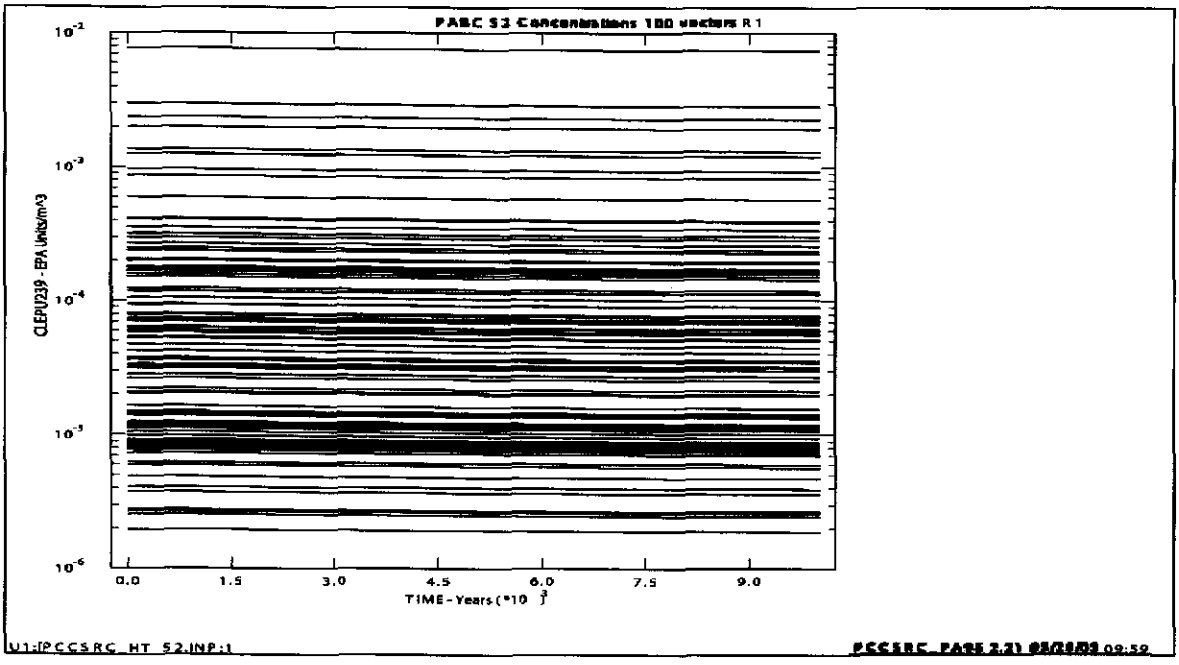
a) PABC



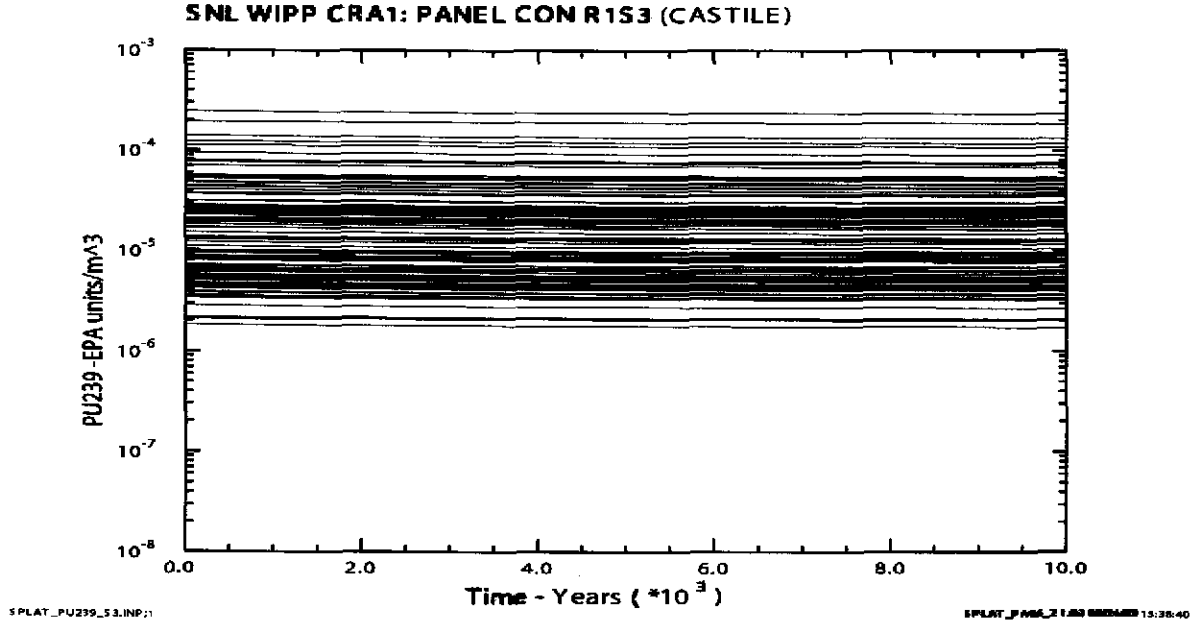
b) CRA1

Figure 36: Time dependent AM241L concentration in Castile brine.

Part a) shows results from the CRA-2004 PABC. Part b) shows results from the CRA-2004.



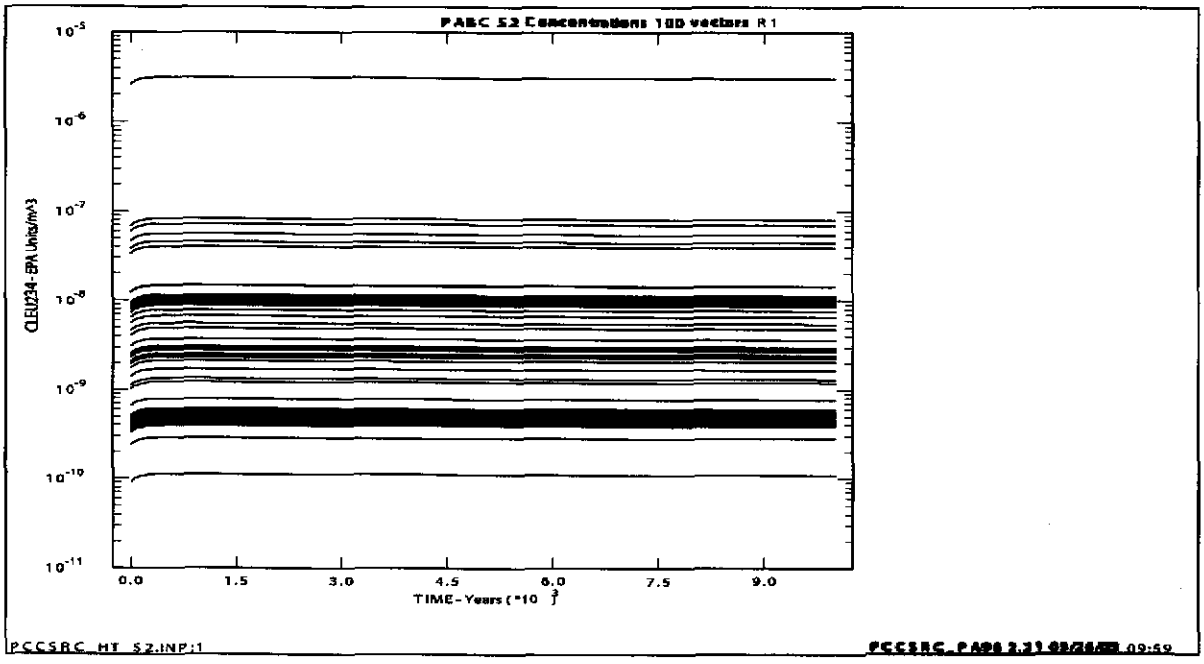
a) PABC



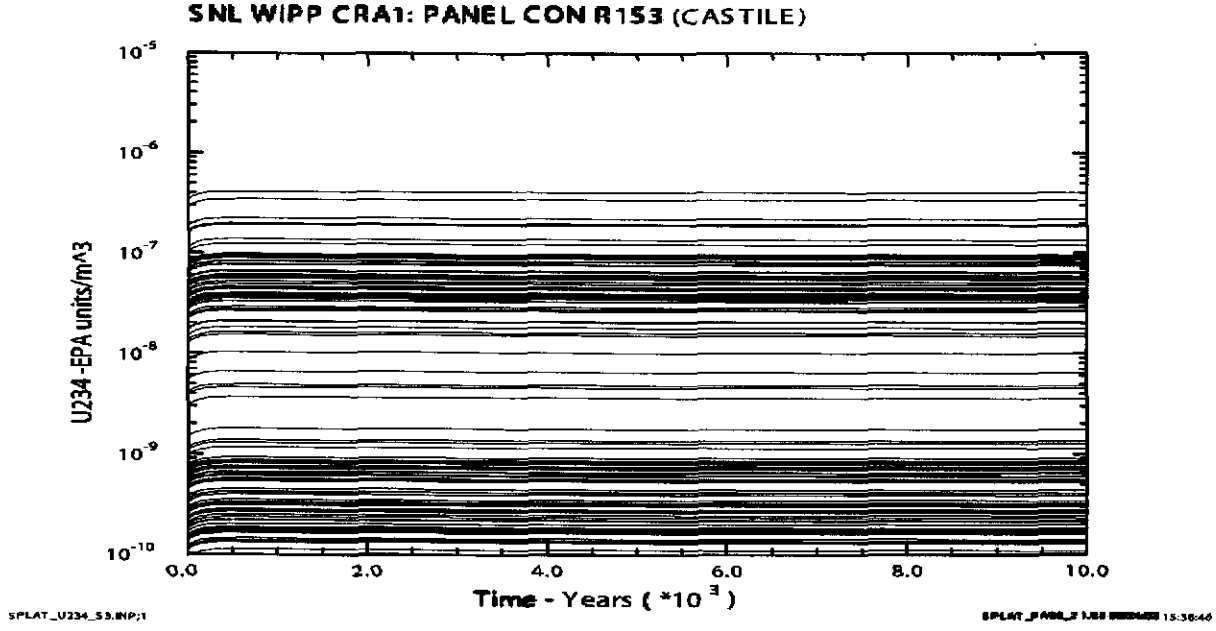
b) CRA1

Figure 37: Time dependent PU239L concentration in Castile brine.

Part a) shows results from the CRA-2004 PABC. Part b) shows results from the CRA-2004.



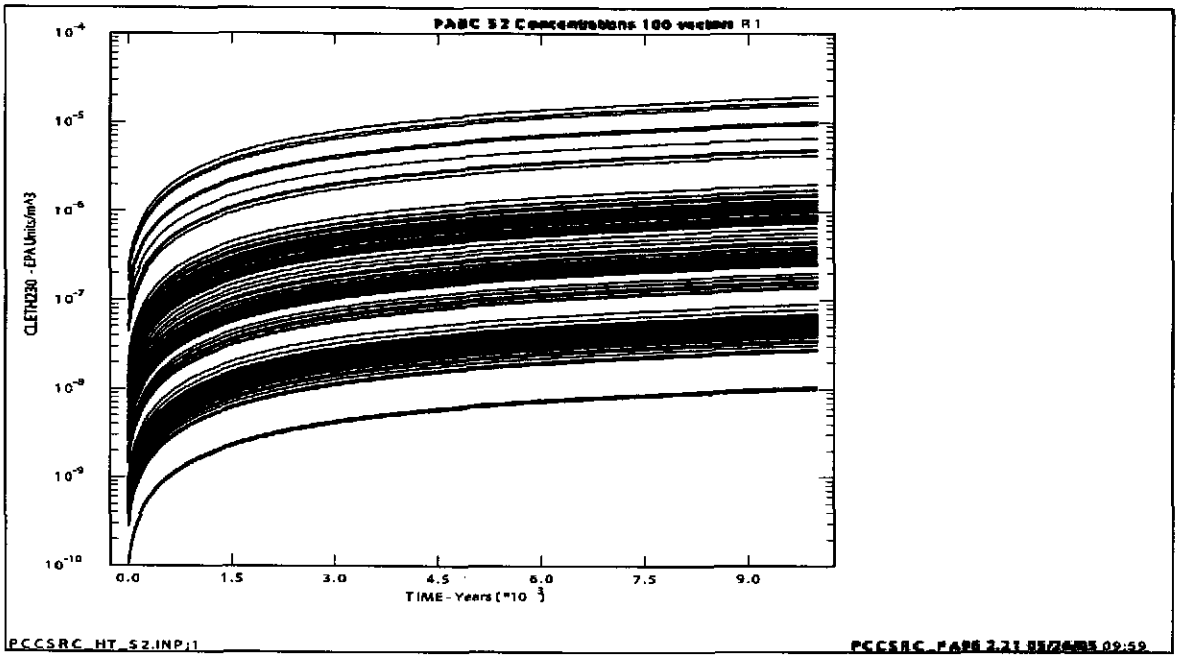
a) PABC



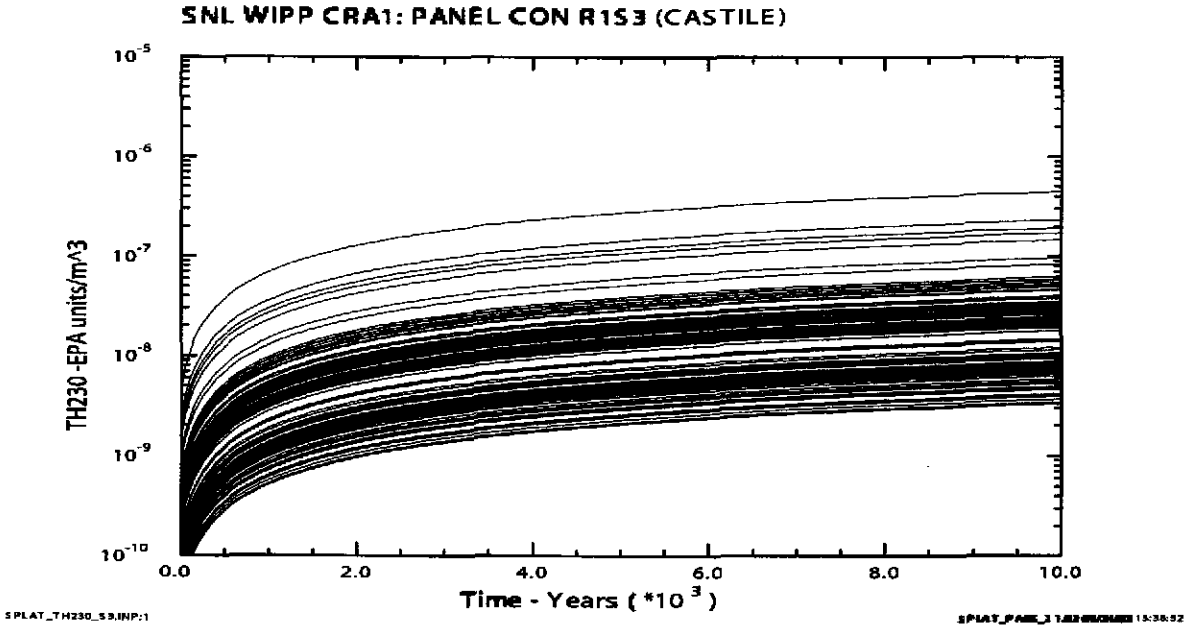
b) CRA1

Figure 38: Time dependent U234L concentration in Castile brine.

Part a) shows results from the CRA-2004 PABC. Part b) shows results from the CRA-2004.



a) PABC



b) CRA1

Figure 39: Time dependent TH230L concentration in Castile brine.

Part a) shows results from the CRA-2004 PABC. Part b) shows results from the CRA-2004.

5.4 RADIONUCLIDES UP THE BOREHOLE (S6)

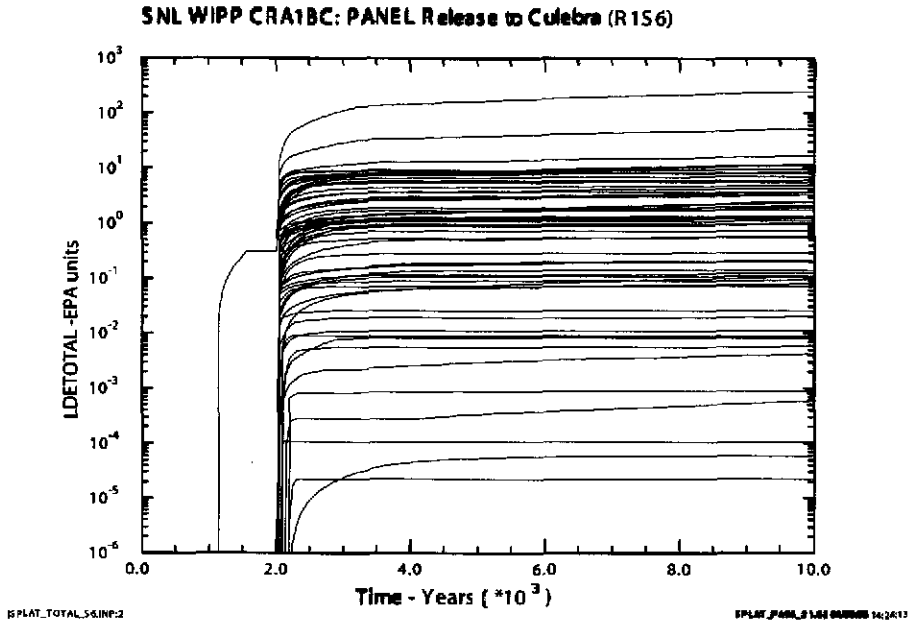
PANEL is run in the STANDARD mode for the S6 scenario to determine the EPA units up the borehole to the Culebra. PANEL calculates the mobilized radionuclide concentrations using panel brine volumes and brine flow volumes from BRAGFLO. The volume of brine in the panel and the flow of brine past the disturbed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

The PANEL results for the EPA units up the borehole to the Culebra are shown in Figures 40 to 53. Figures 40 through 53 are horsetail plots. "Horsetail" plots show values of individual variables for all vectors in a scenario as a function of time for the entire 10,000-year regulatory compliance period. The independent variable (abscissa) in Figures 40 through 53 is time in years. The dependent variable (ordinate) in Figures 40 through 53 is EPA Units up the borehole to the Culebra.

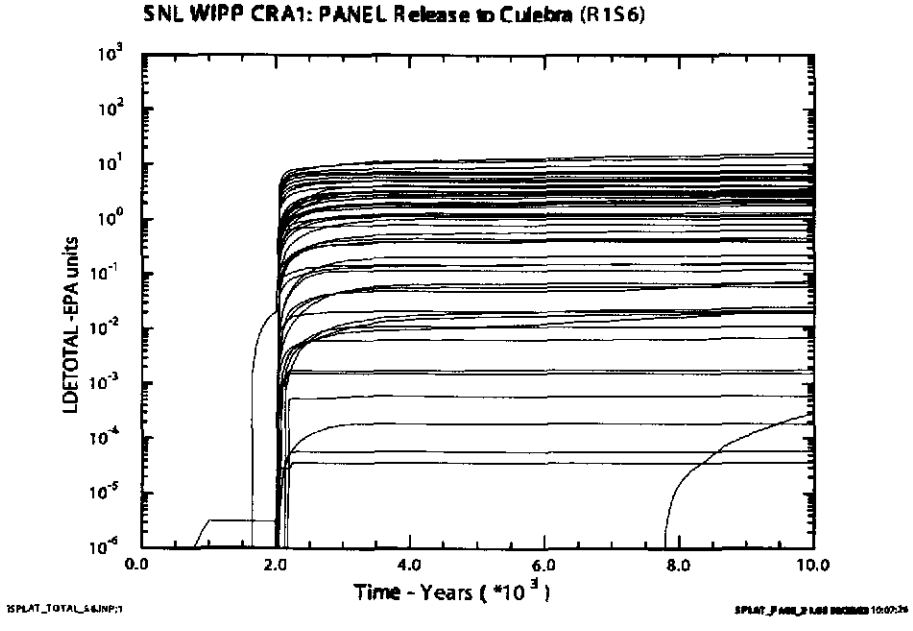
Figure 40 shows the cumulative total EPA Units up the borehole to the Culebra for S6 given an E1 intrusion at 2000 years. Prior to 2000 years, none of the radionuclides move up the borehole to the Culebra. At 2000 years, the time of the E1 intrusion, radionuclides are washed up the borehole to the Culebra. The shape of the curves where there is an immediate rise in the ordinate value at 2000 years followed by almost no increase in the ordinate value as time progresses indicates that movement up the borehole to the Culebra is rapid and essentially complete at the time of the E1 intrusion. The same behavior is apparent for AM241L (Figure 41), PU239L (Figure 42), U234L (Figure 43), and TH230L (Figure 44).
Figures 45 through 50 show the cumulative total EPA Units up the borehole to the Culebra for S6 given an E1 intrusion at 100, 350, 1000, 4000, 6000, and 9000 years respectively. In general, there is more material moved up the borehole to the Culebra in the CRA-2004 PABC than in the CRA-2004.

As a side calculation it is interesting to note the possible contribution that radionuclides other than the "lumped" radionuclides could make if they were tracked to the end of the PA calculation. This is a further response to a request from EPA to examine the impact of leaving NP237 out of the transport calculations (Cotsworth 2004c). Figures 51, 52, and 53 show the EPA Units up the borehole to the Culebra for radionculides that are not tracked in the CCDFGF calculations of Culebra releases. Figure 51 shows the total values. Figure 52 shows the values for NP237, and Figure53 shows the values for Am243.

The maximum contribution in the CRA-2004 PABC seen from radionuclides that not typically tracked in PA is 1.0E-01 EPA Units up the borehole to the Culebra. It was less than 1.0E-01 EPA Units in the CRA-2004. 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 1.0E+03 EPA Units for CRA-2004 PABC. Thus, the contribution made by the radionuclides that are not tracked is several orders of magnitude lower than the ones that are tracked.



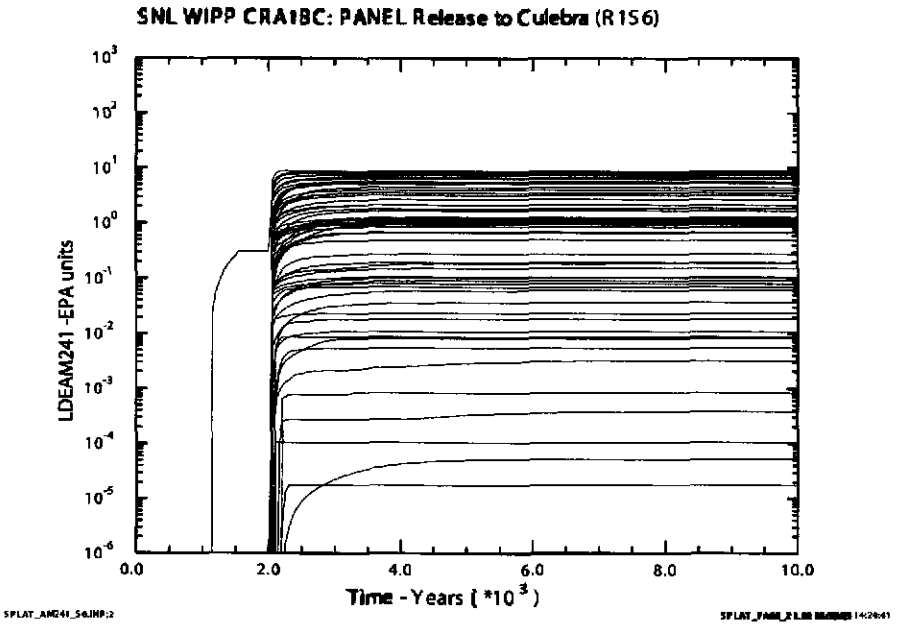
a) PABC



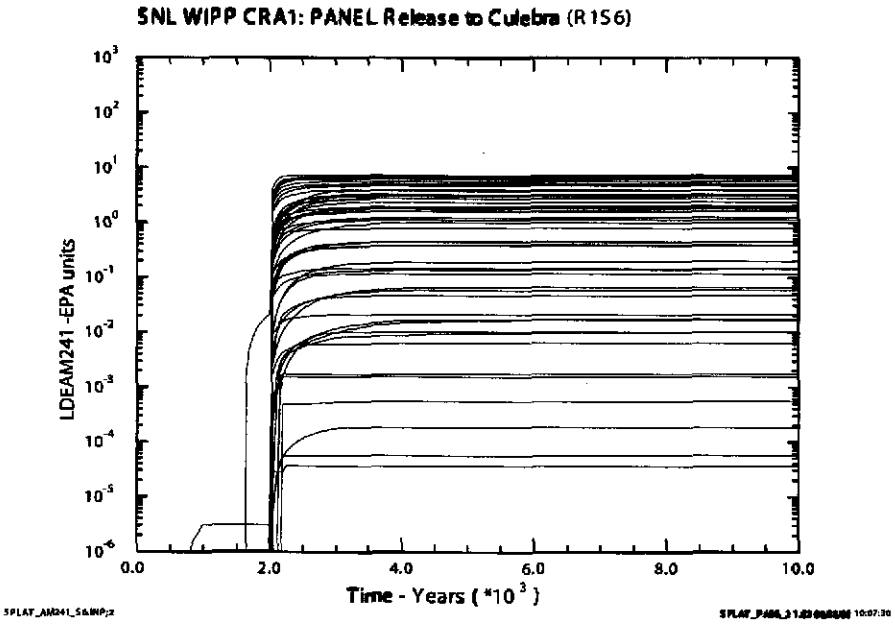
b) CRA1

Figure 40. Cumulative Total EPA Units Up the Borehole to the Culebra for S6 (E1 intrusion at 2000 years).

Part a) shows results from the CRA-2004 PABC. Part b) shows results from the CRA-2004.



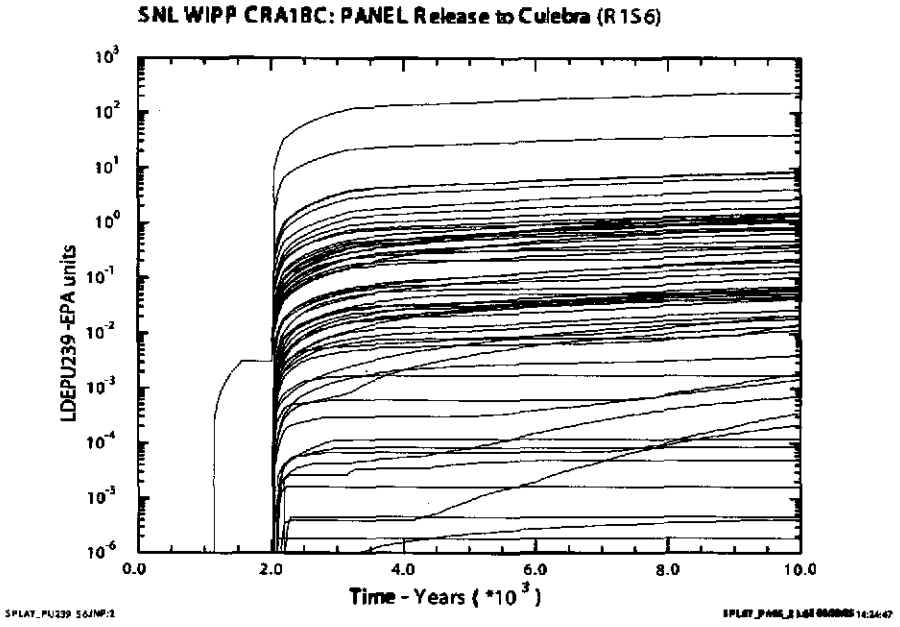
a) PABC



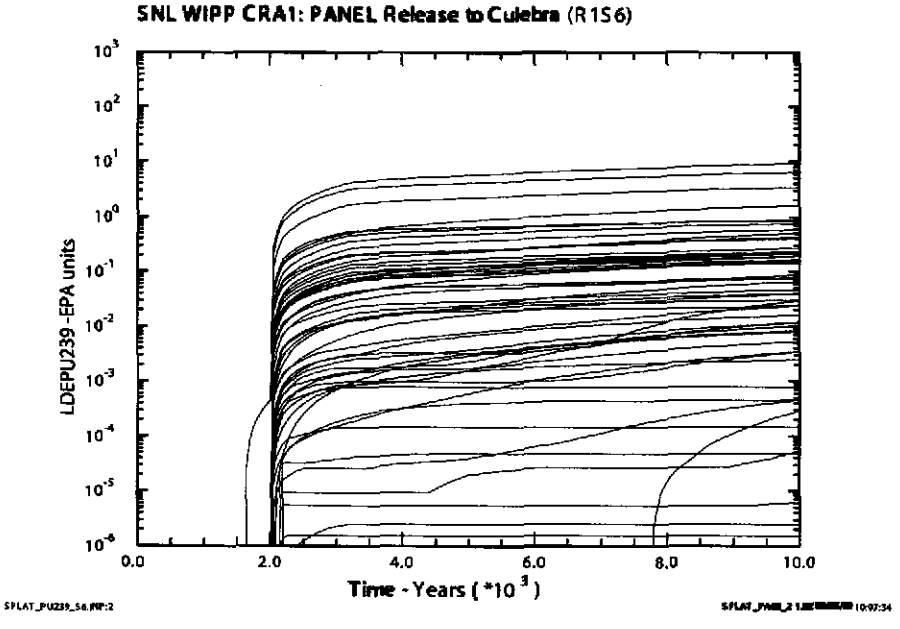
b) CRA1

Figure 41. Cumulative AM241L EPA Units Up the Borehole to the Culebra for S6 (E1 intrusion at 2000 years).

Part a) shows results from the CRA-2004 PABC. Part b) shows results from the CRA-2004.



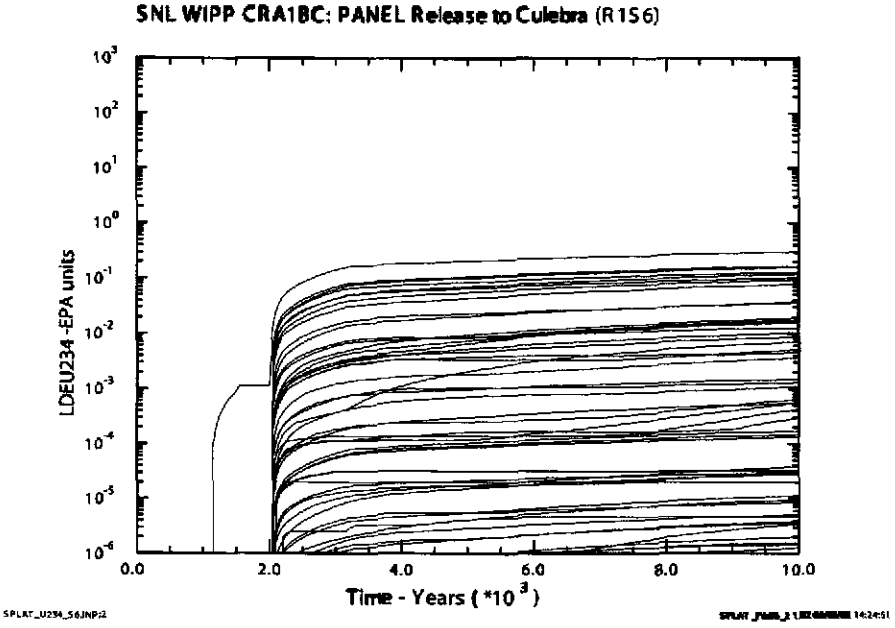
a) PABC



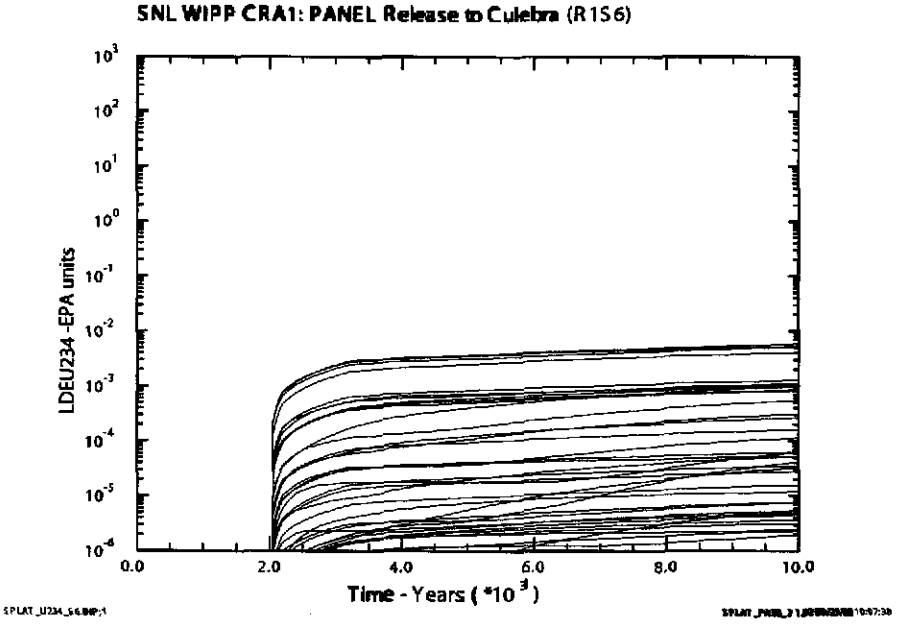
b) CRA1

Figure 42. Cumulative PU239L EPA Units Up the Borehole to the Culebra for S6 (E1 intrusion at 2000 years).

Part a) shows results from the CRA-2004 PABC. Part b) shows results from the CRA-2004.



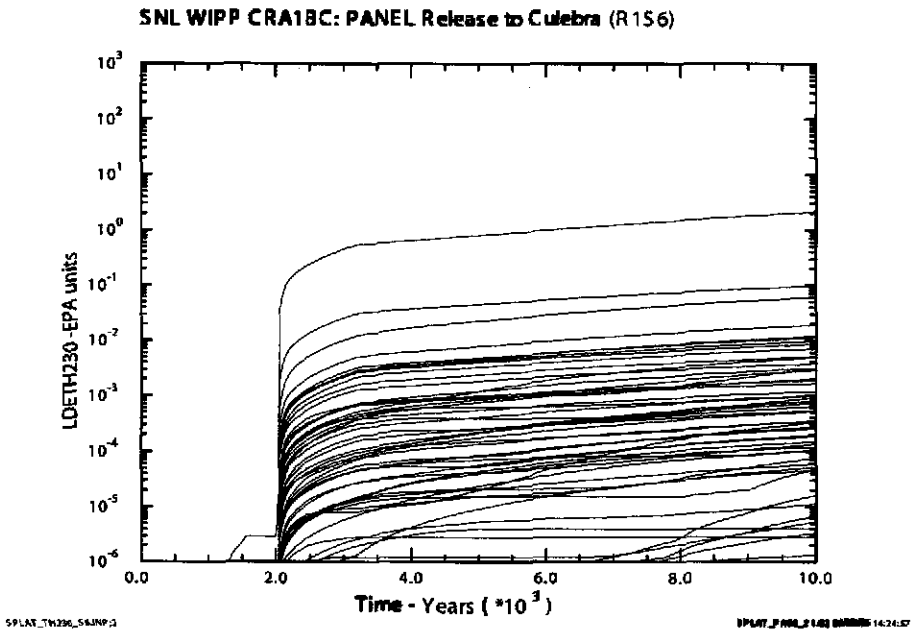
a) PABC



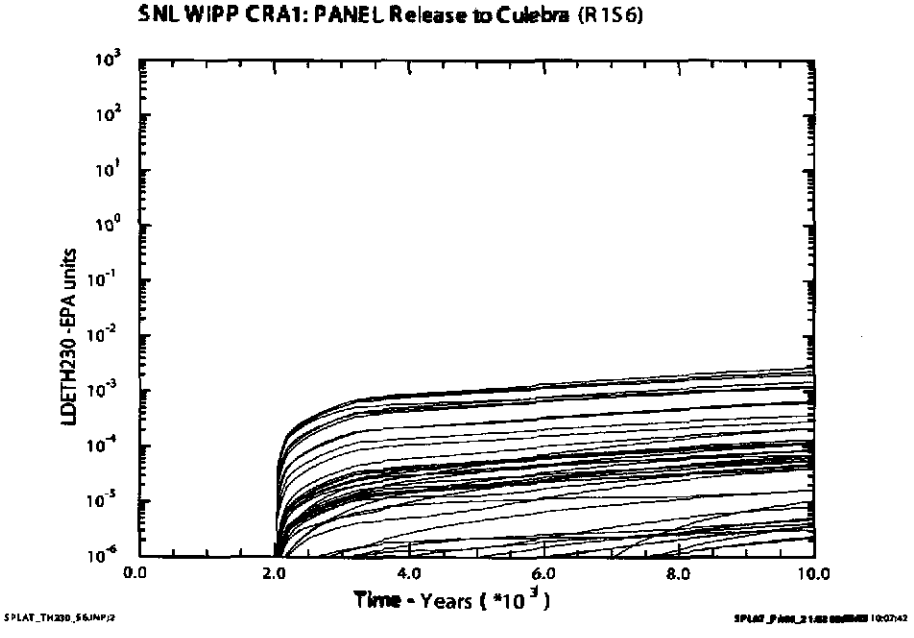
b) CRA1

Figure 43. Cumulative U234L EPA Units Up the Borehole to the Culebra for S6 (E1 intrusion at 2000 years).

Part a) shows results from the CRA-2004 PABC. Part b) shows results from the CRA-2004.



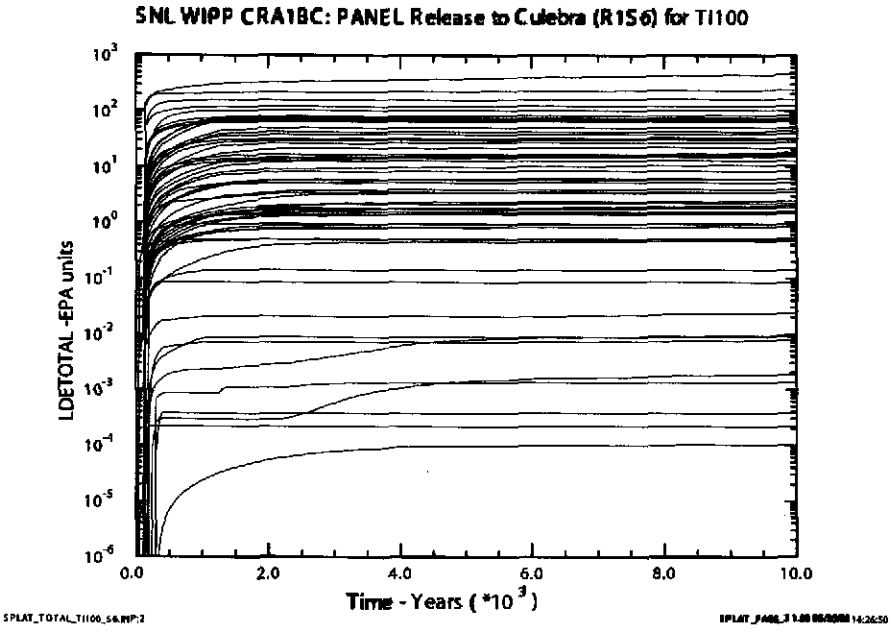
a) PABC



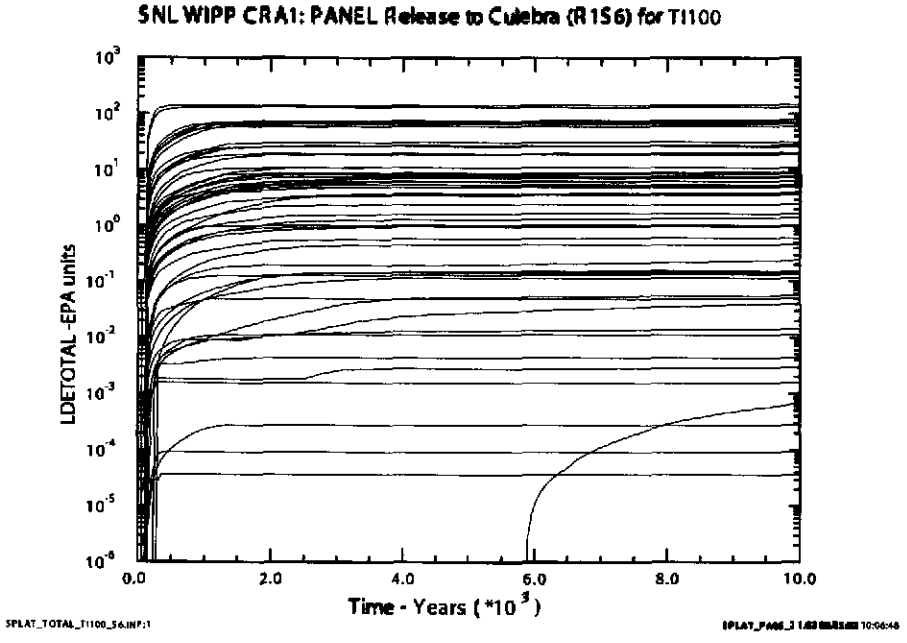
b) CRA1

Figure 44. Cumulative TH230L EPA Units Up the Borehole to the Culebra for S6 (E1 intrusion at 2000 years).

Part a) shows results from the CRA-2004 PABC. Part b) shows results from the CRA-2004.



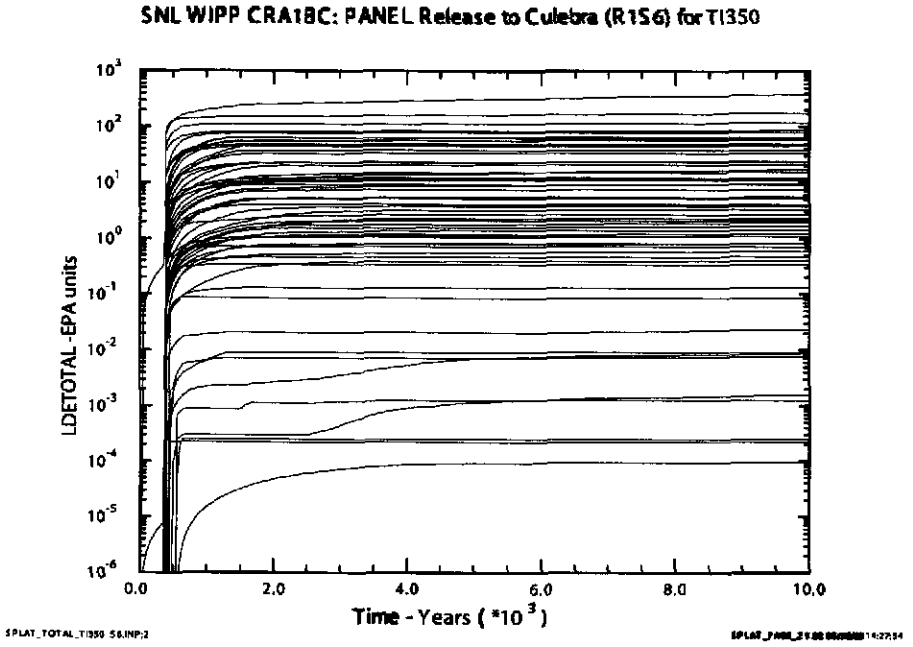
a) PABC



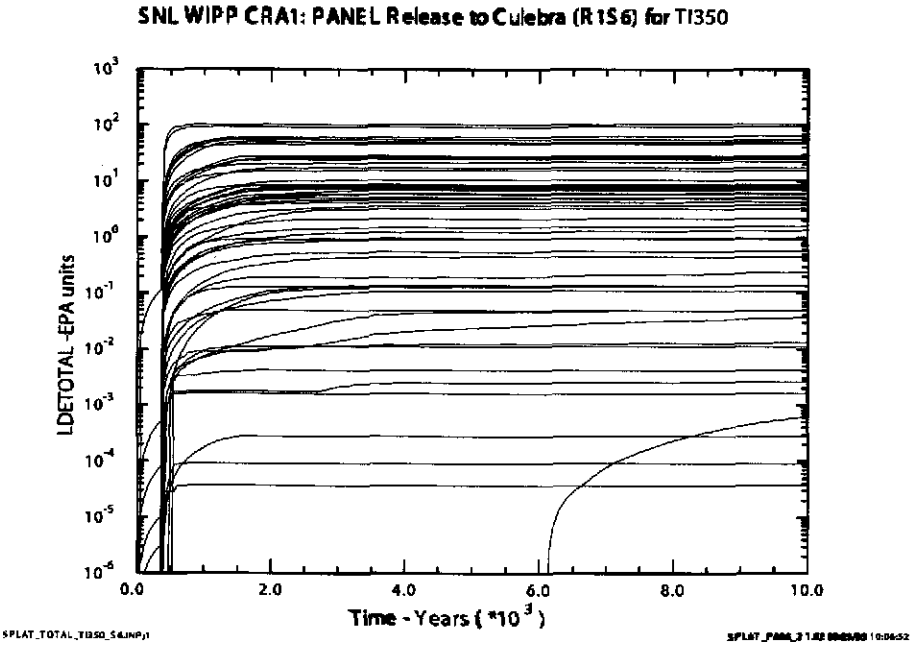
b) CRA1

Figure 45. Cumulative Total EPA Units Up The Borehole to the Culebra for S6 (E1 intrusion at 100 years).

Part a) shows results from the CRA-2004 PABC. Part b) shows results from the CRA-2004.



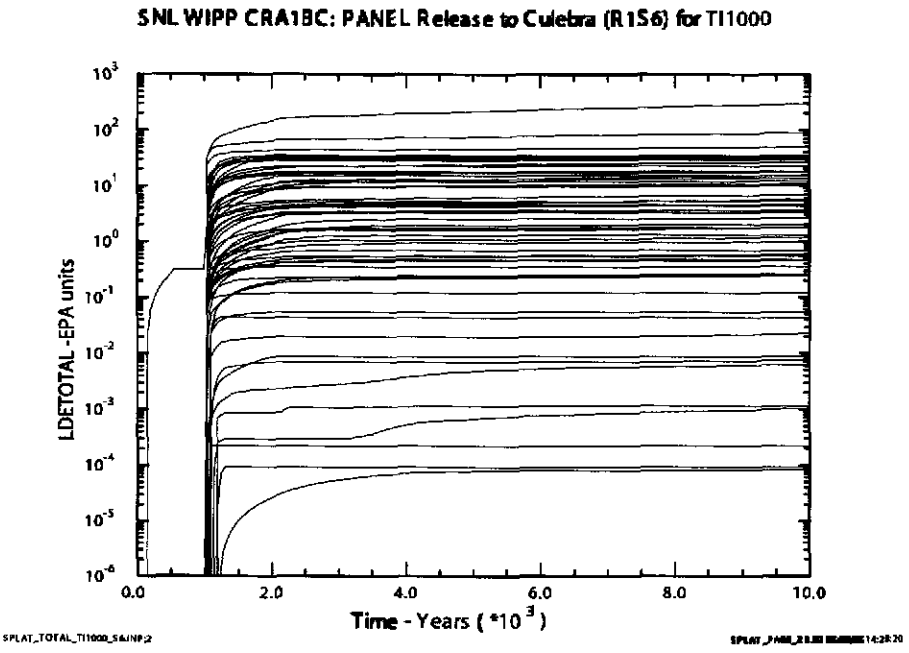
a) PABC



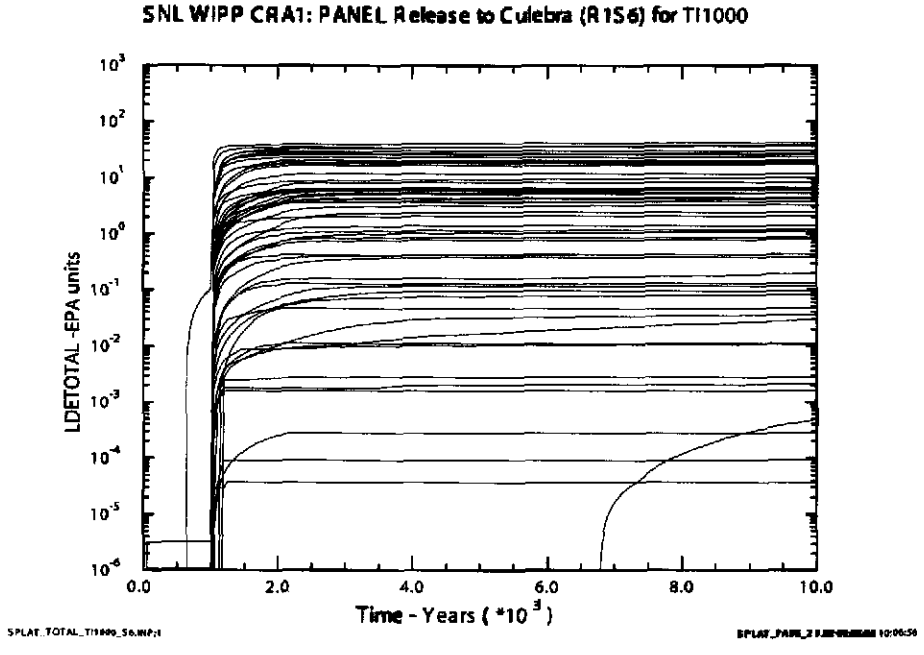
b) CRA1

Figure 46. Cumulative Total EPA Units Up The Borehole to the Culebra for S6 (E1 intrusion at 350 years).

Part a) shows results from the CRA-2004 PABC. Part b) shows results from the CRA-2004.



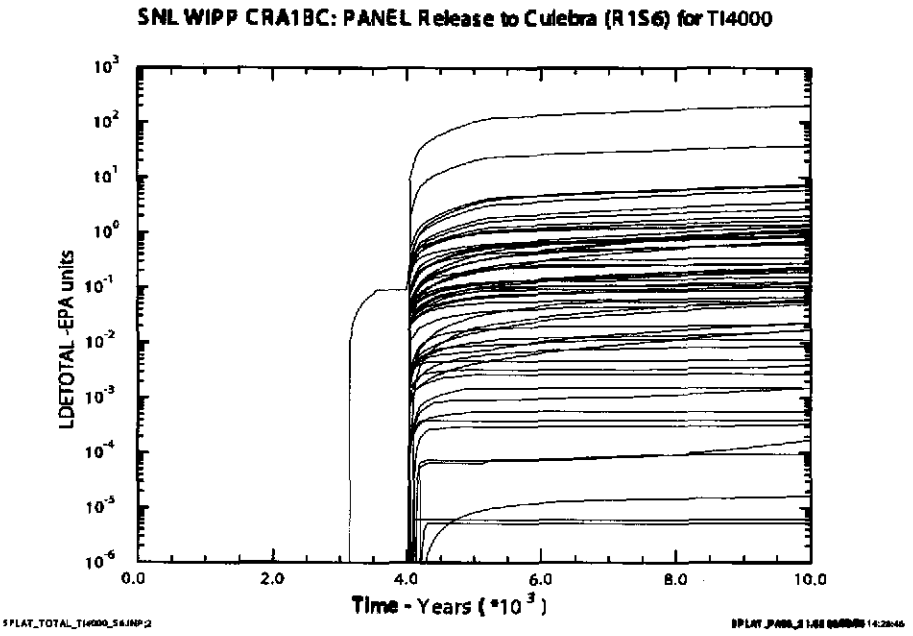
a) PABC



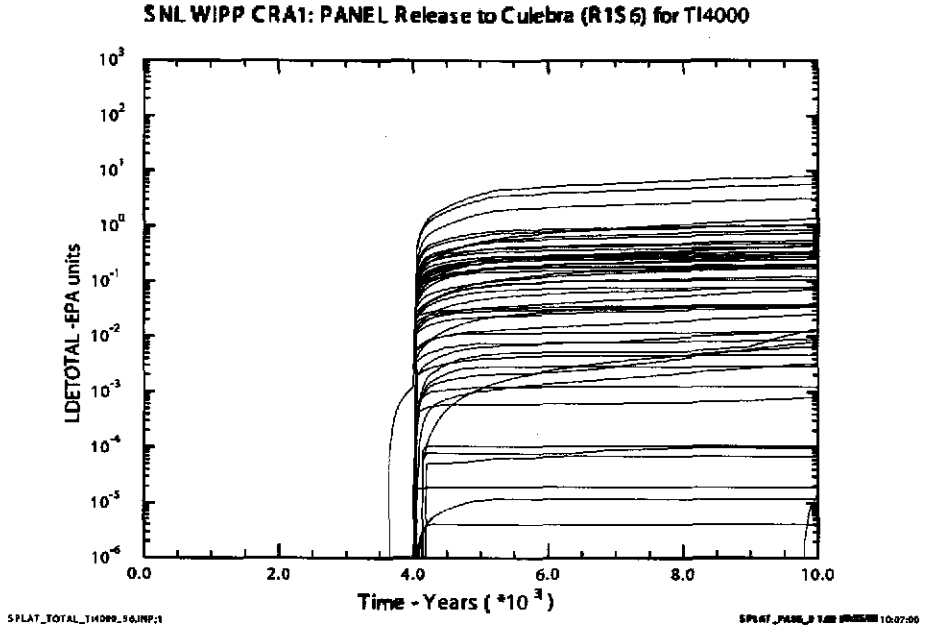
b) CRA1

Figure 47. Cumulative total release to Culebra for S6 (E1 intrusion at 1000 years).

Part a) shows results from the CRA-2004 PABC. Part b) shows results from the CRA-2004.



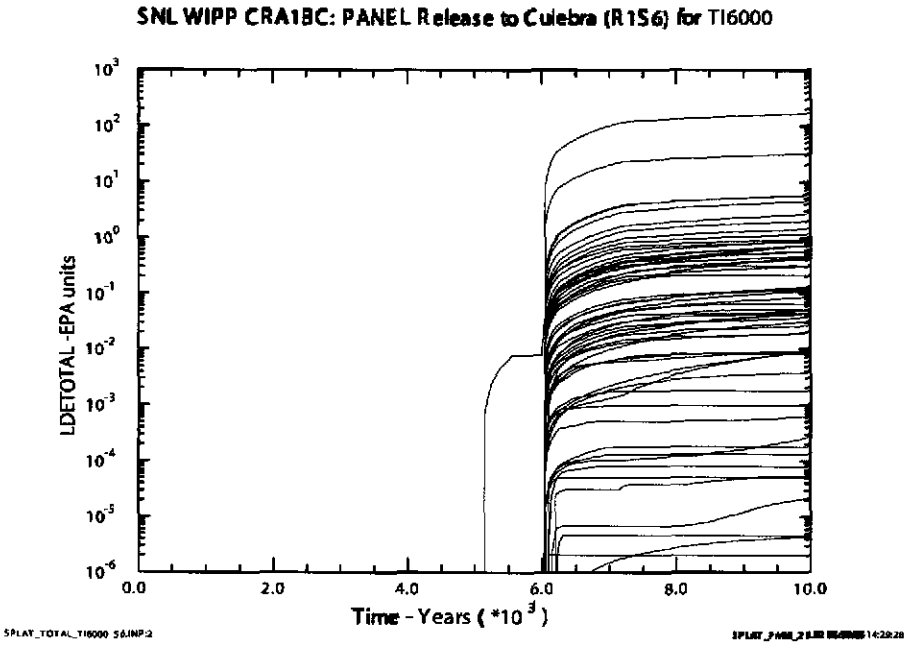
a) PABC



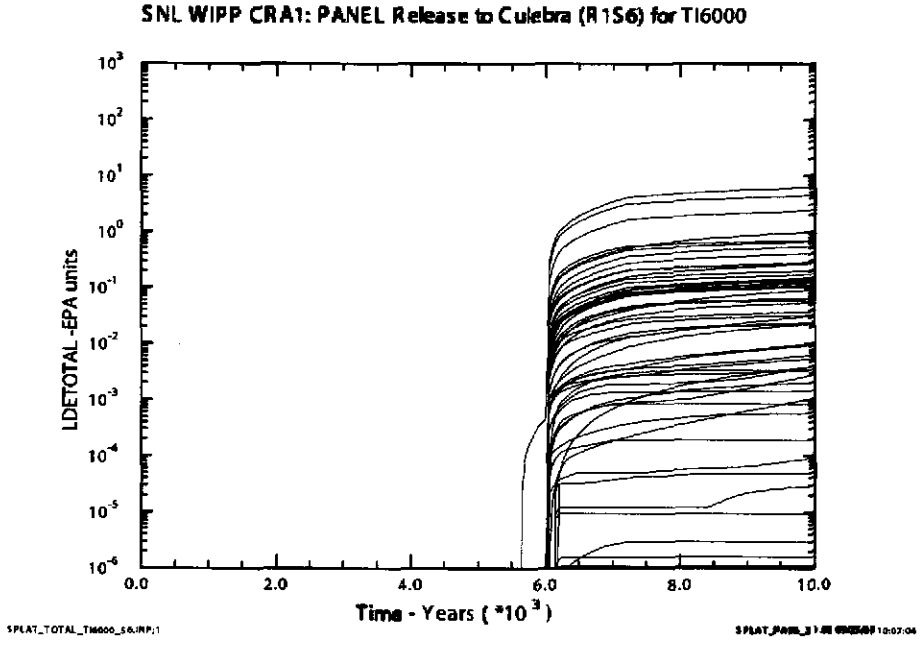
b) CRA1

Figure 48. Cumulative Total EPA Units Up The Borehole to the Culebra for S6 (E1 intrusion at 4000 years).

Part a) shows results from the CRA-2004 PABC. Part b) shows results from the CRA-2004.



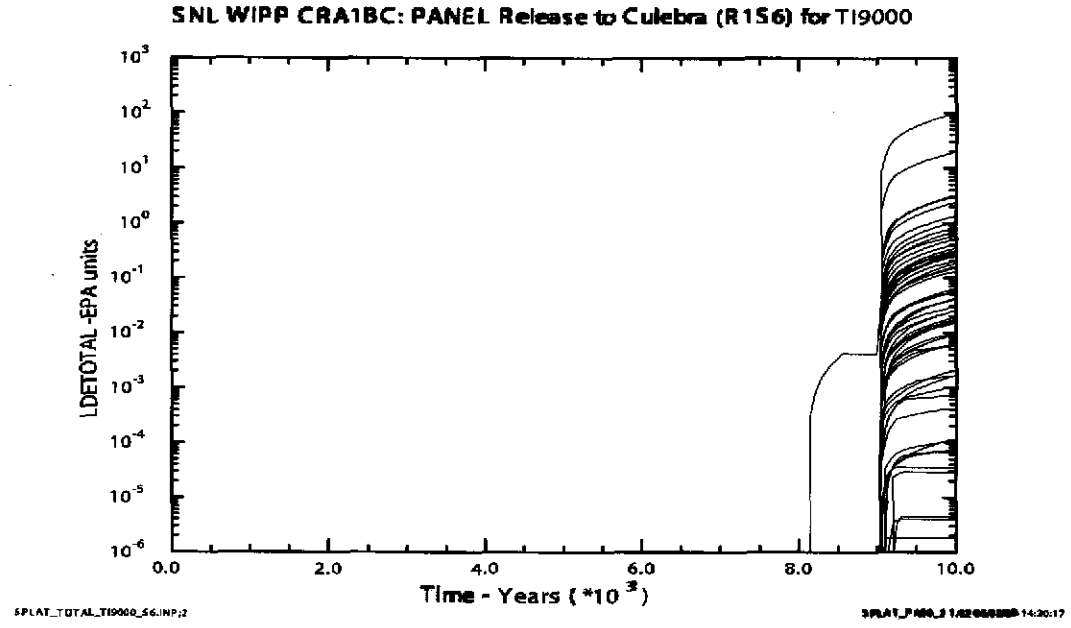
a) PABC



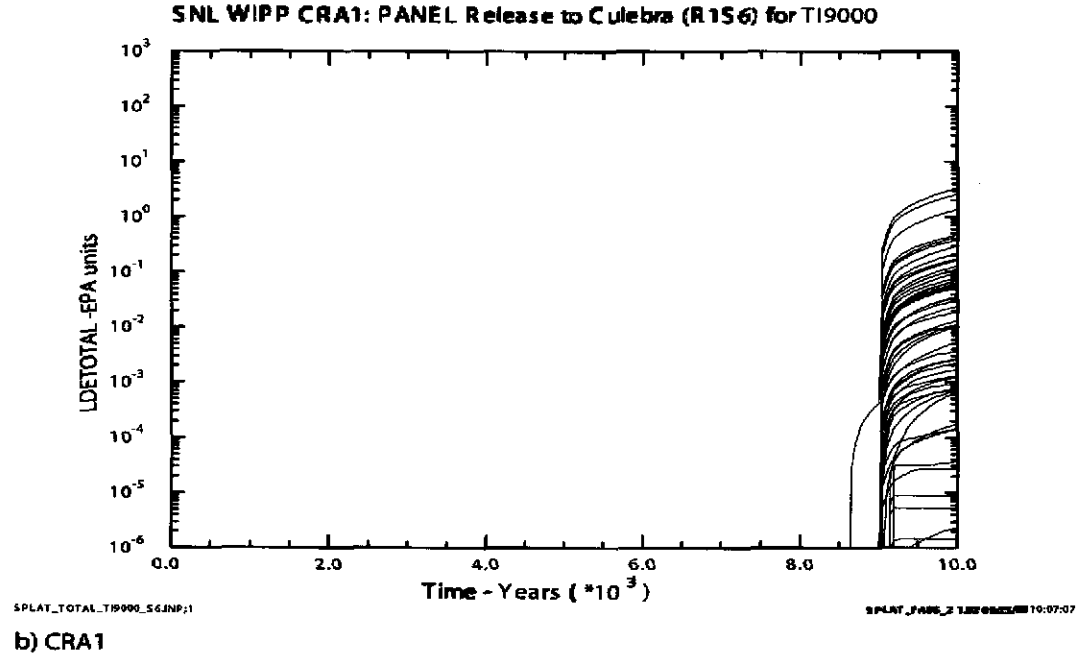
b) CRA1

Figure 49. Cumulative total release to Culebra for S6 (E1 intrusion at 6000 years).

Part a) shows results from the CRA-2004 PABC. Part b) shows results from the CRA-2004.



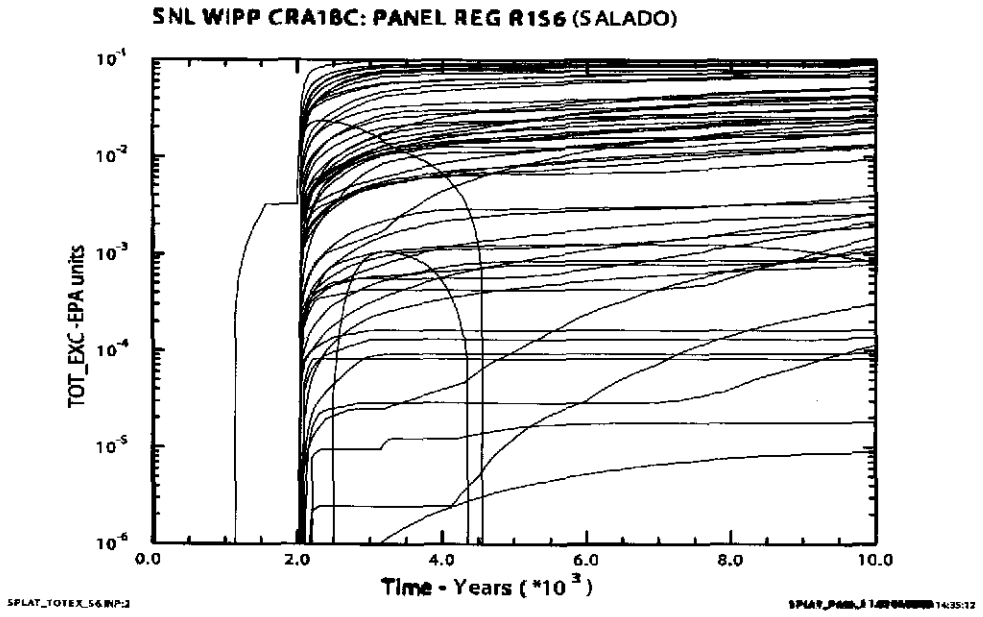
a) PABC



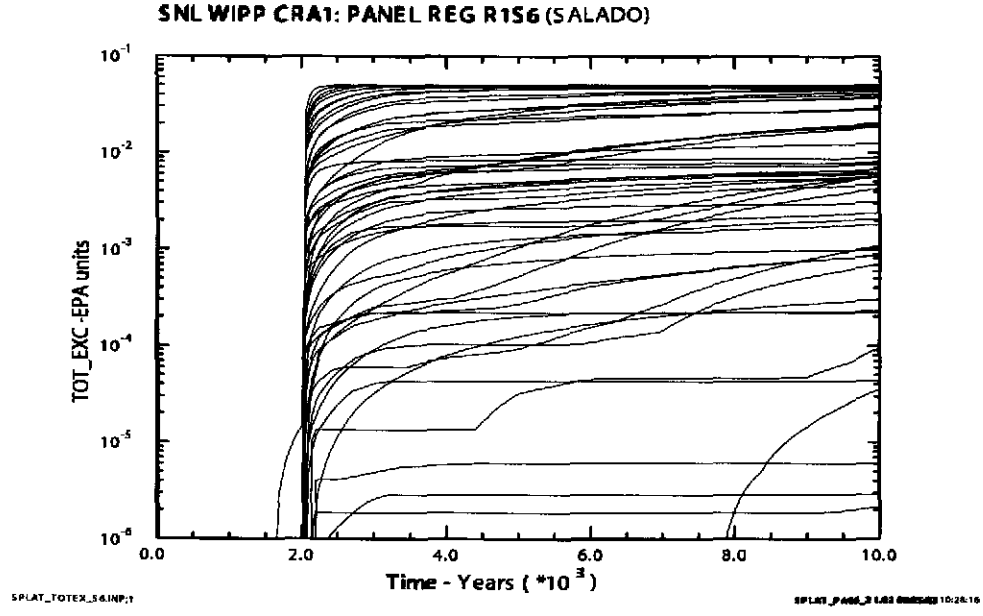
b) CRA1

Figure 50. Cumulative Total EPA Units Up The Borehole to the Culebra for S6 (E1 intrusion at 9000 years).

Part a) shows results from the CRA-2004 PABC. Part b) shows results from the CRA-2004.



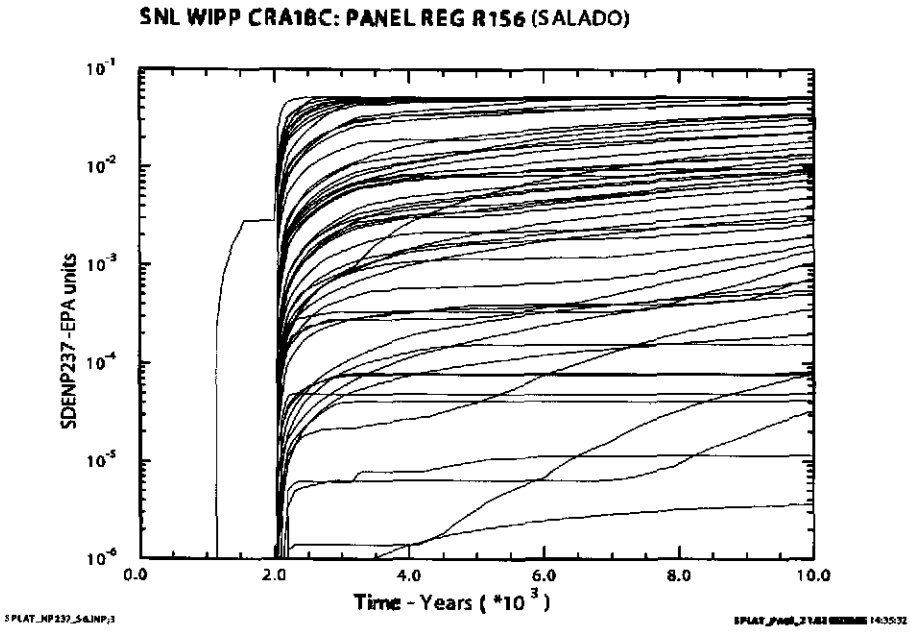
a) PABC



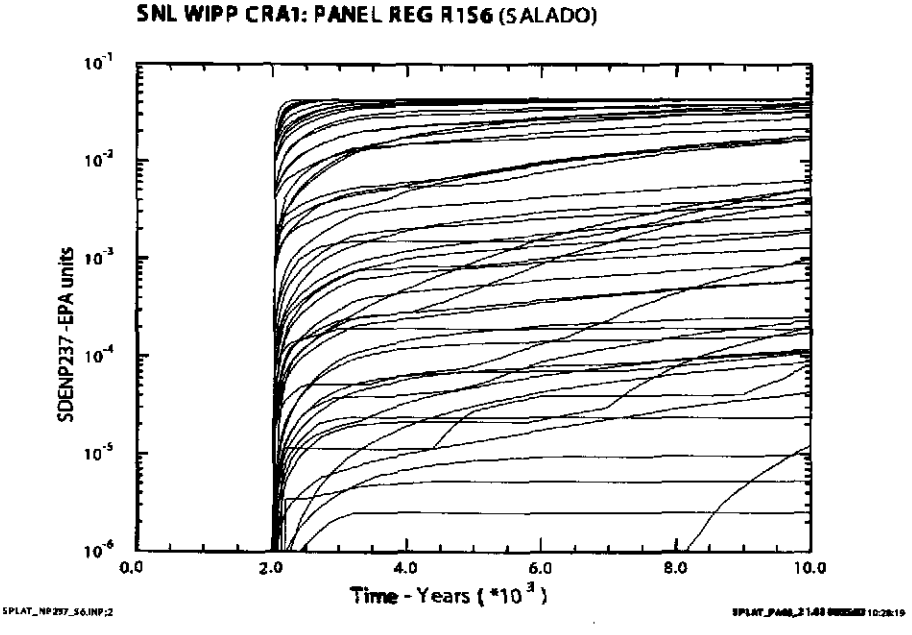
b) CRA1

Figure 51. Cumulative Total EPA Units Up the Borehole to the Culebra for Radionuclides not transported for S6 (E1 intrusion at 2000 years).

Part a) shows results from the CRA-2004 PABC. Part b) shows results from the CRA-2004.



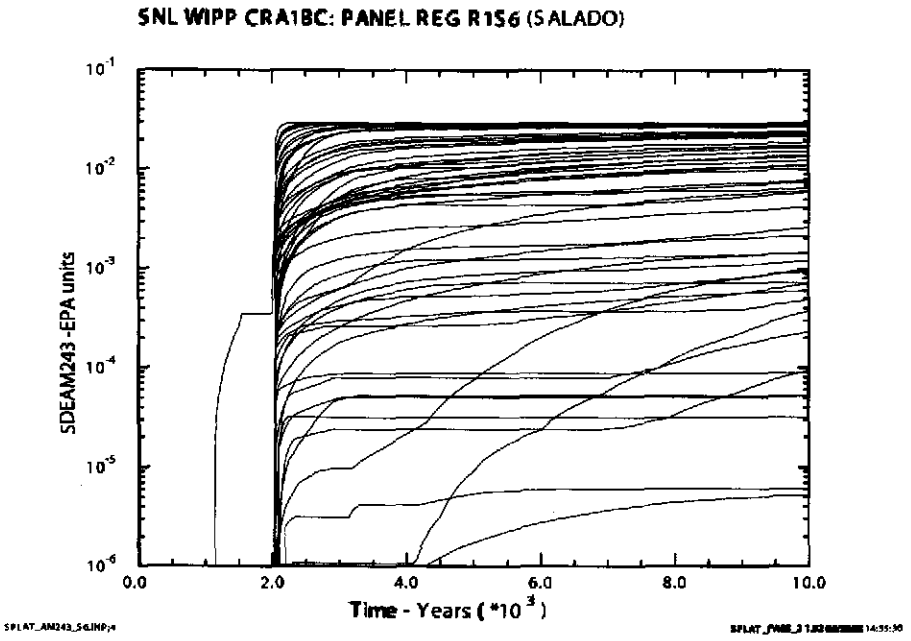
a) PABC



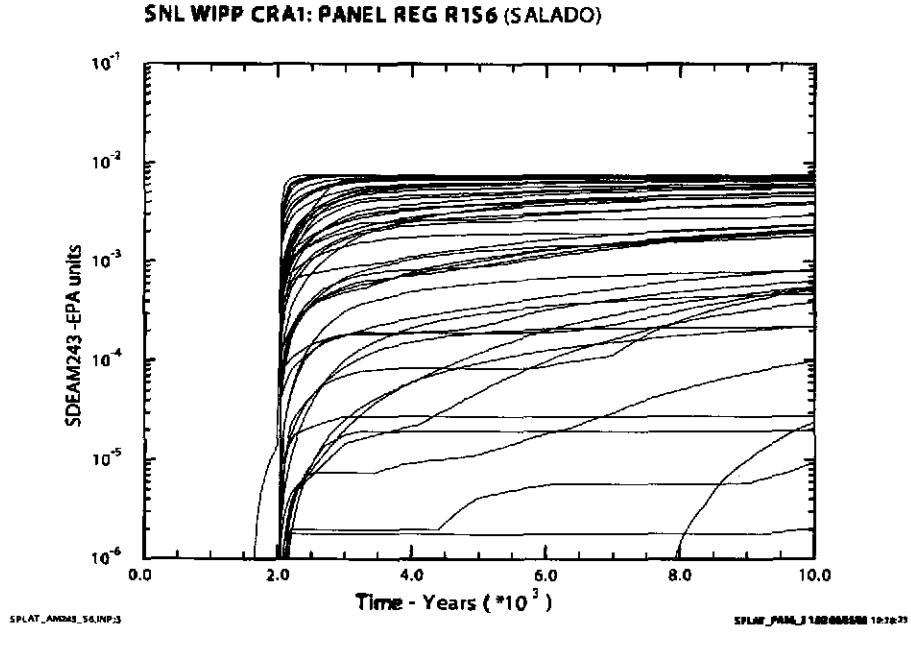
b) CRA1

Figure 52. Cumulative NP237L EPA Units Up the Borehole to the Culebra for S6 [E1 intrusion at 2000 years (Not Transported)].

Part a) shows results from the CRA-2004 PABC. Part b) shows results from the CRA-2004.



a) PABC



b) CRA1

Figure 53. Cumulative AM243L EPA Units Up the Borehole to the Culebra for S6 [E1 intrusion at 2000 years (Not Transported)].

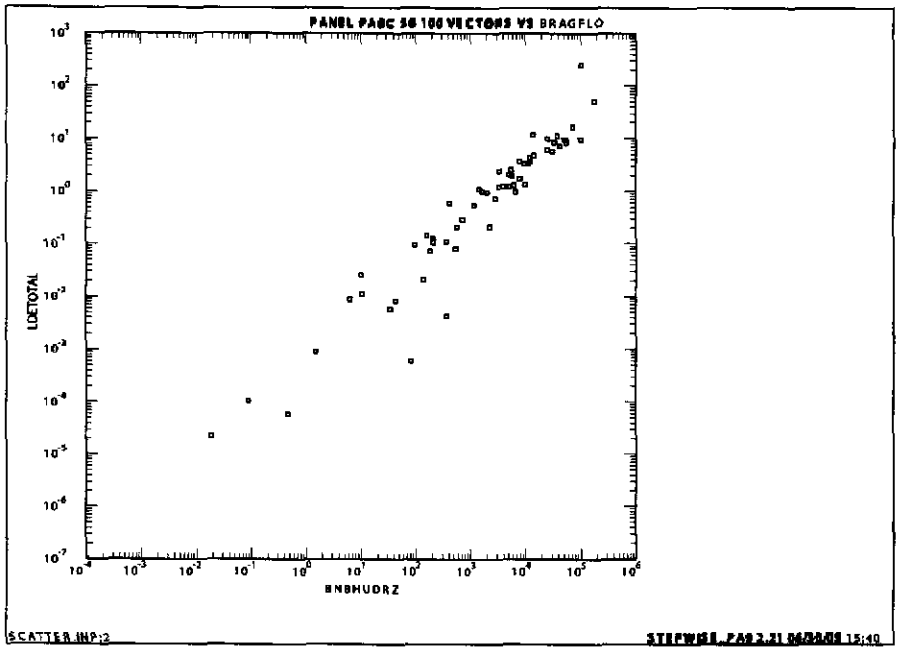
Part a) shows results from the CRA-2004 PABC. Part b) shows results from the CRA-2004.

5.5 SENSITIVITY ANALYSIS

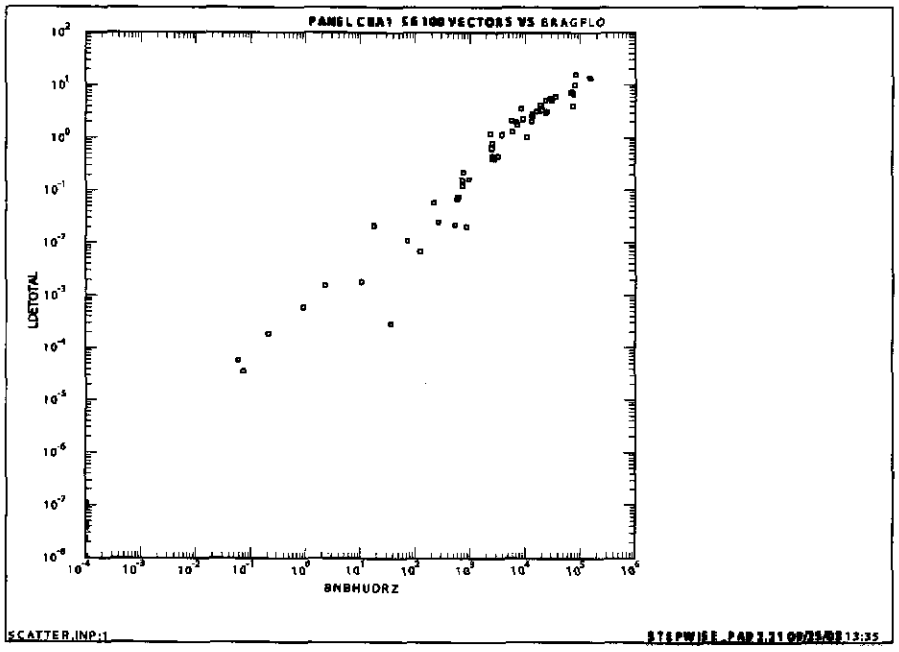
A STEPWISE (Baker 2003a) calculation was performed in order to determine what variables have the most influence on the EPA units up the borehole to the Culebra in the S6 scenario. The sensitivity analysis was performed on the results from Section 5.3 for the cumulative EPA Units up the borehole to the Culebra at 10,000 years for the S6 scenario (E1 intrusion at 2000 years). STEPWISE identifies which uncertain input variables have the strongest correlation to the uncertainty in the output variables.

The strongest correlation identified in all cases was with a BRAGFLO parameter, the borehole permeability (BOREHOLE:BHPERM). The R^2 varied from .723 to .829. 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. To eliminate the effect that the BRAGFLO parameters have on uncertainty in the output and illuminate the effect of the PANEL input parameters, scatter plots of EPA Units versus brine flow were made.

Figures 54 through 58 show the relationship between EPA Units up the borehole to the Culebra and the brine flow (BNBHUDRZ). Figures 54 through 58 are scatter plots with the EPA Units up the borehole to the Culebra as the dependent variable (ordinate) and the brine flow as the independent variable (abscissa). In all of the figures there is a fairly linear relationship with only a little scatter shown between the brine flow and the EPA Units up the borehole to the Culebra. The scatter shown in Figures 54 through 58 is caused by variability in the mobilization potentials (Section 5.1) for the elements. In cases where there are two oxidation states for an element (U which can be +IV or +VI; Pu which can be +III or +IV), there is more scatter seen in the figure because there is more variability in the mobilization potentials. The variability attributed to mobilization potentials is approximately one order of magnitude while the variability attributed to the brine flow is 10 orders of magnitude. The BRAGFLO analysis package (Nemer and Stein 2005) contains an analysis of brine release to the Culebra.



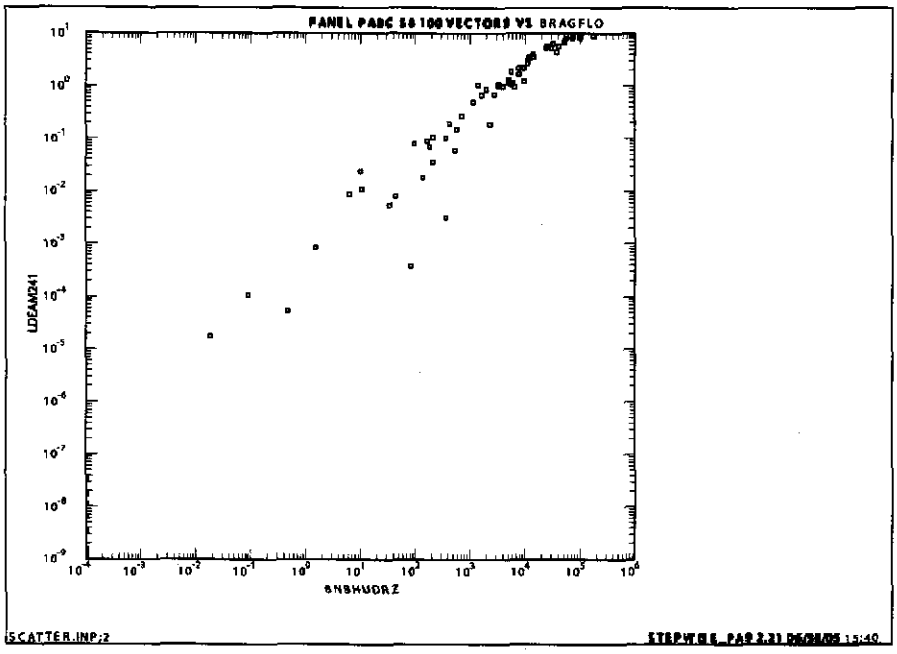
a) PABC



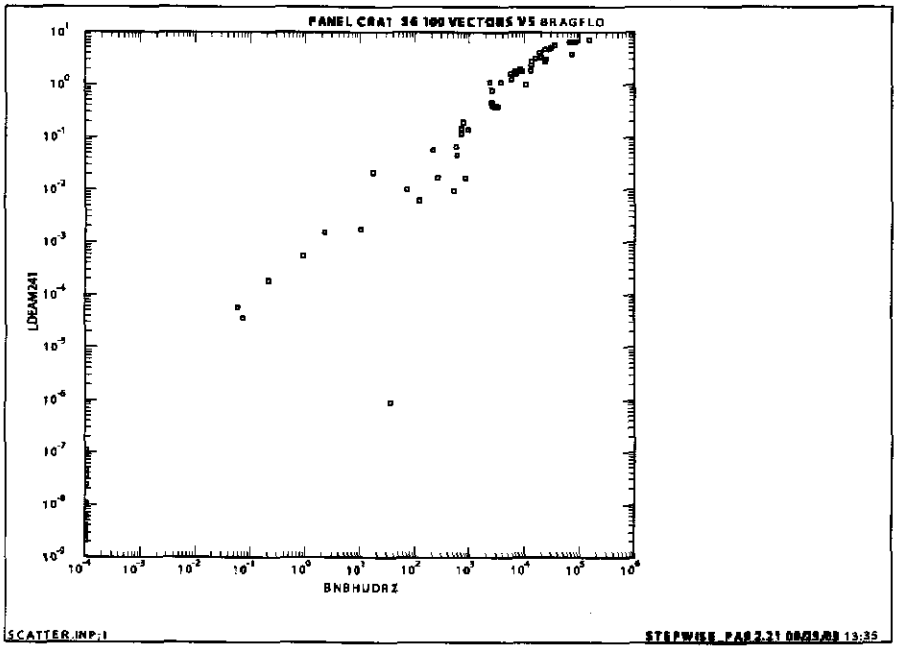
b) CRA1

Figure 54 Cumulative brine release to Culebra for S6 (E1 intrusion at 2000 years) vs. total radionuclide release to Culebra.

Part a) shows results from the CRA-2004 PABC. Part b) shows results from the CRA-2004.



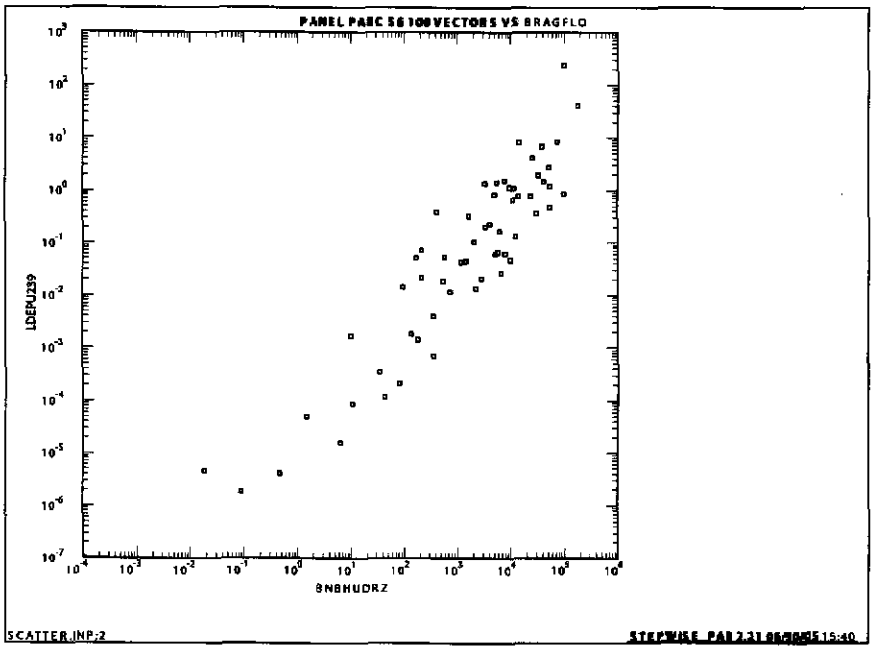
a) PABC



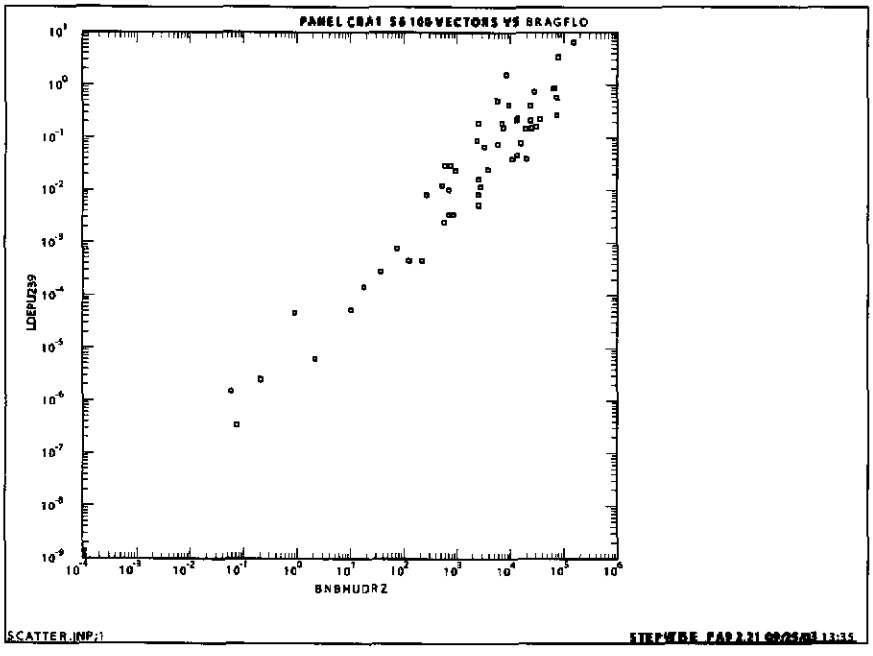
b) CRA1

Figure 55 Cumulative brine release to Culebra for S6 (E1 intrusion at 2000) years vs. Americium release to Culebra.

Part a) shows results from the CRA-2004 PABC. Part b) shows results from the CRA-2004.



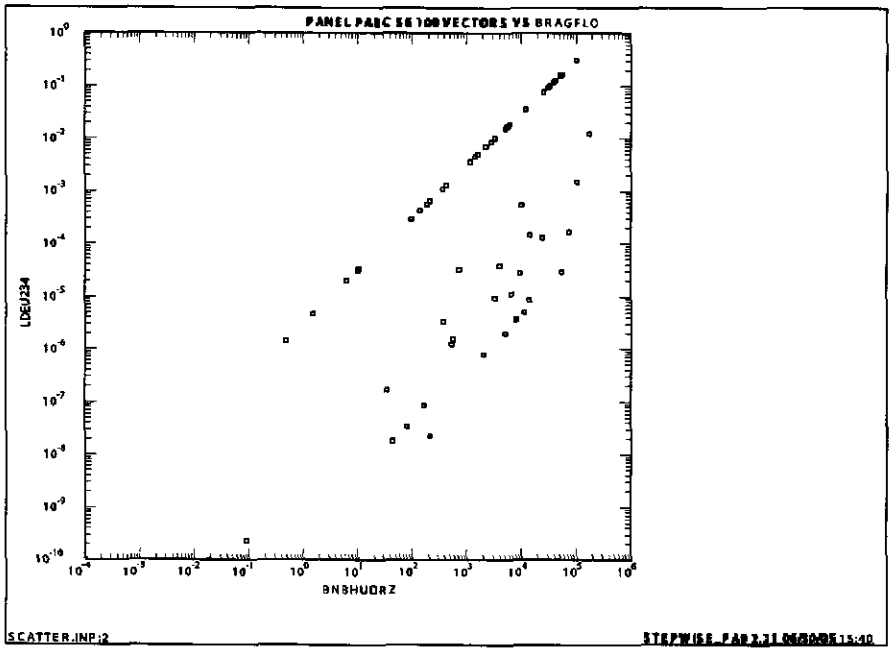
a) PABC



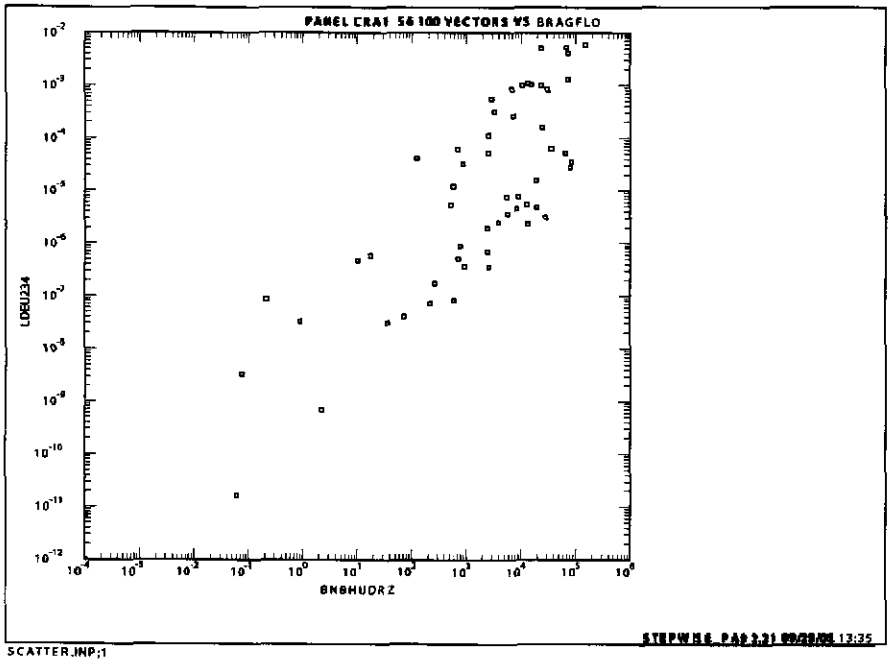
b) CRA1

Figure 56 Cumulative brine release to Culebra for S6 (E1 intrusion at 2000 years) vs. Plutonium release to Culebra.

Part a) shows results from the CRA-2004 PABC. Part b) shows results from the CRA-2004.



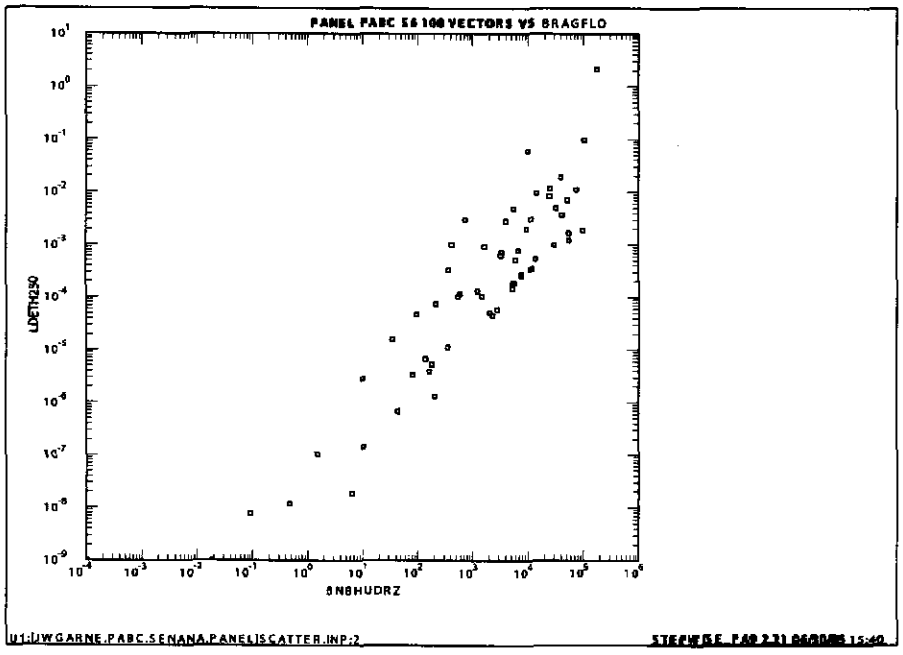
a) PABC



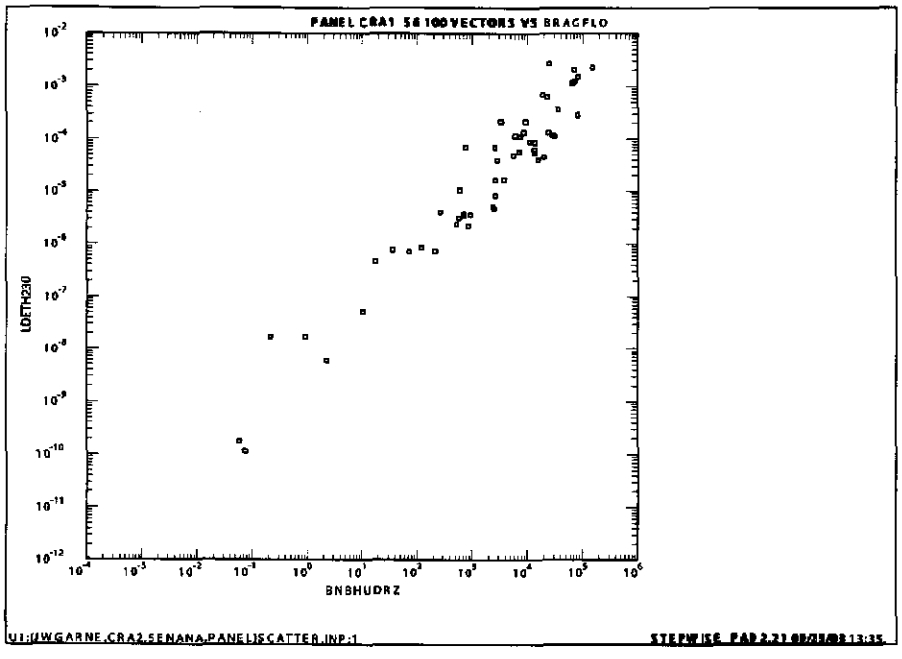
b) CRA1

Figure 57 Cumulative brine release to Culebra for S6 (E1 intrusion at 2000 years) vs. Uranium release to Culebra.

Part a) shows results from the CRA-2004 PABC. Part b) shows results from the CRA-2004.



a) PABC



b) CRA1

Figure 58 Cumulative brine release to Culebra for the S6 (E1 intrusion at 2000 years) vs. Thorium release to Culebra.

Part a) shows results from the CRA-2004 PABC. Part b) shows results from the CRA-2004.

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APPENDIX A: CALCULATION OF LSOLDIF

PANEL supplies information from the CONCENTRATION run to NUTS. For NUTS the values supplied by PANEL are defined in Equation 11 (see Section 3.3).

$$\left\{TC_{brine}^{red/ox}\right\}_{NUTS} = TC_{brine}^{red/ox} \bullet 10^{-L_{dif}^{sol}} \tag{11}$$

Where $\left\{TC_{brine}^{red/ox}\right\}_{NUTS}$ is the potential moles per liter mobilized for the lumped isotopes in Table 13 (see Section 3.3). L_{dif}^{sol} is a multiplicative factor used to account for molar proportions of isotopes in the inventory. $TC_{brine}^{red/ox}$ is an elemental value. It is the potential moles per liter mobilized of an element. It is assumed that isotopes of an element are mobilized in proportion to their molar proportions in the inventory. For example U in the WIPP PA inventory is comprised of several isotopes including but not limited to U235, U238, U232, and U236. Of these, U238 has the highest molar proportions in the inventory. Therefore, for every mole of U that is mobilized, most of it will be U238.

U234L is defined as the amount of U234 plus the amount of U233. Therefore, L_{dif}^{sol} for U234L is defined as:

$$\left(L_{dif}^{sol}\right)_{U234L} = -\log\left\{\frac{N^{U233} + N^{U234}}{\sum_i N^{isotope}}\right\} \tag{A.1}$$

N^{U233} and N^{U234} are the total moles U233 and U234 in the inventory, respectively. $\sum_i N^{isotope}$ is the sum of all isotopes of the element that contains the isotopes of interest. PU238L is defined as the amount of PU238. Therefore, L_{dif}^{sol} for PU238L is defined as:

$$\left(L_{dif}^{sol}\right)_{PU238L} = -\log\left\{\frac{N^{PU238}}{\sum_i N^{isotope}}\right\} \tag{A.2}$$

N^{PU238} is the moles of PU238 in the inventory. TH230L is defined as the amount of TH230 plus the amount of TH229. Therefore, L_{dif}^{sol} for TH230L is defined as

$$\left(L_{dif}^{sol}\right)_{TH230L} = -\log\left\{\frac{N^{TH229} + N^{TH230}}{\sum_i N^{isotope}}\right\} \tag{A.3}$$

N^{TH229} and N^{TH230} are the total moles TH229 and TH230 in the inventory, respectively. AM241L is defined as the amount of AM241 plus the amount of PU241. Since AM241 is the predominant isotope for Am and PU241 quickly decays to Am241, the potential moles per liter mobilized for AM241L is defined as:

$$\left\{TC_{brine}^{red/ox}\right\}_{AM241L} = \left\{TC_{brine}^{red/ox}\right\}_{Am} \quad \text{(A.4)}$$

There is no L_{dif}^{sol} for AM241L. PU239L is defined as the amount of PU239 plus the amount of PU240 plus the amount of PU242 which accounts for almost all of the Pu in the inventory. Therefore, the potential moles per liter mobilized for PU239L is defined as:

$$\left\{TC_{brine}^{red/ox}\right\}_{PU239L} = \left\{TC_{brine}^{red/ox}\right\}_{Pu} \quad \text{(A.5)}$$

There is no L_{dif}^{sol} for PU239L.

Because of radioactive decay and production, the value of L_{dif}^{sol} will change over time. For WIPP PA, a single value for L_{dif}^{sol} is chosen, the maximum value over time. The maximum value is found by running PANEL in the DECAY mode. Using the results from the PANEL DECAY run, L_{dif}^{sol} is calculated at every time step and the maximum value over time is chosen. These values are input manually in MATSET.

A.1 DECAY RUN CALCULATIONS FOR CRA-2004 PABC

PANEL was run in the DECAY mode to produce decayed radionuclide. For this DECAY run, GENMESH and POSTLHS were not needed (see Figure 1). A previous version of the GENMESH binary file was input into the MATSET code.

The analyst ran MATSET which assigns the material property values needed by PANEL. The GENMESH binary file that was input into the MATSET code (GM_ST_CRA.CDB located in CMS library CRA1BC_PANEL class ANALYSIS) and the MATSET input file (MS_PANEL_CRA1BC.INP located in CMS library CRA1BC_PANEL class ANALYSIS), provided the initial material map for the DECAY run. The output files MS.CDB and MS.DBG are located in CMS library CRA1BC_PANEL class ANALYSIS).

ALGEBRACDB was then run to update some input variables and move input data to lumped isotopes. The MS.CDB file was used as input into ALGEBRACDB along with ALG_PANEL_CRA1BC.INP located in CMS library CRA1BC_PANEL class ANALYSIS. The output from this calculation is ALG.CDB located in CMS library CRA1BC_PANEL class ANALYSIS.

PANEL was then run with the ALG.CDB file. This produced DECAY_S1_V001.CDB and DECAY_PABC.DBG located in CMS library CRA1BC_PANEL class ANALYSIS.

ALGEBRACDB was then run again with the DECAY_S1_V001.CDB and ALG_MOLE.INP (located in CMS library CRA1BC_PANEL class ANALYSIS). The following is the ALGEBRACDB input file that was used (ALG_MOLE.INP).

```
ALLTIMES
U_MOLE=SDMU233/ATWEIGHT[27]+SDMU234/ATWEIGHT[28]+SDMU235/ATWEIGHT[29]+ &
       SDMU236/ATWEIGHT[30]+SDMU238/ATWEIGHT[31]
PU_MOLE=SDMPU238/ATWEIGHT[15]+SDMPU239/ATWEIGHT[16]+SDMPU240/ATWEIGHT[17]+ &
        SDMPU241/ATWEIGHT[18]+SDMPU242/ATWEIGHT[19]+SDMPU244/ATWEIGHT[20]
TH_MOLE=SDMTH229/ATWEIGHT[24]+SDMTH230/ATWEIGHT[25]+SDMTH232/ATWEIGHT[26]

MF_U=(SDMU233/ATWEIGHT[27]+SDMU234/ATWEIGHT[28])/U_MOLE
MF_PU=SDMPU238/ATWEIGHT[15]/PU_MOLE
MF_TH=(SDMTH229/ATWEIGHT[24]+SDMTH230/ATWEIGHT[25])/TH_MOLE

EXIT
```

This produced the output DECAY_MOLE_S1_V001.CDB located in CMS library CRA1BC_PANEL class ANALYSIS.

DECAY_MOLE_S1_V001.CDB was then run through the GROPE program to produce the text file GROPE.LIS (located in CMS library CRA1BC_PANEL class ANALYSIS).

A.2 RESULTS

Table A.1 shows the results of running ALG_MOLE.INP on DECAY_S1_V001.CDB. Visual analysis of the 201 time steps shows that the largest mole fraction for Pu238L (Column 7 in Table A.1) occurs at time 0. The value is 6.7416E-03. Therefore,

$$\left(L_{dif}^{sol}\right)_{PU238L} = -\log\{6.7416\text{E-}03\} = 2.17123\,.$$

The largest mole fraction for TH230L occurs at 10,000 years and is 2.14248E-04. Therefore,

$$\left(L_{dif}^{sol}\right)_{TH230L} = -\log\{2.14248\text{E-}04\} = 3.66908$$

The largest mole fraction for U234L occurs at 800 years and is 3.86778E-04. Therefore,

$$\left(L_{dif}^{sol}\right)_{U234L} = -\log\{3.86778\text{E-}04\} = 3.41252$$

These values are input manually into the MATSET input file for the CRA-2004 PABC PANEL calculations.

Table A.1. Mole Fraction of Lumped Isotopes Over Time

Time (Years)	Total Moles Th	Total Moles U	Total Moles Pu	Mole Fraction TH230L	Mole Fraction U234L	Mole Fraction PU238L
0	1.34439E+05	2.72480E+06	4.12570E+04	1.08425E-06	2.86004E-04	[illegible]
50	1.34439E+05	2.72496E+06	4.10843E+04	2.26197E-06	3.19243E-04	4.56091E-03
100	1.34439E+05	2.72508E+06	4.09561E+04	3.51421E-06	3.41611E-04	3.08229E-03
150	1.34439E+05	2.72519E+06	4.08494E+04	4.81519E-06	3.56657E-04	2.08195E-03
200	1.34440E+05	2.72528E+06	4.07564E+04	6.14747E-06	3.66768E-04	1.40581E-03
250	1.34440E+05	2.72537E+06	4.06726E+04	7.49943E-06	3.73559E-04	9.49044E-04
300	1.34440E+05	2.72544E+06	4.05950E+04	8.86314E-06	3.78109E-04	6.40592E-04
350	1.34440E+05	2.72552E+06	4.05217E+04	1.02333E-05	3.81153E-04	4.32347E-04
400	1.34440E+05	2.72559E+06	4.04512E+04	1.16064E-05	3.83181E-04	2.91778E-04
450	1.34441E+05	2.72565E+06	4.03828E+04	1.29799E-05	3.84525E-04	1.96904E-04
500	1.34441E+05	2.72572E+06	4.03157E+04	1.43524E-05	3.85407E-04	1.32875E-04
550	1.34441E+05	2.72579E+06	4.02496E+04	1.57227E-05	3.85979E-04	8.96644E-05
600	1.34441E+05	2.72585E+06	4.01842E+04	1.70901E-05	3.86343E-04	6.05050E-05
650	1.34441E+05	2.72592E+06	4.01193E+04	1.84540E-05	3.86566E-04	4.08280E-05
700	1.34441E+05	2.72598E+06	4.00548E+04	1.98144E-05	3.86693E-04	2.75501E-05
750	1.34442E+05	2.72605E+06	3.99906E+04	2.11708E-05	3.86756E-04	1.85903E-05
800	1.34442E+05	2.72611E+06	3.99266E+04	2.25232E-05	3.86778E-04	1.25443E-05
850	1.34442E+05	2.72617E+06	3.98629E+04	2.38715E-05	3.86769E-04	8.46459E-06
900	1.34442E+05	2.72624E+06	3.97993E+04	2.52156E-05	3.86742E-04	5.71169E-06
950	1.34442E+05	2.72630E+06	3.97359E+04	2.65555E-05	3.86700E-04	3.85410E-06
1000	1.34443E+05	2.72636E+06	3.96726E+04	2.78913E-05	3.86652E-04	2.60064E-06
1050	1.34443E+05	2.72643E+06	3.96094E+04	2.92228E-05	3.86594E-04	1.75483E-06
1100	1.34443E+05	2.72649E+06	3.95464E+04	3.05501E-05	3.86537E-04	1.18412E-06
1150	1.34443E+05	2.72655E+06	3.94835E+04	3.18732E-05	3.86474E-04	7.99007E-07
1200	1.34443E+05	2.72661E+06	3.94208E+04	3.31922E-05	3.86409E-04	5.39147E-07
1250	1.34443E+05	2.72668E+06	3.93582E+04	3.45071E-05	3.86345E-04	3.63800E-07
1300	1.34444E+05	2.72674E+06	3.92957E+04	3.58177E-05	3.86279E-04	2.45481E-07
1350	1.34444E+05	2.72680E+06	3.92333E+04	3.71242E-05	3.86214E-04	1.65644E-07
1400	1.34444E+05	2.72686E+06	3.91710E+04	3.84267E-05	3.86147E-04	1.11771E-07
1450	1.34444E+05	2.72692E+06	3.91089E+04	3.97250E-05	3.86082E-04	7.54196E-08
1500	1.34444E+05	2.72699E+06	3.90469E+04	4.10193E-05	3.86015E-04	5.08908E-08
1550	1.34444E+05	2.72705E+06	3.89850E+04	4.23095E-05	3.85948E-04	3.43394E-08
1600	1.34445E+05	2.72711E+06	3.89232E+04	4.35956E-05	3.85881E-04	2.31711E-08
1650	1.34445E+05	2.72717E+06	3.88615E+04	4.48777E-05	3.85813E-04	1.56351E-08
1700	1.34445E+05	2.72723E+06	3.88000E+04	4.61558E-05	3.85746E-04	1.05501E-08
1750	1.34445E+05	2.72729E+06	3.87386E+04	4.74300E-05	3.85681E-04	7.11883E-09
1800	1.34445E+05	2.72736E+06	3.86773E+04	4.87001E-05	3.85614E-04	4.80355E-09
1850	1.34446E+05	2.72742E+06	3.86161E+04	4.99663E-05	3.85547E-04	3.24127E-09
1900	1.34446E+05	2.72748E+06	3.85551E+04	5.12286E-05	3.85480E-04	2.18709E-09
1950	1.34446E+05	2.72754E+06	3.84941E+04	5.24870E-05	3.85413E-04	1.47578E-09
2000	1.34446E+05	2.72760E+06	3.84333E+04	5.37414E-05	3.85347E-04	9.95801E-10
2050	1.34446E+05	2.72766E+06	3.83726E+04	5.49919E-05	3.85280E-04	6.71931E-10
2100	1.34446E+05	2.72772E+06	3.83120E+04	5.62389E-05	3.85213E-04	4.53394E-10
2150	1.34447E+05	2.72778E+06	3.82515E+04	5.74816E-05	3.85147E-04	3.05934E-10

Table A.1. Mole Fraction of Lumped Isotopes Over Time (continued)

Time (Years)	Total Moles Th	Total Moles U	Total Moles Pu	Mole Fraction TH230L	Mole Fraction U234L	Mole Fraction PU238L
2200	1.34447E+05	2.72784E+06	3.81911E+04	5.87208E-05	3.85080E-04	2.06433E-10
2250	1.34447E+05	2.72790E+06	3.81309E+04	5.99558E-05	3.85015E-04	1.39294E-10
2300	1.34447E+05	2.72796E+06	3.80707E+04	6.11873E-05	3.84948E-04	9.39899E-11
2350	1.34447E+05	2.72802E+06	3.80107E+04	6.24149E-05	3.84882E-04	6.34209E-11
2400	1.34447E+05	2.72808E+06	3.79508E+04	6.36390E-05	3.84815E-04	4.27940E-11
2450	1.34448E+05	2.72814E+06	3.78910E+04	6.48588E-05	3.84749E-04	2.88757E-11
2500	1.34448E+05	2.72820E+06	3.78313E+04	6.60755E-05	3.84682E-04	1.94842E-11
2550	1.34448E+05	2.72826E+06	3.77718E+04	6.72879E-05	3.84616E-04	1.31472E-11
2600	1.34448E+05	2.72832E+06	3.77123E+04	6.84968E-05	3.84549E-04	8.87120E-12
2650	1.34448E+05	2.72838E+06	3.76530E+04	6.97023E-05	3.84483E-04	5.98594E-12
2700	1.34448E+05	2.72844E+06	3.75937E+04	7.09038E-05	3.84416E-04	4.03907E-12
2750	1.34448E+05	2.72850E+06	3.75346E+04	7.21017E-05	3.84352E-04	2.72539E-12
2800	1.34449E+05	2.72855E+06	3.74756E+04	7.32961E-05	3.84285E-04	1.83899E-12
2850	1.34449E+05	2.72861E+06	3.74167E+04	7.44871E-05	3.84219E-04	1.24087E-12
2900	1.34449E+05	2.72867E+06	3.73579E+04	7.56741E-05	3.84152E-04	8.37289E-13
2950	1.34449E+05	2.72873E+06	3.72992E+04	7.68575E-05	3.84088E-04	5.64967E-13
3000	1.34449E+05	2.72879E+06	3.72407E+04	7.80375E-05	3.84021E-04	3.81216E-13
3050	1.34449E+05	2.72885E+06	3.71822E+04	7.92139E-05	3.83955E-04	2.57228E-13
3100	1.34450E+05	2.72890E+06	3.71239E+04	8.03867E-05	3.83890E-04	1.73567E-13
3150	1.34450E+05	2.72896E+06	3.70656E+04	8.15562E-05	3.83824E-04	1.17116E-13
3200	1.34450E+05	2.72902E+06	3.70075E+04	8.27221E-05	3.83758E-04	7.90243E-14
3250	1.34450E+05	2.72908E+06	3.69495E+04	8.38844E-05	3.83693E-04	5.33222E-14
3300	1.34450E+05	2.72914E+06	3.68916E+04	8.50432E-05	3.83627E-04	3.59795E-14
3350	1.34450E+05	2.72919E+06	3.68338E+04	8.61987E-05	3.83562E-04	2.42773E-14
3400	1.34451E+05	2.72925E+06	3.67761E+04	8.73506E-05	3.83498E-04	1.63812E-14
3450	1.34451E+05	2.72931E+06	3.67185E+04	8.84990E-05	3.83431E-04	1.10533E-14
3500	1.34451E+05	2.72937E+06	3.66610E+04	8.96441E-05	3.83365E-04	7.45829E-15
3550	1.34451E+05	2.72942E+06	3.66037E+04	9.07859E-05	3.83301E-04	5.03251E-15
3600	1.34451E+05	2.72948E+06	3.65464E+04	9.19242E-05	3.83235E-04	3.39570E-15
3650	1.34451E+05	2.72954E+06	3.64893E+04	9.30592E-05	3.83168E-04	2.29127E-15
3700	1.34451E+05	2.72959E+06	3.64322E+04	9.41910E-05	3.83104E-04	1.54604E-15
3750	1.34452E+05	2.72965E+06	3.63753E+04	9.53192E-05	3.83038E-04	1.04319E-15
3800	1.34452E+05	2.72971E+06	3.63185E+04	9.64438E-05	3.82973E-04	7.03897E-16
3850	1.34452E+05	2.72976E+06	3.62617E+04	9.75655E-05	3.82907E-04	4.74956E-16
3900	1.34452E+05	2.72982E+06	3.62051E+04	9.86840E-05	3.82841E-04	3.20478E-16
3950	1.34452E+05	2.72988E+06	3.61485E+04	9.97989E-05	3.82777E-04	2.16244E-16
4000	1.34452E+05	2.72993E+06	3.60921E+04	1.00911E-04	3.82711E-04	1.45910E-16
4050	1.34453E+05	2.72999E+06	3.60359E+04	1.02019E-04	3.82647E-04	9.84531E-17
4100	1.34453E+05	2.73005E+06	3.59796E+04	1.03124E-04	3.82581E-04	6.64312E-17
4150	1.34453E+05	2.73010E+06	3.59235E+04	1.04226E-04	3.82515E-04	4.48245E-17
4200	1.34453E+05	2.73016E+06	3.58675E+04	1.05325E-04	3.82450E-04	3.02454E-17
4250	1.34453E+05	2.73021E+06	3.58116E+04	1.06421E-04	3.82384E-04	2.04080E-17
4300	1.34453E+05	2.73027E+06	3.57558E+04	1.07513E-04	3.82320E-04	1.37703E-17
4350	1.34453E+05	2.73032E+06	3.57002E+04	1.08602E-04	3.82254E-04	9.29151E-18

Table A.1. Mole Fraction of Lumped Isotopes Over Time (continued)

Time (Years)	Total Moles Th	Total Moles U	Total Moles Pu	Mole Fraction TH230L	Mole Fraction U234L	Mole Fraction PU238L
4400	1.34454E+05	2.73038E+06	3.56446E+04	1.09688E-04	3.82190E-04	6.26944E-18
4450	1.34454E+05	2.73044E+06	3.55891E+04	1.10771E-04	3.82124E-04	4.23030E-18
4500	1.34454E+05	2.73049E+06	3.55337E+04	1.11851E-04	3.82060E-04	2.85439E-18
4550	1.34454E+05	2.73055E+06	3.54784E+04	1.12928E-04	3.81994E-04	1.92599E-18
4600	1.34454E+05	2.73060E+06	3.54232E+04	1.14001E-04	3.81930E-04	1.29956E-18
4650	1.34454E+05	2.73066E+06	3.53681E+04	1.15072E-04	3.81864E-04	8.76874E-19
4700	1.34454E+05	2.73071E+06	3.53132E+04	1.16139E-04	3.81802E-04	5.91669E-19
4750	1.34455E+05	2.73077E+06	3.52583E+04	1.17203E-04	3.81736E-04	3.99227E-19
4800	1.34455E+05	2.73082E+06	3.52035E+04	1.18265E-04	3.81672E-04	2.69376E-19
4850	1.34455E+05	2.73087E+06	3.51488E+04	1.19323E-04	3.81606E-04	1.81761E-19
4900	1.34455E+05	2.73093E+06	3.50943E+04	1.20378E-04	3.81542E-04	1.22642E-19
4950	1.34455E+05	2.73098E+06	3.50398E+04	1.21431E-04	3.81476E-04	8.27525E-20
5000	1.34455E+05	2.73104E+06	3.49854E+04	1.22480E-04	3.81412E-04	5.58368E-20
5050	1.34455E+05	2.73109E+06	3.49312E+04	1.23526E-04	3.81347E-04	3.76757E-20
5100	1.34456E+05	2.73115E+06	3.48770E+04	1.24569E-04	3.81283E-04	2.54214E-20
5150	1.34456E+05	2.73120E+06	3.48229E+04	1.25609E-04	3.81217E-04	1.71529E-20
5200	1.34456E+05	2.73125E+06	3.47689E+04	1.26646E-04	3.81153E-04	1.15739E-20
5250	1.34456E+05	2.73131E+06	3.47150E+04	1.27681E-04	3.81087E-04	7.80939E-21
5300	1.34456E+05	2.73136E+06	3.46613E+04	1.28713E-04	3.81024E-04	5.26934E-21
5350	1.34456E+05	2.73141E+06	3.46076E+04	1.29741E-04	3.80960E-04	3.55546E-21
5400	1.34456E+05	2.73147E+06	3.45540E+04	1.30767E-04	3.80896E-04	2.39903E-21
5450	1.34457E+05	2.73152E+06	3.45005E+04	1.31790E-04	3.80832E-04	1.61872E-21
5500	1.34457E+05	2.73157E+06	3.44471E+04	1.32810E-04	3.80766E-04	1.09222E-21
5550	1.34457E+05	2.73163E+06	3.43938E+04	1.33827E-04	3.80702E-04	7.36968E-22
5600	1.34457E+05	2.73168E+06	3.43406E+04	1.34841E-04	3.80637E-04	4.97263E-22
5650	1.34457E+05	2.73173E+06	3.42875E+04	1.35852E-04	3.80573E-04	3.35523E-22
5700	1.34457E+05	2.73179E+06	3.42345E+04	1.36861E-04	3.80509E-04	2.26392E-22
5750	1.34457E+05	2.73184E+06	3.41816E+04	1.37866E-04	3.80444E-04	1.52756E-22
5800	1.34457E+05	2.73189E+06	3.41287E+04	1.38870E-04	3.80380E-04	1.03071E-22
5850	1.34458E+05	2.73194E+06	3.40760E+04	1.39870E-04	3.80315E-04	6.95459E-23
5900	1.34458E+05	2.73200E+06	3.40234E+04	1.40867E-04	3.80251E-04	4.69255E-23
5950	1.34458E+05	2.73205E+06	3.39709E+04	1.41862E-04	3.80189E-04	3.16624E-23
6000	1.34458E+05	2.73210E+06	3.39184E+04	1.42854E-04	3.80123E-04	2.13639E-23
6050	1.34458E+05	2.73215E+06	3.38661E+04	1.43843E-04	3.80060E-04	1.44152E-23
6100	1.34458E+05	2.73221E+06	3.38138E+04	1.44829E-04	3.79996E-04	9.72644E-24
6150	1.34458E+05	2.73226E+06	3.37617E+04	1.45813E-04	3.79931E-04	6.56281E-24
6200	1.34459E+05	2.73231E+06	3.37096E+04	1.46794E-04	3.79867E-04	4.42818E-24
6250	1.34459E+05	2.73236E+06	3.36577E+04	1.47772E-04	3.79803E-04	2.98786E-24
6300	1.34459E+05	2.73241E+06	3.36058E+04	1.48748E-04	3.79738E-04	2.01602E-24
6350	1.34459E+05	2.73246E+06	3.35540E+04	1.49721E-04	3.79674E-04	1.36029E-24
6400	1.34459E+05	2.73252E+06	3.35023E+04	1.50691E-04	3.79612E-04	9.17839E-25
6450	1.34459E+05	2.73257E+06	3.34507E+04	1.51659E-04	3.79547E-04	6.19300E-25
6500	1.34459E+05	2.73262E+06	3.33992E+04	1.52624E-04	3.79484E-04	4.17865E-25
6550	1.34459E+05	2.73267E+06	3.33478E+04	1.53586E-04	3.79420E-04	2.81948E-25
6600	1.34460E+05	2.73272E+06	3.32965E+04	1.54546E-04	3.79355E-04	1.90241E-25

Table A.1. Mole Fraction of Lumped Isotopes Over Time (continued)

Time (Years)	Total Moles Th	Total Moles U	Total Moles Pu	Mole Fraction TH230L	Mole Fraction U234L	Mole Fraction PU238L
6650	1.34460E+05	2.73277E+06	3.32452E+04	1.55503E-04	3.79291E-04	1.28362E-25
6700	1.34460E+05	2.73282E+06	3.31941E+04	1.56458E-04	3.79228E-04	8.66109E-26
6750	1.34460E+05	2.73287E+06	3.31430E+04	1.57410E-04	3.79164E-04	5.84396E-26
6800	1.34460E+05	2.73293E+06	3.30921E+04	1.58359E-04	3.79101E-04	3.94312E-26
6850	1.34460E+05	2.73298E+06	3.30412E+04	1.59306E-04	3.79037E-04	2.66057E-26
6900	1.34460E+05	2.73303E+06	3.29905E+04	1.60250E-04	3.78974E-04	1.79517E-26
6950	1.34460E+05	2.73308E+06	3.29397E+04	1.61192E-04	3.78909E-04	1.21127E-26
7000	1.34461E+05	2.73313E+06	3.28892E+04	1.62131E-04	3.78845E-04	8.17285E-27
7050	1.34461E+05	2.73318E+06	3.28387E+04	1.63068E-04	3.78782E-04	5.51451E-27
7100	1.34461E+05	2.73323E+06	3.27882E+04	1.64002E-04	3.78718E-04	3.72082E-27
7150	1.34461E+05	2.73328E+06	3.27379E+04	1.64934E-04	3.78653E-04	2.51057E-27
7200	1.34461E+05	2.73333E+06	3.26877E+04	1.65864E-04	3.78592E-04	1.69397E-27
7250	1.34461E+05	2.73338E+06	3.26375E+04	1.66790E-04	3.78528E-04	1.14297E-27
7300	1.34461E+05	2.73343E+06	3.25875E+04	1.67715E-04	3.78465E-04	7.71203E-28
7350	1.34461E+05	2.73348E+06	3.25375E+04	1.68637E-04	3.78402E-04	5.20356E-28
7400	1.34462E+05	2.73353E+06	3.24876E+04	1.69556E-04	3.78337E-04	3.51101E-28
7450	1.34462E+05	2.73358E+06	3.24378E+04	1.70473E-04	3.78273E-04	2.36899E-28
7500	1.34462E+05	2.73363E+06	3.23881E+04	1.71387E-04	3.78212E-04	1.59843E-28
7550	1.34462E+05	2.73368E+06	3.23385E+04	1.72300E-04	3.78148E-04	1.07852E-28
7600	1.34462E+05	2.73373E+06	3.22890E+04	1.73210E-04	3.78084E-04	7.27709E-29
7650	1.34462E+05	2.73377E+06	3.22395E+04	1.74117E-04	3.78020E-04	4.91008E-29
7700	1.34462E+05	2.73382E+06	3.21902E+04	1.75022E-04	3.77957E-04	3.31298E-29
7750	1.34462E+05	2.73387E+06	3.21409E+04	1.75925E-04	3.77894E-04	2.23538E-29
7800	1.34463E+05	2.73392E+06	3.20917E+04	1.76825E-04	3.77831E-04	1.50828E-29
7850	1.34463E+05	2.73397E+06	3.20426E+04	1.77723E-04	3.77769E-04	1.01768E-29
7900	1.34463E+05	2.73402E+06	3.19936E+04	1.78619E-04	3.77704E-04	6.86659E-30
7950	1.34463E+05	2.73407E+06	3.19447E+04	1.79512E-04	3.77641E-04	4.63310E-30
8000	1.34463E+05	2.73412E+06	3.18959E+04	1.80403E-04	3.77578E-04	3.12609E-30
8050	1.34463E+05	2.73417E+06	3.18471E+04	1.81291E-04	3.77515E-04	2.10926E-30
8100	1.34463E+05	2.73421E+06	3.17984E+04	1.82178E-04	3.77453E-04	1.42318E-30
8150	1.34463E+05	2.73426E+06	3.17498E+04	1.83062E-04	3.77390E-04	9.60264E-31
8200	1.34464E+05	2.73431E+06	3.17013E+04	1.83944E-04	3.77327E-04	6.47918E-31
8250	1.34464E+05	2.73436E+06	3.16530E+04	1.84823E-04	3.77262E-04	4.37169E-31
8300	1.34464E+05	2.73441E+06	3.16046E+04	1.85700E-04	3.77199E-04	2.94970E-31
8350	1.34464E+05	2.73446E+06	3.15564E+04	1.86576E-04	3.77136E-04	1.99025E-31
8400	1.34464E+05	2.73450E+06	3.15082E+04	1.87449E-04	3.77075E-04	1.34288E-31
8450	1.34464E+05	2.73455E+06	3.14601E+04	1.88319E-04	3.77012E-04	9.06076E-32
8500	1.34464E+05	2.73460E+06	3.14121E+04	1.89187E-04	3.76949E-04	6.11355E-32
8550	1.34464E+05	2.73465E+06	3.13642E+04	1.90054E-04	3.76886E-04	4.12497E-32
8600	1.34464E+05	2.73470E+06	3.13164E+04	1.90917E-04	3.76823E-04	2.78324E-32
8650	1.34465E+05	2.73474E+06	3.12686E+04	1.91779E-04	3.76761E-04	1.87793E-32
8700	1.34465E+05	2.73479E+06	3.12210E+04	1.92638E-04	3.76697E-04	1.26708E-32
8750	1.34465E+05	2.73484E+06	3.11734E+04	1.93496E-04	3.76634E-04	8.54935E-33
8800	1.34465E+05	2.73489E+06	3.11259E+04	1.94351E-04	3.76571E-04	5.76848E-33
8850	1.34465E+05	2.73493E+06	3.10785E+04	1.95204E-04	3.76508E-04	3.89213E-33

Table A.1. Mole Fraction of Lumped Isotopes Over Time (continued)

Time (Years)	Total Moles Th	Total Moles U	Total Moles Pu	Mole Fraction TH230L	Mole Fraction U234L	Mole Fraction PU238L
8900	1.34465E+05	2.73498E+06	3.10312E+04	1.96055E-04	3.76447E-04	2.62613E-33
8950	1.34465E+05	2.73503E+06	3.09840E+04	1.96904E-04	3.76384E-04	1.77191E-33
9000	1.34465E+05	2.73507E+06	3.09368E+04	1.97750E-04	3.76321E-04	1.19556E-33
9050	1.34465E+05	2.73512E+06	3.08897E+04	1.98595E-04	3.76258E-04	8.06673E-34
9100	1.34466E+05	2.73517E+06	3.08427E+04	1.99437E-04	3.76195E-04	5.44282E-34
9150	1.34466E+05	2.73521E+06	3.07958E+04	2.00277E-04	3.76134E-04	3.67241E-34
9200	1.34466E+05	2.73526E+06	3.07489E+04	2.01116E-04	3.76071E-04	2.47786E-34
9250	1.34466E+05	2.73531E+06	3.07022E+04	2.01951E-04	3.76008E-04	1.67188E-34
9300	1.34466E+05	2.73535E+06	3.06555E+04	2.02786E-04	3.75945E-04	1.12805E-34
9350	1.34466E+05	2.73540E+06	3.06089E+04	2.03618E-04	3.75883E-04	7.61125E-35
9400	1.34466E+05	2.73545E+06	3.05624E+04	2.04447E-04	3.75821E-04	5.13549E-35
9450	1.34466E+05	2.73549E+06	3.05159E+04	2.05275E-04	3.75759E-04	3.46503E-35
9500	1.34467E+05	2.73554E+06	3.04696E+04	2.06101E-04	3.75696E-04	2.33794E-35
9550	1.34467E+05	2.73559E+06	3.04233E+04	2.06925E-04	3.75633E-04	1.57746E-35
9600	1.34467E+05	2.73563E+06	3.03771E+04	2.07746E-04	3.75570E-04	1.06435E-35
9650	1.34467E+05	2.73568E+06	3.03310E+04	2.08566E-04	3.75509E-04	7.18141E-36
9700	1.34467E+05	2.73572E+06	3.02849E+04	2.09384E-04	3.75447E-04	4.84546E-36
9750	1.34467E+05	2.73577E+06	3.02390E+04	2.10200E-04	3.75384E-04	3.26934E-36
9800	1.34467E+05	2.73581E+06	3.01931E+04	2.11013E-04	3.75321E-04	2.20590E-36
9850	1.34467E+05	2.73586E+06	3.01473E+04	2.11825E-04	3.75260E-04	1.48837E-36
9900	1.34467E+05	2.73591E+06	3.01016E+04	2.12634E-04	3.75197E-04	1.00423E-36
9950	1.34467E+05	2.73595E+06	3.00559E+04	2.13442E-04	3.75135E-04	6.77578E-37
10000	1.34468E+05	2.73600E+06	3.00103E+04	2.14248E-04	3.75072E-04	4.57176E-37

APPENDIX B : INPUT FILES USED FOR PANEL CRA-2004 PABC CALCULATIONS

B.1 GM_PANEL_CRA1BC.INP

The following MATSET input file is used to set the values needed for PANEL for a CRA1BC (PABC) run for concentration and standard type runs.

```
!-------------------------------------------------------------
! Analysis    : CRA-2004 PA Baseline Calculation (PABC) AP-122
! Analysis ID : CRA1BC
! Remark      : This input file is unchanged from previous
!             : analyses. See original description below.
!-------------------------------------------------------------
!=============================================================================
!   FILETYPE: GENMESH input text file
!   TITLE: Simple GENMESH to set up Source Term CDB
!   ANALYSTS: Christine Stockman
!   DATE: May 31, 1996
!=============================================================================
!
  *SETUP
    DIM=     3
    ORIGIN= 0.0, 0.0, 0.0
    IJKMAX= 2, 2, 2
  *GRID
!   ==================== X direction ====================
    DEL, COORD=X, DEL=   1.00, INRANGE=  1,  2, FACTOR= 1.0
!   ==================== Y direction ====================
    DEL, COORD=Y, DEL=   1.00, INRANGE=  1,  2, FACTOR= 1.0
!   ==================== Z direction ====================
    DEL, COORD=Z, DEL=   1.00, INRANGE=  1,  2, FACTOR= 1.0
!
  *REGIONS
   REGION= 1, IRANGE= 1,2, JRANGE= 1,2 KRANGE= 1, 2
 !=============================================================================
  *END
```

B.2 MS_PANEL_CRA1BC.INP

The following MATSET input file is used to set the values needed for PANEL for a CRA1BC (PABC) run for concentration and standard type runs.

```
!=============================================================================
! TITLE:    MATSET input file for PANEL (CRA1BC for SOURCE term in PANEL runs)
!  This input file if for the 2004 CRA Baseline Calculation (AP-122)
! ANALYSTS: J. W. GARNER
! CREATED:  Apr 20, 2005
! A modification of the 2003 CRA Source Term MATSET input file
! PURPOSE:  PREPARE INPUT CDB FOR  PANEL
!=============================================================================
!
*HEADING
 RUN=0
 SCALE=SOURCE
 SCENARIO=00
 TITLE=SOURCE TERM
!
*PRINT_ASSIGNED_VALUES
!
*UNITS=SI
!
*CREATE_BLOCK
  BLOCKID=      2,  3,  4,  5,  6,  7,  8,  9, 10, 11, 12, 13, 14, 15, &
           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, 42, 43, 44, 45, &
           46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60, &
           61, 62, 63, 64, 65
*RETRIEVE*NAME
 COORDINATE, DIM=3, NAMES=X, Y, Z
 MATERIAL,    1=GLOBAL, 2=REFCON, &
```

```
    3=AM241,  4=AM243,  5=CF252,  6=CM243,  7=CM244,  8=CM245, &
    9=CM248, 10=CS137, 11=NP237, 12=PA231, 13=PB210, 14=PM147, &
   15=PU238, 16=PU239, 17=PU240, 18=PU241, 19=PU242, 20=PU244, &
   21=RA226, 22=RA228, 23=SR90,  24=TH229, 25=TH230, 26=TH232, &
   27=U233,  28=U234,  29=U235,  30=U236,  31=U238,  &
   32=AM, 33=CF, 34=CM, 35=CS, 36=NP, 37=PA, 38=PB, 39=PM, 40=PU, &
   41=RA, 42=SR, 43=TH, 44=U,  &
   45=SOLMOD3, 46=SOLMOD4, 47=SOLMOD5, 48=SOLMOD6, &
   49=PHUMOX3, 50=PHUMOX4, 51=PHUMOX5, 52=PHUMOX6, &
   53=SOLAM3,  54=SOLPU3,  55=SOLPU4,  56=SOLTH4,  57=SOLU4,  58=SOLU6, &
   59=AM241L, 60=PU238L, 61=PU239L, 62=TH230L, 63=U234L,  64=BOREHOLE, &
   65=WAS_AREA
!MATERIALS 59-63 ARE LUMPED PARAMETERS FOR NUTS
!
 PROPERTY   MATERIAL=WAS_AREA,  NAMES =PROBDEG
 PROPERTY   MATERIAL=Global,    NAMES =OXSTAT
 PROPERTY   MATERIAL=REFCON,    NAMES =YRSEC,INVSCALE,PANDFVOL
!ISOTOPES
 PROPERTY   MATERIAL=Am241,     NAMES =InvCHD,InvRHD,ATWEIGHT,HALFLIFE,EPAREL
 PROPERTY   MATERIAL=Am243,     NAMES =InvCHD,InvRHD,ATWEIGHT,HALFLIFE,EPAREL
 PROPERTY   MATERIAL=Cf252,     NAMES =InvCHD,InvRHD,ATWEIGHT,HALFLIFE,EPAREL
 PROPERTY   MATERIAL=Cm243,     NAMES =InvCHD,InvRHD,ATWEIGHT,HALFLIFE,EPAREL
 PROPERTY   MATERIAL=Cm244,     NAMES =InvCHD,InvRHD,ATWEIGHT,HALFLIFE,EPAREL
 PROPERTY   MATERIAL=Cm245,     NAMES =InvCHD,InvRHD,ATWEIGHT,HALFLIFE,EPAREL
 PROPERTY   MATERIAL=Cm248,     NAMES =InvCHD,InvRHD,ATWEIGHT,HALFLIFE,EPAREL
 PROPERTY   MATERIAL=Cs137,     NAMES =InvCHD,InvRHD,ATWEIGHT,HALFLIFE,EPAREL
 PROPERTY   MATERIAL=Np237,     NAMES =InvCHD,InvRHD,ATWEIGHT,HALFLIFE,EPAREL
 PROPERTY   MATERIAL=Pa231,     NAMES =InvCHD,InvRHD,ATWEIGHT,HALFLIFE,EPAREL
 PROPERTY   MATERIAL=Pb210,     NAMES =InvCHD,InvRHD,ATWEIGHT,HALFLIFE,EPAREL
 PROPERTY   MATERIAL=Pm147,     NAMES =InvCHD,InvRHD,ATWEIGHT,HALFLIFE,EPAREL
 PROPERTY   MATERIAL=Pu238,     NAMES =InvCHD,InvRHD,ATWEIGHT,HALFLIFE,EPAREL
 PROPERTY   MATERIAL=Pu239,     NAMES =InvCHD,InvRHD,ATWEIGHT,HALFLIFE,EPAREL
 PROPERTY   MATERIAL=Pu240,     NAMES =InvCHD,InvRHD,ATWEIGHT,HALFLIFE,EPAREL
 PROPERTY   MATERIAL=Pu241,     NAMES =InvCHD,InvRHD,ATWEIGHT,HALFLIFE,EPAREL
 PROPERTY   MATERIAL=Pu242,     NAMES =InvCHD,InvRHD,ATWEIGHT,HALFLIFE,EPAREL
 PROPERTY   MATERIAL=Pu244,     NAMES =InvCHD,InvRHD,ATWEIGHT,HALFLIFE,EPAREL
 PROPERTY   MATERIAL=Ra226,     NAMES =InvCHD,InvRHD,ATWEIGHT,HALFLIFE,EPAREL
 PROPERTY   MATERIAL=Ra228,     NAMES =InvCHD,InvRHD,ATWEIGHT,HALFLIFE,EPAREL
 PROPERTY   MATERIAL=Sr90 ,     NAMES =InvCHD,InvRHD,ATWEIGHT,HALFLIFE,EPAREL
 PROPERTY   MATERIAL=Th229,     NAMES =InvCHD,InvRHD,ATWEIGHT,HALFLIFE,EPAREL
 PROPERTY   MATERIAL=Th230,     NAMES =InvCHD,InvRHD,ATWEIGHT,HALFLIFE,EPAREL
 PROPERTY   MATERIAL=Th232,     NAMES =InvCHD,InvRHD,ATWEIGHT,HALFLIFE,EPAREL
 PROPERTY   MATERIAL=U233,      NAMES =InvCHD,InvRHD,ATWEIGHT,HALFLIFE,EPAREL
 PROPERTY   MATERIAL=U234,      NAMES =InvCHD,InvRHD,ATWEIGHT,HALFLIFE,EPAREL
 PROPERTY   MATERIAL=U235,      NAMES =InvCHD,InvRHD,ATWEIGHT,HALFLIFE,EPAREL
 PROPERTY   MATERIAL=U236,      NAMES =InvCHD,InvRHD,ATWEIGHT,HALFLIFE,EPAREL
 PROPERTY   MATERIAL=U238,      NAMES =InvCHD,InvRHD,ATWEIGHT,HALFLIFE,EPAREL
!LUMPED ISOTOPES
 PROPERTY   MATERIAL=AM241L,    NAMES =InvCHD,InvRHD
 PROPERTY   MATERIAL=PU238L,    NAMES =InvCHD,InvRHD,LSOLDIFF
 PROPERTY   MATERIAL=PU239L,    NAMES =InvCHD,InvRHD
 PROPERTY   MATERIAL=TH230L,    NAMES =InvCHD,InvRHD,LSOLDIFF
 PROPERTY   MATERIAL=U234L,     NAMES =InvCHD,InvRHD,LSOLDIFF
!ELEMENTS
 PROPERTY   MATERIAL=AM,        NAMES =CONCMIN,CONCINT,CAPHUM,CAPMIC,PROPMIC
 PROPERTY   MATERIAL=NP,        NAMES =CONCMIN,CONCINT,CAPHUM,CAPMIC,PROPMIC
 PROPERTY   MATERIAL=PU,        NAMES =CONCMIN,CONCINT,CAPHUM,CAPMIC,PROPMIC
 PROPERTY   MATERIAL=TH,        NAMES =CONCMIN,CONCINT,CAPHUM,CAPMIC,PROPMIC
 PROPERTY   MATERIAL=U,         NAMES =CONCMIN,CONCINT,CAPHUM,CAPMIC,PROPMIC
!OXIDATION STATES
 PROPERTY   MATERIAL=SOLMOD3,   NAMES =SOLSOH,SOLCOH,SOLVAR
 PROPERTY   MATERIAL=SOLMOD4,   NAMES =SOLSOH,SOLCOH,SOLVAR
 PROPERTY   MATERIAL=SOLMOD5,   NAMES =SOLSOH,SOLCOH
 PROPERTY   MATERIAL=SOLMOD6,   NAMES =SOLSOH,SOLCOH
 PROPERTY   MATERIAL=PHUMOX3,   NAMES =PHUMSIM,PHUMCIM
 PROPERTY   MATERIAL=PHUMOX4,   NAMES =PHUMSIM,PHUMCIM
 PROPERTY   MATERIAL=PHUMOX5,   NAMES =PHUMSIM,PHUMCIM
 PROPERTY   MATERIAL=PHUMOX6,   NAMES =PHUMSIM,PHUMCIM
!WASTE UNIT FACTOR
 PROPERTY   MATERIAL=BOREHOLE,  NAMES=WUF
!=============================================================================
*SET*VALUES
!INVSCALE AND PANDFVOL NEEDED UNTIL ADDED TO DATA BASE
 PROPERTY   MATERIAL=REFCON,    NAMES*VALUE: INVSCALE=.1044,PANDFVOL=1045.
!
! PROPERTY   MATERIAL=PU238L,   NAMES*VALUE: LSOLDIFF=2.17519 CCA Value
! PROPERTY   MATERIAL=PU238L,   NAMES*VALUE: LSOLDIFF=2.18488 CRA Value
 PROPERTY   MATERIAL=PU238L,   NAMES*VALUE: LSOLDIFF=2.17123
! PROPERTY   MATERIAL=TH230L,   NAMES*VALUE: LSOLDIFF=2.900 CCA Value
! PROPERTY   MATERIAL=TH230L,   NAMES*VALUE: LSOLDIFF=3.95623 CRA Value
 PROPERTY   MATERIAL=TH230L,   NAMES*VALUE: LSOLDIFF=3.66908
```

```
! PROPERTY   MATERIAL=U234L,     NAMES*VALUE: LSOLDIFF=2.550 CCA Value
! PROPERTY   MATERIAL=U234L,     NAMES*VALUE: LSOLDIFF=3.25069 CRA Value
 PROPERTY   MATERIAL=U234L,     NAMES*VALUE: LSOLDIFF=3.41252
!
*END
!------------------------------------------------------------------------
[End of file]
```

A.3 ALG_PANEL_CRA1BC.INP

The following ALGEBRA input file is used for all PANEL runs for the CCA1BC (PABC). Since there is always microbial activity in this calculation, values for SOLS and SOLC are set to the values of SOLSOH and SOLCOH. It also sets the half-lives and atomic weights for the lumped isotopes. In this calculation, we sample only on solubility variability for oxidation state III and IV. These samples values are propagated to the appropriate 10 variables and the solubility variability of oxidation state VI is set to zero.

```
!
! This input file is for the CRA-2004 PABC, AP-122
!
!
! NOW, DEFINE SOLS AND SOLC
!
LIMIT BLOCK 45 ! (SOLMOD3)
SOLS=MAKEPROP(SOLSOH)
SOLC=MAKEPROP(SOLCOH)
!
LIMIT BLOCK 46 ! (SOLMOD4)
SOLS=MAKEPROP(SOLSOH)
SOLC=MAKEPROP(SOLCOH)
!
LIMIT BLOCK 47 ! (SOLMOD5)
SOLS=MAKEPROP(SOLSOH)
SOLC=MAKEPROP(SOLCOH)
!
LIMIT BLOCK 48 ! (SOLMOD6)
SOLS=MAKEPROP(SOLSOH)
SOLC=MAKEPROP(SOLCOH)
!
!PROPOGATE THE SOLUBILITY VARIABILITY TO VARIABLES NEEDED FOR PANEL
!
LIMIT BLOCK 53 ! (SOLAM3)
SOLSIM=MAKEPROP(SOLVAR[B:45])
SOLCIM=MAKEPROP(SOLVAR[B:45])
!
LIMIT BLOCK 54 ! (SOLPU3)
SOLSIM=MAKEPROP(SOLVAR[B:45])
SOLCIM=MAKEPROP(SOLVAR[B:45])
!
LIMIT BLOCK 55 ! (SOLPU4)
SOLSIM=MAKEPROP(SOLVAR[B:46])
SOLCIM=MAKEPROP(SOLVAR[B:46])
!
LIMIT BLOCK 57 ! (SOLU4)
SOLSIM=MAKEPROP(SOLVAR[B:46])
SOLCIM=MAKEPROP(SOLVAR[B:46])
!
LIMIT BLOCK 56 ! (SOLTH4)
SOLSIM=MAKEPROP(SOLVAR[B:46])
SOLCIM=MAKEPROP(SOLVAR[B:46])
!
LIMIT BLOCK 58 ! (SOLU6)
SOLSIM=MAKEPROP(0.)
SOLCIM=MAKEPROP(0.)
!
! SET HALFLIFE AND ATWEIGHT FOR AM241L SAME AS FOR AM241
!
LIMIT BLOCK 59 ! (AM241L)
ATWEIGHT=MAKEPROP(ATWEIGHT[B:3])
HALFLIFE=MAKEPROP(HALFLIFE[B:3])
!
! SET HALFLIFE AND ATWEIGHT FOR PU238L SAME AS FOR PU238
!
LIMIT BLOCK 60 ! (PU238L)
ATWEIGHT=MAKEPROP(ATWEIGHT[B:15])
```

```
HALFLIFE=MAKEPROP(HALFLIFE[B:15])
!
! SET HALFLIFE AND ATWEIGHT FOR PU239L SAME AS FOR PU239
!
LIMIT BLOCK 61 ! (PU239L)
ATWEIGHT=MAKEPROP(ATWEIGHT[B:16])
HALFLIFE=MAKEPROP(HALFLIFE[B:16])
!
! SET HALFLIFE AND ATWEIGHT FOR TH230L SAME AS FOR TH230
!
LIMIT BLOCK 62 ! (TH230L)
ATWEIGHT=MAKEPROP(ATWEIGHT[B:25])
HALFLIFE=MAKEPROP(HALFLIFE[B:25])
!
! SET HALFLIFE AND ATWEIGHT FOR U234L SAME AS FOR U234
!
LIMIT BLOCK 63 ! (U234L)
ATWEIGHT=MAKEPROP(ATWEIGHT[B:28])
HALFLIFE=MAKEPROP(HALFLIFE[B:28])
!
END
```

A.4 LHS3_DUMMY.INP

```
This file is not read by LHS3, but its presence is required.

[End of file]
```

APPENDIX C

List of values from database used in the source term calculation from MATSET

AM	CONCMIN	2.6000E-08	SDB: AM,CONCMIN
AM	CONCINT	0.0000E+00	SDB: AM,CONCINT
AM	CAPHUM	1.1000E-05	SDB: AM,CAPHUM
AM	CAPMIC	1.0000E+00	SDB: AM,CAPMIC
AM	PROPMIC	3.6000E+00	SDB: AM,PROPMIC
NP	CONCMIN	2.6000E-08	SDB: NP,CONCMIN
NP	CONCINT	0.0000E+00	SDB: NP,CONCINT
NP	CAPHUM	1.1000E-05	SDB: NP,CAPHUM
NP	CAPMIC	2.7000E-03	SDB: NP,CAPMIC
NP	PROPMIC	1.2000E+01	SDB: NP,PROPMIC
PU	CONCMIN	2.6000E-08	SDB: PU,CONCMIN
PU	CONCINT	1.0000E-09	SDB: PU,CONCINT
PU	CAPHUM	1.1000E-05	SDB: PU,CAPHUM
PU	CAPMIC	6.8000E-05	SDB: PU,CAPMIC
PU	PROPMIC	3.0000E-01	SDB: PU,PROPMIC
TH	CONCMIN	2.6000E-08	SDB: TH,CONCMIN
TH	CONCINT	0.0000E+00	SDB: TH,CONCINT
TH	CAPHUM	1.1000E-05	SDB: TH,CAPHUM
TH	CAPMIC	1.9000E-03	SDB: TH,CAPMIC
TH	PROPMIC	3.1000E+00	SDB: TH,PROPMIC
U	CONCMIN	2.6000E-08	SDB: U,CONCMIN
U	CONCINT	0.0000E+00	SDB: U,CONCINT
U	CAPHUM	1.1000E-05	SDB: U,CAPHUM
U	CAPMIC	2.1000E-03	SDB: U,CAPMIC
U	PROPMIC	2.1000E-03	SDB: U,PROPMIC
SOLMOD3	SOLSOH	3.8700E-07	SDB: SOLMOD3,SOLSOH
SOLMOD3	SOLCOH	2.8800E-07	SDB: SOLMOD3,SOLCOH
SOLMOD3	***SOLVAR***	***-3.0682E-02***	***SDB: SOLMOD3,SOLVAR***
SOLMOD4	SOLSOH	5.6400E-08	SDB: SOLMOD4,SOLSOH
SOLMOD4	SOLCOH	6.7900E-08	SDB: SOLMOD4,SOLCOH
SOLMOD4	***SOLVAR***	***7.5000E-02***	***SDB: SOLMOD4,SOLVAR***
SOLMOD5	SOLSOH	3.5500E-07	SDB: SOLMOD5,SOLSOH
SOLMOD5	SOLCOH	8.2400E-07	SDB: SOLMOD5,SOLCOH
SOLMOD6	SOLSOH	1.0000E-03	SDB: SOLMOD6,SOLSOH
SOLMOD6	SOLCOH	1.0000E-03	SDB: SOLMOD6,SOLCOH
PHUMOX3	PHUMSIM	1.9000E-01	SDB: PHUMOX3,PHUMSIM
PHUMOX3	***PHUMCIM***	***1.3700E+00***	***SDB: PHUMOX3,PHUMCIM***
PHUMOX4	PHUMSIM	6.3000E+00	SDB: PHUMOX4,PHUMSIM
PHUMOX4	PHUMCIM	6.3000E+00	SDB: PHUMOX4,PHUMCIM
PHUMOX5	PHUMSIM	9.1000E-04	SDB: PHUMOX5,PHUMSIM
PHUMOX5	PHUMCIM	7.4000E-03	SDB: PHUMOX5,PHUMCIM
PHUMOX6	PHUMSIM	1.2000E-01	SDB: PHUMOX6,PHUMSIM
PHUMOX6	PHUMCIM	5.1000E-01	SDB: PHUMOX6,PHUMCIM
BOREHOLE	WUF	2.3200E+00	SDB: BOREHOLE,WUF
GLOBAL	***OXSTAT***	***5.0000E-01***	***SDB: GLOBAL,OXSTAT***

Items above in bold and italics indicated that the values listed are replaced by sampled values before use in the source term calculations.

Rigali, Mark J

From: dskesse@sandia.gov
Sent: Thursday, July 21, 2005 5:18 PM
To: Rigali, Mark J
Cc: Kessel, David S
Subject: Notification of Role Assignment Delegation

Subject: Notification of Role Assignment Delegation
Date: Jul-21-2005
To: *Distribution*

Person making delegation: KESSEL,DAVID S.

Individual acting as delegate:
RIGALI,MARK J.

Role assignment(s) being delegated:
Timecard_Final_Reviewer (06821)

Dates delegation in effect:

From: 7/19/2005
To: 12/20/2005