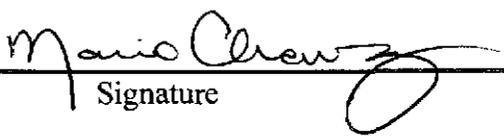


**Sandia National Laboratories
Waste Isolation Pilot Plant**

**Analysis Package for PANEL:
CRA-2009 Performance Assessment Baseline Calculation**

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CONTENTS

EXECUTIVE SUMMARY	7
1. INTRODUCTION	8
1.1 BACKGROUND	8
1.2 OBJECTIVES FOR THE CRA-2009 PABC PANEL ANALYSIS.....	9
2. CHANGES FROM THE CRA-2004 PABC TO THE CRA-2009 PABC THAT AFFECT PANEL CALCULATIONS	9
2.1 ACTINIDE SOLUBILITY UPDATE	9
2.2 SOLUBILITY UNCERTAINTY UPDATE.....	12
2.3 INVENTORY UPDATE	13
2.4 PANEL IMPLEMENTATION.....	15
3. THEORETICAL BASIS FOR PANEL CALCULATIONS	16
3.1 RADIOACTIVE DECAY	17
3.2 POTENTIAL FOR DISSOLUTION AND MOBILIZATION.....	19
3.3 MOBILIZED RADIONUCLIDE CONCENTRATIONS	22
3.4 RADIONUCLIDES UP THE BOREHOLE TO THE CULEBRA (S6).....	26
4. PANEL MODELING PROCESS.....	26
4.1 GENMESH: SINGLE-ELEMENT GRID GENERATION	27
4.2 MATSET: MATERIAL PROPERTY ASSIGNMENTS	27
4.3 POSTLHS: UNCERTAIN PARAMETER VALUES.....	28
4.4 ALGEBRACDB: DATA MODIFICATION.....	28
4.5 BRAGFLO OUTPUT TO PANEL.....	29
4.6 PANEL OUTPUT FILES	29
5. PANEL RESULTS	31
5.1 PANEL SOURCE TERM.....	32
5.2 RADIONUCLIDE DECAY.....	58
5.3 PANEL CONCENTRATIONS	66
5.4 RADIONUCLIDES UP THE BOREHOLE (S6).....	77
6. REFERENCES	77
APPENDIX A: CALCULATION OF LSOLDIF.....	82
APPENDIX B: INPUT FILES USED FOR PANEL CRA-2009 PABC CALCULATIONS.....	84
B.1 GM_PANEL_PABC09.INP	84
B.2 MS_PANEL_PABC09.INP.....	84
B.3 ALG1_PANEL_PABC09.INP	86
B.4 ALG2_PANEL_PABC09.INP	86
B.5 ALG3_PANEL_PABC09.INP	87
B.6 LHS3_DUMMY.INP.....	88

APPENDIX C89

TABLES

Table 1. Actinide-Solubility Parameters Used for the CRA-2004 PABC and the
CRA-2009 PABC(a) 11

Table 2. Actinide Solubility Uncertainty Parameters Used for the CRA-2004
PABC and the CRA-2009 PABC. 13

Table 3. Updated Radionuclide Inventory Values That Are Relevant to the
PANEL Calculations for the CRA-2009 PABC. 14

Table 4. WIPP PA modeling scenarios 16

Table 5. Atomic Weights and Radionuclide Half-lives for CRA-2009 PABC 18

Table 6. Parameters related to humic colloids for the CRA-2009 PABC 20

Table 7. Parameters related to mineral fragment colloids for the
CRA-2009 PABC..... 21

Table 8. Parameters related to intrinsic colloids for the CRA-2009 PABC 21

Table 9. Parameters related to microbial colloids for the CRA-2009 PABC 21

Table 10. EPA release limits used in PANEL ($L_{isotope}$ from Equation 10)..... 24

Table 11: Radionuclides Modeled in PANEL Concentration Calculations..... 25

Table 12. Software Version Numbers Used for PANEL Calculations for the
CRA-2009 PABC..... 27

Table 13. Definitions of Variables Plotted in Figures 2 through 23 33

Table 14. Definitions of Variables Plotted in Figures 24 through 29 58

FIGURES

Figure 1. The run sequence for PANEL in the CRA-2009 PABC. Here
PANDFVOL is the Panel Default Volume, see Section 3.3..... 30

Figure 2. Scatter Plot of Dissolution Potential for Am in Salado Brine for all 100
Vectors in Scenario S1, Replicate 1..... 35

Figure 3. Scatter Plot of Mobilization Potential for Humic Colloids for Am in
Salado Brine for all 100 Vectors in Scenario S1, Replicate 1. 36

Figure 4. Scatter Plot of Mobilization Potential for Microbial Colloids for Am in Salado Brine for all 100 Vectors in Scenario S1, Replicate 1. 37

Figure 5. Scatter Plot of Mobilization Potential for Mineral Fragments for Am in Salado Brine for all 100 Vectors in Scenario S1, Replicate 1. 38

Figure 6. Scatter Plot of Total Mobilization Potential for Am in Salado Brine. 39

Figure 7. Scatter Plot of Dissolution Potential for Am in Castile Brine for all 100 Vectors in Scenario S1, Replicate 1..... 40

Figure 8. Scatter Plot of Mobilization Potential for Humic Colloids for Am in Castile Brine for all 100 Vectors in Scenario S1, Replicate 1. 41

Figure 9. Scatter Plot of Mobilization Potential for Microbial Colloids for Am in Castile Brine for all 100 Vectors in Scenario S1, Replicate 1. 42

Figure 10. Scatter Plot of Mobilization Potential for Mineral Fragments for Am in Salado Brine for all 100 Vectors in Scenario S1, Replicate 1. 43

Figure 11. Scatter Plot of Total Mobilization Potential for Am in Castile Brine. 44

Figure 12. Scatter Plot of Dissolution Potential for Pu in Salado Brine for all 100 Vectors in Scenario S1, Replicate 1..... 46

Figure 13. Scatter Plot of Mobilization Potential for Humic Colloids for Plutonium in Salado Brine for all 100 Vectors in Scenario S1, Replicate 1. 47

Figure 14. Scatter Plot of Mobilization Potential for Microbial Colloids for Pu in Salado Brine for all 100 Vectors in Scenario S1, Replicate 1. 48

Figure 15. Scatter Plot of Mobilization Potential for Intrinsic Colloids for Pu in Salado Brine for all 100 Vectors in Scenario S1, Replicate 1. 49

Figure 16. Scatter Plot of Mobilization Potential for Mineral Fragments for Pu in Salado Brine for all 100 Vectors in Scenario S1, Replicate 1. 50

Figure 17. Scatter Plot of Total Mobilization Potential for Pu in Salado Brine. 51

Figure 18. Scatter Plot of Dissolution Potential for Pu in Castile Brine for all 100 Vectors in Scenario S1, Replicate 1..... 52

Figure 19. Scatter Plot of Mobilization Potential for Humic Colloids for Pu in Castile Brine for all 100 Vectors in Scenario S1, Replicate 1. 53

Figure 20. Scatter Plot of Mobilization Potential for Microbial Colloids for Pu in Castile Brine for all 100 Vectors in Scenario S1, Replicate 1. 54

Figure 21. Scatter Plot of Mobilization Potential for Intrinsic Colloids for Pu in Castile Brine for all 100 Vectors in Scenario S1, Replicate 1.....	55
Figure 22. Scatter Plot of Mobilization Potential for Mineral Fragments for Pu in Castile Brine for all 100 Vectors in Scenario S1, Replicate 1.....	56
Figure 23. Scatter Plot of Total Potential Mobilized Pu in Castile Brine.....	57
Figure 24. Time dependent inventories of Am and Pu isotopes.....	60
Figure 25. Time dependent inventories of U isotopes.....	61
Figure 26. Time dependent inventories of various isotopes.....	62
Figure 27. Time dependent inventories of Sr and Cs isotopes.....	63
Figure 28. Time dependent inventories of various minor isotopes.....	64
Figure 29. Time dependent inventories of lumped isotopes.....	65
Figure 30. Time dependent total concentrations in Salado brine.....	67
Figure 31. Time dependent AM241L concentration in Salado brine.....	68
Figure 32. Time dependent PU239L concentration in Salado brine.....	69
Figure 33. Time dependent U234L concentration in Salado brine.....	70
Figure 34. Time dependent TH230L concentration in Salado brine.....	71
Figure 35. Time dependent total concentrations in Castile brine.....	72
Figure 36. Time dependent AM241L concentration in Castile brine.....	73
Figure 37. Time dependent PU239L concentration in Castile brine.....	74
Figure 38. Time dependent U234L concentration in Castile brine.....	75
Figure 39. Time dependent TH230L concentration in Castile brine.....	76

Acronyms

AP	Analysis Plan
CCA	Compliance Certification Application
CFR	Code of Federal Regulations
CMS	Configuration Management System
CRA	Compliance Recertification Application
DBR	Direct Brine Release
DCL	Digital Command Language
DOE	U.S. 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
SNL	Sandia National Laboratories
TRU	Transuranic
WIPP	Waste Isolation Pilot Plant

EXECUTIVE SUMMARY

For the CRA-2009 PABC PANEL calculations in this document, there were four changes that affected the results.

- 1) Radionuclide inventory
- 2) Base solubilities
- 3) Solubility uncertainties
- 4) Minimum brine volume

The radionuclide inventory changes had almost no effect since all releases are normalized by the unit of waste (WUF) which is a function of the radionuclide inventory.

The base solubility limits increased for the +III oxidation state by a factor of 4.29 to 5.24, depending on the brine type; there were minimal changes for the +IV and +V oxidation state base solubility limits. This increased the concentration in the brine for +III oxidation state radionuclides that were solubility limited.

For the CRA-2009 PABC, the solubility uncertainties for the +III and +IV oxidation states have larger ranges and similar medians. The larger ranges cause more variability in the radionuclide concentration in the brines.

The minimum repository brine volume required for a DBR increased from 10,000 to 17,400 cubic meters. This reduced the concentration in the brine for radionuclides that are inventory limited.

Overall, the average radionuclide concentrations are similar to those used in the CRA-2009, but the higher and lower extremes have shifted higher and lower, respectively.

1. INTRODUCTION

1.1 BACKGROUND

The Waste Isolation Pilot Plant (WIPP), located in southeastern New Mexico, has been developed by the U.S. Department of Energy (DOE) for the geologic (deep underground) disposal of transuranic (TRU) waste. Containment of TRU waste at the WIPP is regulated by the U.S. Environmental Protection Agency (EPA) according to the regulations set forth in Title 40 of the Code of Federal Regulations (CFR), Part 191. The DOE demonstrates compliance with the containment requirements according to the Certification Criteria in Title 40 CFR Part 194 by means of performance assessment (PA) calculations performed by Sandia National Laboratories (SNL). WIPP PA calculations estimate the probability and consequence of potential radionuclide releases from the repository to the accessible environment for a regulatory period of 10,000 years after facility closure. The models are maintained and updated with new information as part of a recertification process that occurs at five-year intervals after the first waste is received at the site.

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

Since the CRA-2004 PABC, additional PA calculations were completed for and documented in the 2009 Compliance Recertification Application (CRA-2009). The CRA-2009 PA resulted from continued review of the CRA-2004 PABC, including a number of technical changes and corrections, as well as updates to parameters and improvements to the PA computer codes (Clayton et al. 2008). The EPA has requested that additional information, which was received between the commencement of the CRA-2009 PA (December 2007) and the submittal of the CRA-2009 (March 2009), be included in an additional PA calculation (Cotsworth 2009), referred to as the CRA-2009 Performance Assessment Baseline Calculation (PABC-2009). The PABC-2009 analysis is guided by Analysis Plan AP-145 (Clayton 2009b). This report documents the PANEL analysis for the PABC-2009 and is compared with the results from the CRA-2004 PABC (same as the CRA-2009 PA).

1.2 OBJECTIVES FOR THE CRA-2009 PABC PANEL ANALYSIS

The EPA required that DOE revise the CRA-2009 analysis and present results before EPA would judge the CRA-2009 complete (Cotsworth 2009). The EPA noted a number of technical changes and corrections to the CRA-2009 PA that it deemed necessary. The issues and changes affecting the PANEL portion of WIPP PA include the following:

- 1) Actinide solubilities were updated.
- 2) Implementation of uncertainty for the actinide solubilities was updated.
- 3) Inventory information was updated.

2. CHANGES FROM THE CRA-2004 PABC TO THE CRA-2009 PABC THAT AFFECT PANEL CALCULATIONS

2.1 ACTINIDE SOLUBILITY UPDATE

Brush and Xiong (2009a) described the establishment of actinide solubilities for the CRA-2009 PABC. The WIPP Th(IV), Np(V), and Am(III) thermodynamic speciation and solubility models, implemented in the Fracture-Matrix Transport (FMT) code (Babb and Novak 1997 and addenda; Wang 1998), were used to calculate the solubilities of actinide (An) elements in the +IV, +V, and +III oxidation states, respectively, in WIPP brines under expected near-field chemical conditions.

Prediction of the long-term near-field chemical conditions expected in WIPP disposal rooms comprised: (1) use of WIPP-relevant standard brines to simulate fluids that could enter the repository. In particular GWB brine (Generic Weep Brine), which represents brine that could enter the repository from the Salado Formation, and ERDA-6 brine (Energy Research and Development Administration), which represents brine that could enter the repository from the Castile Formation; (2) the assumption that instantaneous, reversible equilibria among these brines, major Salado minerals, and MgO hydration and carbonation products will control chemical conditions; and (3) use of a thermodynamic model in the speciation and solubility code FMT to calculate these chemical conditions. Brush and Xiong (2009a, Subsection 2.1) described these assumptions, brines, and methods in detail.

Predictions of An(III), An(IV)m, and An(V) solubilities involved: (1) use of speciation and solubility models for Th(IV), Np(V), and Am(III); (2) use of WIPP-relevant standard brines to simulate fluids that could enter the repository. In particular GWB brine, which represents brine that could enter the repository from the Salado Formation and ERDA-6 brine, which represents brine that could enter the repository from the Castile Formation; (3) use of FMT to calculate the solubilities of Th(IV), Np(V), and Am(III); (4) use of the current FMT thermodynamic database; (5) use of uncertainty ranges and probability distributions for the Th(IV), Np(V), and Am(III) solubility predictions; (6) predictions of the redox speciation of Th, U, Np, Pu, and Am under the near-field chemical conditions expected in the WIPP; (7) use of the oxidation-state analogy to apply the solubilities calculated for Th(IV), Np(V), and Am(III) to other actinides in the WIPP; and (8) use of a solubility estimate for U(VI) (see below). Brush and Xiong (2009a, Subsection 2.2) discussed the predictions of actinide solubilities in detail.

Most of the assumptions, brines, databases, and methods used to predict near-field chemical conditions and the solubilities of Th(IV), Np(V), and Am(III) for the CRA-2009 PABC (Brush and Xiong 2009a; 2009c) were identical to those used for the CRA-2004 PABC (Brush and Xiong 2005a; Brush, 2005). However, two changes requested by the EPA (see Xiong et al. 2009 for a description of the EPA's request) necessitated the following analyses for the CRA-2009 PABC: (1) Brush and Xiong (2009b, Table 5) used the CRA-2009 PABC inventory (Crawford et al. 2009) and a new minimum brine volume (Clayton 2008) to calculate new organic-ligand concentrations, which replaced those calculated by Brush and Xiong (2005b) for the CRA-2004 PABC; and (2) Xiong et al. (2009) re-established the uncertainty ranges and probability distributions for the Th(IV) and Am(III) solubility models, which replaced those established by Xiong et al. (2005) for the CRA-2004 PABC.

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

$$\left(s_{brine}^{red/ox} \right) \tag{1}$$

where red/ox is the actinide oxidation state (+III, +IV, +V, +VI), brine is the brine type (Salado or Castile), and the units are in moles/liter. Table 1 provides the solubilities established for the CRA-2009 PABC (Brush and Xiong 2009c) and compares them to those established for the CRA-2004 PABC (Brush 2005). Table 2 provides a list of the solubility uncertainty values.

Table 1. Actinide-Solubility Parameters Used for the CRA-2004 PABC and the CRA-2009 PABC(a)

Material	Property	Description	CRA-2004 PABC	CRA-2009 PABC	Units
SOLMOD3	SOLCOH	Solubility of +III actinides in Castile brine, including organic ligands with a brucite-hydromagnesite buffer	2.88E-07	1.51E-06	moles/liter
SOLMOD3	SOLSOH	Solubility of +III actinides in Salado brine, including organic ligands with a brucite- hydromagnesite buffer	3.87E-07	1.66E-06	moles/liter
SOLMOD4	SOLCOH	Solubility of +IV actinides in Castile brine, including organic ligands with a brucite-hydromagnesite buffer	6.79E-08	6.98E-08	moles/liter
SOLMOD4	SOLSOH	Solubility of +IV actinides in Salado brine, including organic ligands with a brucite- hydromagnesite buffer	5.64E-08	5.63E-08	moles/liter
SOLMOD5	SOLCOH	Solubility of +V actinides in Castile brine, including organic ligands with a brucite- hydromagnesite buffer	8.24E-07	8.75E-07	moles/liter
SOLMOD5	SOLSOH	Solubility of +V actinides in Salado brine, including organic ligands with a brucite- hydromagnesite buffer	3.55E-07	3.90E-07	moles/liter
SOLMOD6	SOLCOH	Solubility of +VI actinides in Castile brine, including organic ligands with a brucite-hydromagnesite buffer	1.00E-03	1.00E-03	moles/liter
SOLMOD6	SOLSOH	Solubility of +VI actinides in Salado brine, including organic ligands with a brucite- hydromagnesite buffer	1.00E-03	1.00E-03	moles/liter

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

2.2 SOLUBILITY UNCERTAINTY UPDATE

Actinide solubilities used in PA are calculated by

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

where $s_{brine}^{red/ox}$ is the solubility estimate for a given vector calculated by FMT (see Equation 1), and M is the uncertainty in the solubility estimate. The term M is a function of the oxidation state, and is a sampled parameter as shown in Table 2.

Xiong et al. (2009) re-established the uncertainty range and probability distribution for the Th(IV) and Am(III) thermodynamic speciation and solubility models in response to an EPA request (see Xiong et al. 2009 for a description of the EPA's request).

The Xiong et al. (2009) Th(IV) comparison included a total of 140 comparisons between experimentally-measured and FMT-predicted Th(IV) solubilities. This is an increase of 95 comparisons over the 45 comparisons of Xiong et al. (2005), which established the actinide solubility uncertainty range and probability distributions for the CRA-2004 PABC. In Xiong et al. (2009), it is shown that the WIPP Th(IV) model overpredicts measured solubilities. This overprediction resulted in the mean and median values of M in Equation 2 for the +IV oxidation state to be -0.346 and -0.520 , respectively (see Table 7 of Xiong et al. 2009). In contrast, for the CRA-2004 PABC Xiong et al. (2005) used the same model, database, and code; but slightly underpredicted the measured solubilities in their analysis.

The Xiong et al. (2009) Am(III) comparison included a total of 346 comparisons between experimentally measured and FMT-predicted Nd(III) and Am(III) solubilities. This is an increase of 103 comparisons from the 243 comparisons of Xiong et al. (2005). The Xiong et al. (2009) comparison included more underpredictions than overpredictions, although there was a significant negative skew in the distribution. The mean and median values of M for the +III oxidation state are -0.142 and 0.072 , respectively (Table 11 of Xiong et al. 2009). Xiong et al. (2005) used the same model, database, and code; but obtained more overpredictions than underpredictions, with a significant positive skew in the distribution from their analysis.

The EPA specified that a fixed value be used for U(VI). For both the CRA-2004 PABC and the CRA-2009 PABC, the U(VI) solubility is fixed at 1×10^{-3} moles/liter.

Table 2. Actinide Solubility Uncertainty Parameters Used for the CRA-2004 PABC and the CRA-2009 PABC.

Material	Property	CRA-2009 PABC Value ^(b)	CRA-2004 PABC Value ^(b)	Units	Distribution Type
SOLMOD3	SOLVAR ^(a)	7.20E-02	-3.07E-02	NONE	Cumulative
SOLMOD4	SOLVAR ^(a)	-5.20E-01	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). SOLMOD3 is used for all actinides in the +III oxidation state and SOLMOD4 is used for the +IV oxidation state.

(b) A cumulative distribution is represented in the WIPP Performance Assessment Parameter Database (PAPDB) with a single value that is the median value. The reader can reference Tierney (1990) for the conversion to the cumulative distribution. Xiong et al. (2009) shows the distributions in more detail.

(c) If GLOBAL:OXSTAT is less than or equal to 0.5, Pu will be in oxidation state +III. If it is greater than 0.5, the oxidation state for plutonium will be +IV.

2.3 INVENTORY UPDATE

The EPA requested (Cotsworth 2009) that the waste inventory used for the CRA-2009 PABC be updated to reflect corrections and changes that had occurred during the completeness review of the CRA-2009. The update to the CRA-2009 inventory was conducted by Los Alamos National Laboratory (LANL) (Crawford et al. 2009). Calculation of the parameters needed for the CRA-2009 PABC PA was conducted by SNL (Fox et al. 2009). Table 3 shows the updated inventory values that are relevant for the PANEL calculations.

Table 3. Updated Radionuclide Inventory Values That Are Relevant to the PANEL Calculations for the CRA-2009 PABC.

Material	Property	CRA-2009 PABC Value	CRA-2004 PABC Value	Units
BOREHOLE	WUF(a)	2.60E+00	2.32E+00	Curies
AM241	INVCHD(b)	4.68E+05	5.01E+05	Curies
AM241	INVRHD(c)	4.48E+03	1.65E+04	Curies
AM241L	INVCHD	4.85E+05	5.15E+05	Curies
AM241L	INVRHD	4.61E+03	1.74E+04	Curies
AM243	INVCHD	7.17E+01	7.75E+01	Curies
AM243	INVRHD	7.80E-00	1.13E+00	Curies
CF252	INVCHD	3.28E-02	3.85E-05	Curies
CF252	INVRHD	1.83E-04	1.98E-05	Curies
CM243	INVCHD	1.34E+00	1.82E-01	Curies
CM243	INVRHD	2.09E+00	2.32E-01	Curies
CM244	INVCHD	2.61E+03	1.81E+03	Curies
CM244	INVRHD	4.36E+02	3.20E+02	Curies
CM245	INVCHD	5.86E-01	6.13E-03	Curies
CM245	INVRHD	8.26E-02	1.10E-02	Curies
CM248	INVCHD	1.24E-01	6.51E-02	Curies
CM248	INVRHD	7.63E-03	9.16E-03	Curies
CS137	INVCHD	5.48E+02	3.52E+03	Curies
CS137	INVRHD	8.89E+04	2.03E+05	Curies
NP237	INVCHD	3.65E+01	1.13E+01	Curies
NP237	INVRHD	2.49E+00	8.32E-01	Curies
PA231	INVCHD	3.78E-01	8.69E-01	Curies
PA231	INVRHD	1.87E-01	8.26E-04	Curies
PB210	INVCHD	1.75E+00	3.59E+00	Curies
PB210	INVRHD	1.43E+01	3.02E-05	Curies
PM147	INVCHD	5.09E-02	3.74E-04	Curies
PM147	INVRHD	1.18E+00	1.30E-01	Curies
PU238	INVCHD	1.47E+06	1.13E+06	Curies
PU238	INVRHD	5.11E+03	2.96E+03	Curies
PU238L	INVCHD	1.47E+06	1.13E+06	Curies
PU238L	INVRHD	5.11E+03	2.96E+03	Curies
PU239	INVCHD	5.10E+05	5.77E+05	Curies
PU239	INVRHD	2.92E+03	5.24E+03	Curies
PU239L	INVCHD	6.55E+05	6.71E+05	Curies
PU239L	INVRHD	3.92E+03	6.83E+03	Curies
PU240	INVCHD	1.44E+05	9.38E+04	Curies
PU240	INVRHD	9.89E+02	1.58E+03	Curies
PU241	INVCHD	5.06E+05	4.20E+05	Curies
PU241	INVRHD	3.94E+03	2.80E+04	Curies

Table 3. Updated Radionuclide Inventory Values That Are Relevant to the PANEL Calculations for the CRA-2009 PABC (continued)

Material	Property	CRA-2009 PABC Value	CRA-2004 PABC Value	Units
PU242	INVCHD	7.46E+01	1.22E+01	Curies
PU242	INVRHD	1.25E+00	4.80E-01	Curies
PU244	INVCHD	3.48E-04	1.26E-06	Curies
PU244	INVRHD	2.34E-06	5.53E-03	Curies
RA226	INVCHD	2.21E+00	4.56E+00	Curies
RA226	INVRHD	1.83E+01	9.34E-05	Curies
RA228	INVCHD	3.08E-01	2.88E+00	Curies
RA228	INVRHD	7.69E-02	1.06E+00	Curies
SR90	INVCHD	5.03E+02	2.62E+04	Curies
SR90	INVRHD	7.99E+04	1.50E+05	Curies
TH229	INVCHD	8.81E+00	4.65E+00	Curies
TH229	INVRHD	4.19E+00	5.64E-01	Curies
TH230	INVCHD	5.87E-01	1.69E-01	Curies
TH230	INVRHD	9.20E-03	1.07E-02	Curies
TH230L	INVCHD	9.40E+00	4.82E+00	Curies
TH230L	INVRHD	4.20E+00	5.75E-01	Curies
TH232	INVCHD	2.75E-01	2.50E+00	Curies
TH232	INVRHD	6.86E-02	9.20E-01	Curies
U233	INVCHD	1.56E+02	1.10E+03	Curies
U233	INVRHD	5.09E+01	1.27E+02	Curies
U234	INVCHD	3.04E+02	3.13E+02	Curies
U234	INVRHD	5.18E+00	3.08E+01	Curies
U234L	INVCHD	4.60E+02	1.41E+03	Curies
U234L	INVRHD	5.61E+01	1.58E+02	Curies
U235	INVCHD	4.42E+00	3.92E+00	Curies
U235	INVRHD	7.04E-02	1.09E+00	Curies
U236	INVCHD	1.35E+00	1.56E+00	Curies
U236	INVRHD	2.48E-01	1.32E+00	Curies
U238	INVCHD	2.71E+01	7.91E+01	Curies
U238	INVRHD	2.96E-01	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.

2.4 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 1998) 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 to version 4.03 (Garner 2005a) to set the default volume of a panel via MATSET. PANEL 4.03 was validated according to the requirements of NP 19-1 (Garner 2005b) and used in both the CRA-2004 PABC and the CRA-2009 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, Latin Hypercube Sampling (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 4). 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 4. 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. (Helton et al. 1998)

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 flows induced by 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 (Helton et al. 1998).

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 3), PANEL needs the atomic weight and half-life of the radionuclides. These values are shown in Table 5 and have not changed since the CCA. In the DECAY mode, PANEL decays those radionuclides shown in Table 5.

Table 5. Atomic Weights and Radionuclide Half-lives for CRA-2009 PABC

Material	Property	CRA-2009 PABC Value	Units	Material	Property	CRA-2009 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 2.2. The base solubility value, $(s_{brine}^{red/ox})$, 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 and CRA-2009 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 2 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).

$$H_{brine}^{red/ox} = \begin{cases} (S_{brine}^{red/ox}) \cdot (h_{brine}^{red/ox}) & \text{if } (S_{brine}^{red/ox}) \cdot (h_{brine}^{red/ox}) \leq (H_{elem}^{max}) \\ (H_{elem}^{max}) & \text{if } (S_{brine}^{red/ox}) \cdot (h_{brine}^{red/ox}) > (H_{elem}^{max}) \end{cases} \quad (3)$$

$H_{brine}^{red/ox}$ is the mobilization potential for humic colloids. $(S_{brine}^{red/ox})$ is defined in Equation 2. $(h_{brine}^{red/ox})$ is a factor for humic colloids that is defined for each oxidation state and brine type as shown in Table 6. (H_{elem}^{max}) is the maximum allowed for mobilized humic colloids for the element (also shown in Table 6). None of the values in Table 6 were updated for the CRA-2009 PABC.

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

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

$MF_{brine}^{red/ox}$ is the mobilization potential for mineral fragment colloids. $(mf_{brine}^{red/ox})$ is a constant value for each element that is independent of brine type as shown in Table 7. None of the values in Table 7 were updated for the CRA-2009 PABC.

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

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

$IC_{brine}^{red/ox}$ is the mobilization potential for intrinsic colloids. ($ic_{brine}^{red/ox}$) is a constant value for each element that is independent of brine of type as shown in Table 8. None of the values in Table 8 were updated for the CRA-2009 PABC.

The mobilization potential for microbial colloids is zero if there is no microbial activity. However all vectors have microbial activity in the CRA-2009 PABC. The mobilization potential for microbial colloids is calculated using Equation 6.

Table 6. Parameters related to humic colloids for the CRA-2009 PABC

Material	Property	Description	CRA-2009 PABC Value	Units
PHUMOX3	PHUMCIM(b)	Multiplicative factor to calculate humic colloids for actinides in the +III oxidation state in Castile brine	(a) 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) This is 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 ($h_{brine}^{red/ox}$) in Equation 3.

(c) Corresponds to (H_{clom}^{max}) in Equation 3.

Table 7. Parameters related to mineral fragment colloids for the CRA-2009 PABC

Material	Property	Description	CRA-2009 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 $(m_{f_{brine}}^{red/ox})$ in Equation 4.

Table 8. Parameters related to intrinsic colloids for the CRA-2009 PABC

Material	Property	Description	CRA-2009 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 $(i_{c_{brine}}^{red/ox})$ in Equation 5.

Table 9. Parameters related to microbial colloids for the CRA-2009 PABC

Material	Property	Description	CRA-2009 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 $(m_{c_{brine}}^{red/ox})$ in Equation 6.

(b) Corresponds to (MC_{elem}^{max}) in Equation 6.

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

$MC_{brine}^{red/ox}$ is the mobilization potential for microbial colloids. $(S_{brine}^{red/ox})$ is defined in Equation 2. $(H_{brine}^{red/ox})$ is defined in Equation 3. $(MF_{brine}^{red/ox})$ is defined in Equation 4. $(IC_{brine}^{red/ox})$ is defined in Equation 5. $(mc_{brine}^{red/ox})$ is a factor for microbial colloids that is defined for each element independent of brine type as shown in Table 9. (MC_{elem}^{max}) is a value that limits the amount of microbial colloids that can be mobilized in the presence of other mobilization processes. The values for (MC_{elem}^{max}) are shown in Table 9. None of the values in Table 9 were updated for the CRA-2009 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.

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

$TC_{brine}^{red/ox}$ 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 (used for CRA-2004 PABC). 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). For CRA-2009 PABC, the fraction of the inventory is calculated in an ALGEBRA step before PANEL is executed (Clayton 2009a).

The concentration is given in Equation 8.

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

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 (not including scenario S6), the brine volume, V_{brine} (Panel Default Volume or PANDFVOL), is a constant value based on Stein (2005) for the CRA-2004 PABC and Clayton (2008) for the CRA-2009 PABC. The value derived in Stein (2005) or Clayton (2008) 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,

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

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.

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

Where $W^{isotope}$ is the activity concentration in EPA Units/liter for the isotope (see Section 2.1 of Helton et al. 1998). $L_{isotope}$ is the EPA release limit for the isotope (shown in Table 10), and f_w is the waste unit factor (shown in Table 3, defined in Leigh and Trone 2005b). None of the values in Table 10 were updated for the CRA-2009 PABC.

Table 10. EPA release limits used in PANEL ($L_{isotope}$ from Equation 10).

Material	Property	CRA-2009 PABC 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 25 individual radionuclides and five “lumped” radionuclides shown in Table 11. 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 11: 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 because their half lives are less than 20 years.

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

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

Where $\left\{ TC_{brine}^{red/ox} \right\}_{NUTS}$ is the potential moles per liter mobilized for the lumped isotopes in Table 11. L_{dif}^{sol} is a multiplicative factor used to account for molar proportions of isotopes in the inventory. The multiplicative factors are calculated in two ALGEBRACDB steps and set in the parameters, PU238L:LSOLDIF, TH230L:LSOLDIF, U234L:LSOLDIF. Calculation of these values is discussed in Clayton, 2009a and in Appendix A.

The total concentration in EPA units for the 25 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 25 individual isotopes in Table 11. For the calculation of Culebra releases (S1-S5) in CCDFGF, the values supplied by PANEL are defined by Equation 13.

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

W_{lumped}^{total} is the total EPA Units per liter for the lumped isotopes in Table 11.

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 (Nemer 2006). 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 PABC09_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 PABC09-9 of the CMS libraries (Long 2010).

Figure 1 (left hand side) shows the run sequence for PANEL. For the CRA-2009 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. Two ALGEBRACDB runs follow the DECAY run to set parameters for the following PANEL runs.

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 2003b) provides input to MATSET (Gilkey 2003b). MATSET provides input to POSTLHS (Vugrin 2005b), and POSTLHS provides input to ALGEBRACDB (Gilkey 2003a). Output from this third ALGEBRACDB run 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 2003a) and ALGEBRACDB is also input to PANEL. The software version numbers used for the PANEL calculations for the CRA-2009 PABC are given in Table 12.

Table 12. Software Version Numbers Used for PANEL Calculations for the CRA-2009 PABC

Software Application	Version
GENMESH	6.08
MATSET	9.10
POSTLHS	4.07A
ALGEBRACDB	2.35
SUMMARIZE	3.01
SPLAT	1.02
STEPWISE	2.21
PCCSRC	2.21
BLOTII2	1.59A

4.1 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 2003b). The analyst supplies input for GENMESH in an ASCII input file. The CRA-2009 PABC analysis uses the file: GM_PANEL_PABC09.INP (see Appendix B) located in CMS library: PABC09_PANEL.

4.2 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_PABC09.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-2009 PABC is MS_PANEL_PABC09.INP (see Appendix B) and is located in the CMS library: PABC09_PANEL.

For the CRA-2009 PABC calculations, three additional steps were added before the POSTLHS step. PANEL was executed in the decay mode and then ALGEBRA was run twice. These steps were done in order that the mole fractions for the lumped variables and the fraction of inventory in one panel could be calculated as part of the run stream instead of being done offline (Clayton 2009b).

4.3 POSTLHS: UNCERTAIN PARAMETER VALUES

The sixth step in the run sequence employs the POSTLHS code, which takes the binary output from the second algebra step (ALG2_PANEL_PABC09.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. The sampled parameter WAS_AREA:PROBDEG no longer has any impact on the source term since the distribution has been changed, so there is always microbial degradation. POSTLHS requires that a dummy ASCII file be specified, which is not used in the calculations. The dummy file used for the CRA-2009 PABC is LHS3_DUMMY.INP (see Appendix B) and is located in CMS library: LIBPABC09_LHS. Output from LHS (LHS2_PANEL_PABC09_R1.TRN, LHS2_PANEL_PABC09_R2.TRN, LHS2_PANEL_PABC09_R3.TRN for the three replicates) are also used by POSTLHS in this step. These files are stored in CMS library: PABC09_LHS.

4.4 ALGEBRACDB: DATA MODIFICATION

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). Three Algebra steps are included in the modeling process both before and after POSTLHS.

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 files used for the Algebra 1, 2, and 3 steps in the CRA-2009 PABC are ALG1_PANEL_PABC09.INP, ALG2_PANEL_PABC09.INP, and ALG3_PANEL_PABC09.INP (see Appendix B) and are located in CMS library: LIBPABC09_PANEL. The Algebra 3 step executes the mathematical instructions to modify the output data from POSTLHS:

- LHS3_PANEL_PABC09_R1_V001.CDB - LHS3_PANEL_PABC09_R1_V100.CDB;
 - LHS3_PANEL_PABC09_R2_V001.CDB - LHS3_PANEL_PABC09_R2_V100.CDB;
- and
- LHS3_PANEL_PABC09_R3_V001.CDB - LHS3_PANEL_PABC09_R3_V100.CDB

which are stored in the CMS library: PABC09_PANEL.

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

- ALG3_PANEL_PABC09_R1_V001.CDB – ALG3_PANEL_PABC09_R1_V100.CDB;
 - ALG3_PANEL_PABC09_R2_V001.CDB – ALG3_PANEL_PABC09_R2_V100.CDB;
- and
- ALG3_PANEL_PABC09_R3_V001.CDB – ALG3_PANEL_PABC09_R3_V100.CDB

Which are stored in the CMS library: PABC09_PANEL.

4.5 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_PABC09_R1_S6_V001.CDB through ALG2_BF_PABC09_R3_S6_V100.CDB which are stored in the CMS libraries PABC09_BFRxS6, where x = 1, 2, or 3.

4.6 PANEL OUTPUT FILES

Panel output files are stored in CMS library PABC09_PANEL. For scenario S6 (standard type run), the output files are named PANEL_INT_PABC09_R1_S6_TI2000_V001.CDB through PANEL_INT_PABC09_R3_S6_TI2000_V001.CDB and same with TI = 0100, 0350, 1000, 4000, 6000, 9000.

The panel decay run is named PANEL_DECAY_PABC09_R1_S1_V001.CDB and Panel concentration runs are named PANEL_CON_PABC09_R1_S1_V001.CDB to PANEL_CON_PABC09_R3_S5_V100.CDB.

Used for DECAY and CONCENTRATION runs.

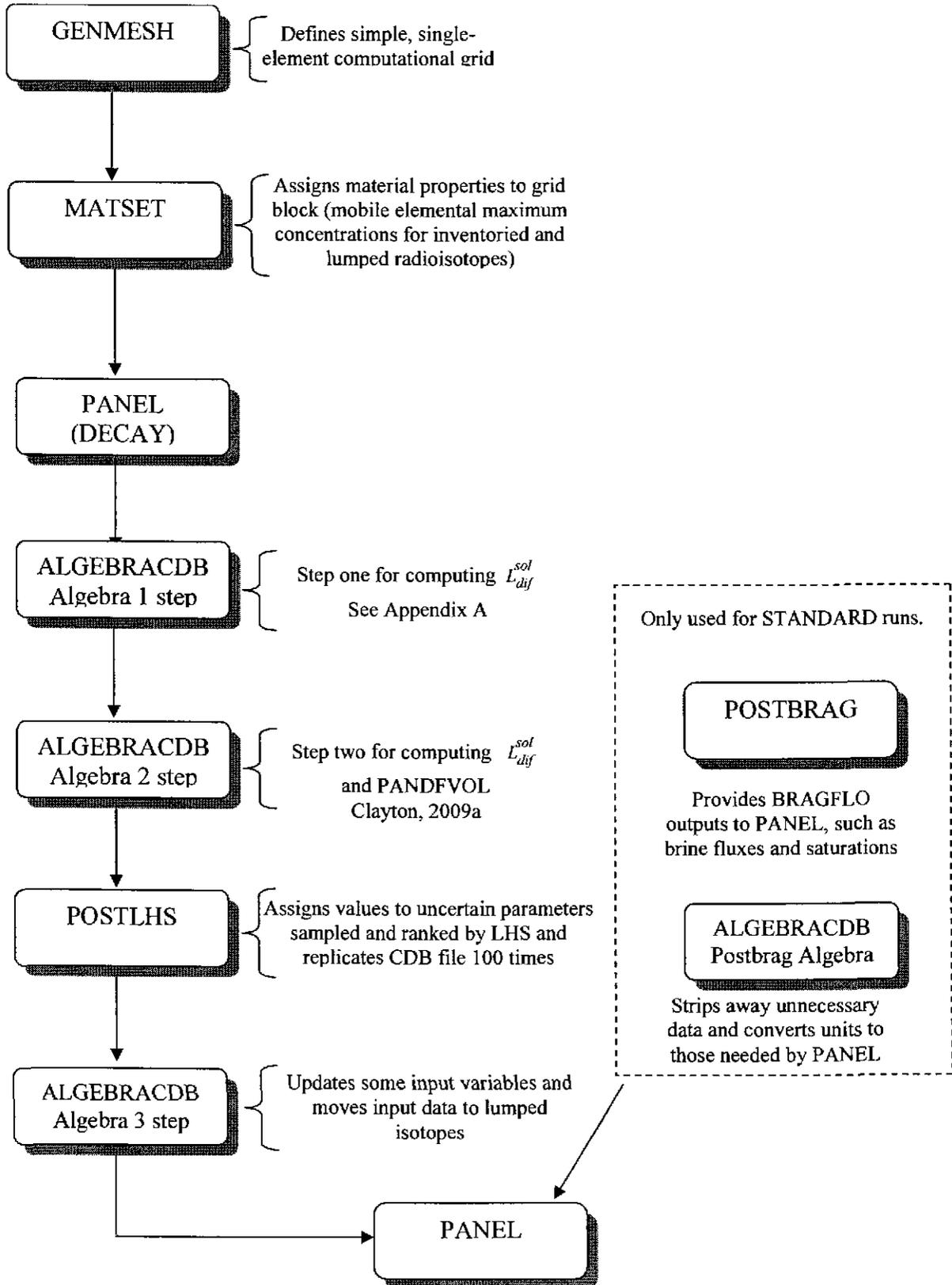


Figure 1. The run sequence for PANEL in the CRA-2009 PABC. Here PANDFVOL is the Panel Default Volume, see Section 3.3.

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 11 (the non-bold isotopes in Table 11). 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 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 be removed from the panel. 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 Clayton (2008) for the CRA-2009 PABC. Clayton (2008) gives an estimate of the volume of brine in the repository that would lead to a brine release. This value is 17,400 cubic meters. To determine the fraction of that volume that would be in a panel, the 17,400 cubic meter value is multiplied by the volume fraction of one panel to the entire repository. 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-2009 PABC results and the CRA-2004 PABC results. The CRA-2004 PABC for PANEL was used in the CRA-2009 PA. 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 11. 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 11. 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 calculates the source term for all runs. The runs used are from concentration type runs. 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 PABC results (Part b in each figure) and the CRA-2009 PABC results (Part a in each figure) presented. There were no changes that affected PANEL Concentration (or Decay) type runs between CRA-2004 PABC and CRA-2009 PA. This is why we compare the CRA-2009 PABC results and the CRA-2004 PABC results. 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 13 provides definitions for the variables plotted in Figures 2 through 23.

Table 13. 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 and CRA-2009 PABC)
WSOLPU	dimensionless	This variable is the sampled value of the solubility variability for Pu (used in CRA-2004 PABC and CRA-2009 PABC) depending on the oxidation state of Pu

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 as the range of the uncertainty variable SOLMOD3:SOLVAR.

Figures 2 to 6 are for Am in Salado brine. Figure 2 indicates that the potential dissolved component for Am in Salado are very similar for both CRA-2004 PABC and CRA-2009 PABC. There is an approximate factor of 4.3 different for the same value of WSOLVAR3 because of the solubility (Table 1) and also a larger uncertainty range.

Figure 3 indicates that the range of values for the potential humic component of mobilized Am in Salado brine is larger in the CRA-2009 PABC than it was in CRA-2004 PABC. This is to be expected since, even though the multiplier $(h_{brine}^{red/ox})$ in Equation 3 was not updated for the CRA-2009 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 reach the maximum value $[(H_{elem}^{max})$ in Equation 3] in both the CRA-2004 PABC and in CRA-2009 PABC. This is apparent on the far right-hand-side of Figure 3 where the vectors have values equivalent to the maximum, 1.10E-05 moles/liter.

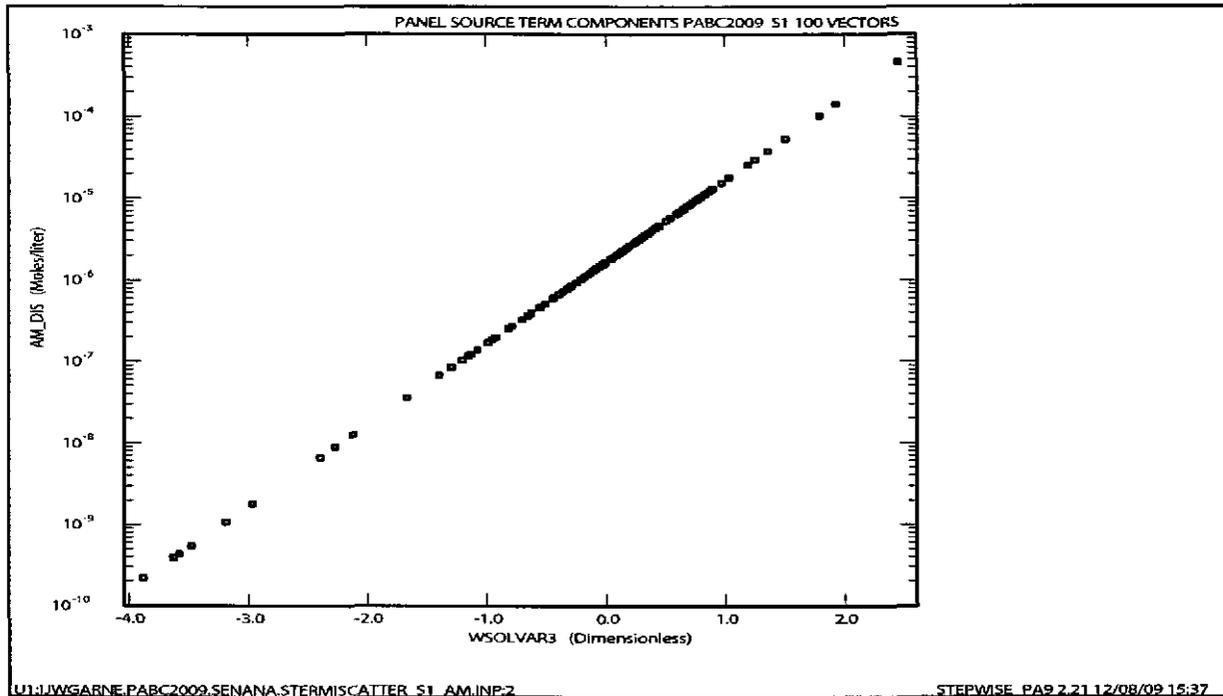
Figure 4 indicates the mobilization potential of microbial colloids. The results are again about a factor of 4.3 larger because of the dissolved value with an extended range from the uncertainty variable.

Figure 5 indicates that the mobilization potential for mineral fragments for Am did not change from CRA-2004 PABC to CRA-2009 PABC. It has a constant value of 2.60E-08 moles/liter.

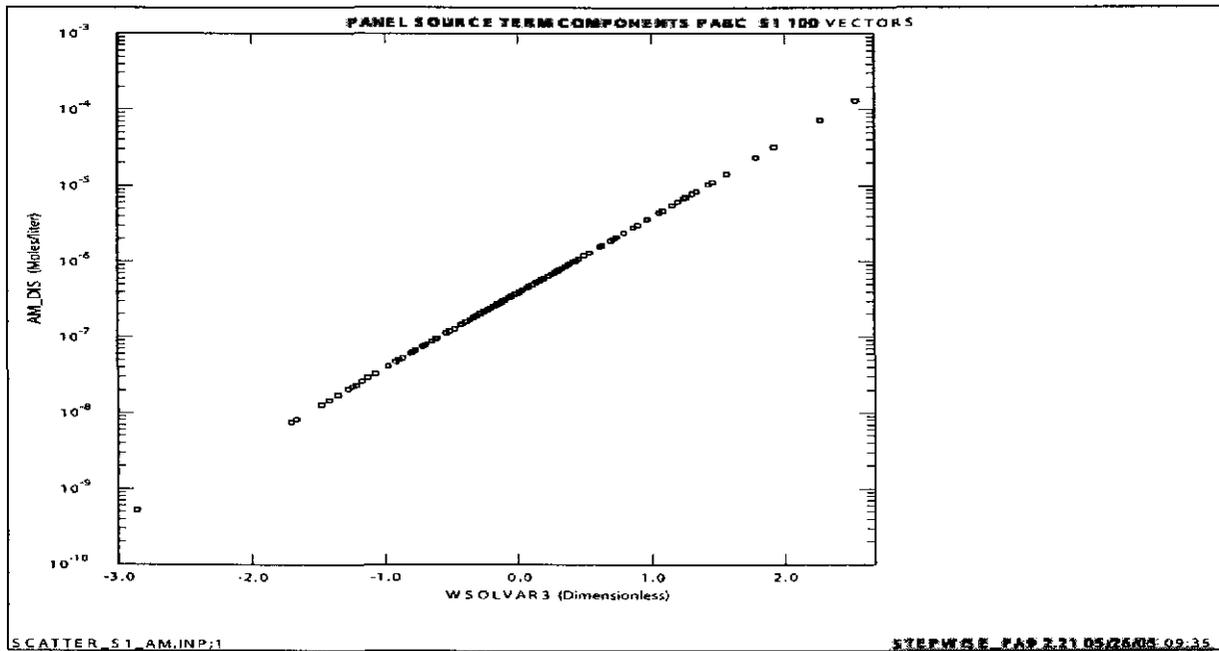
Figure 6 shows the total mobilization potential for Am in Salado brine.

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. There is a factor of 5.24 in the solubility instead of 4.3 for the Salado 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 $(h_{brine}^{red/ox})$ in Equation 3 is not a constant but is instead a sampled variable (see Table 6). The result is more “scatter” in the figure. Figure 8 also shows that humic colloids can reach the maximum value of 1.1×10^{-5} moles/liter in both the CRA-2004 PABC and the CRA-2009 PABC. In Figure 11, both Part a and Part b shows a fairly continuous curve.

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.



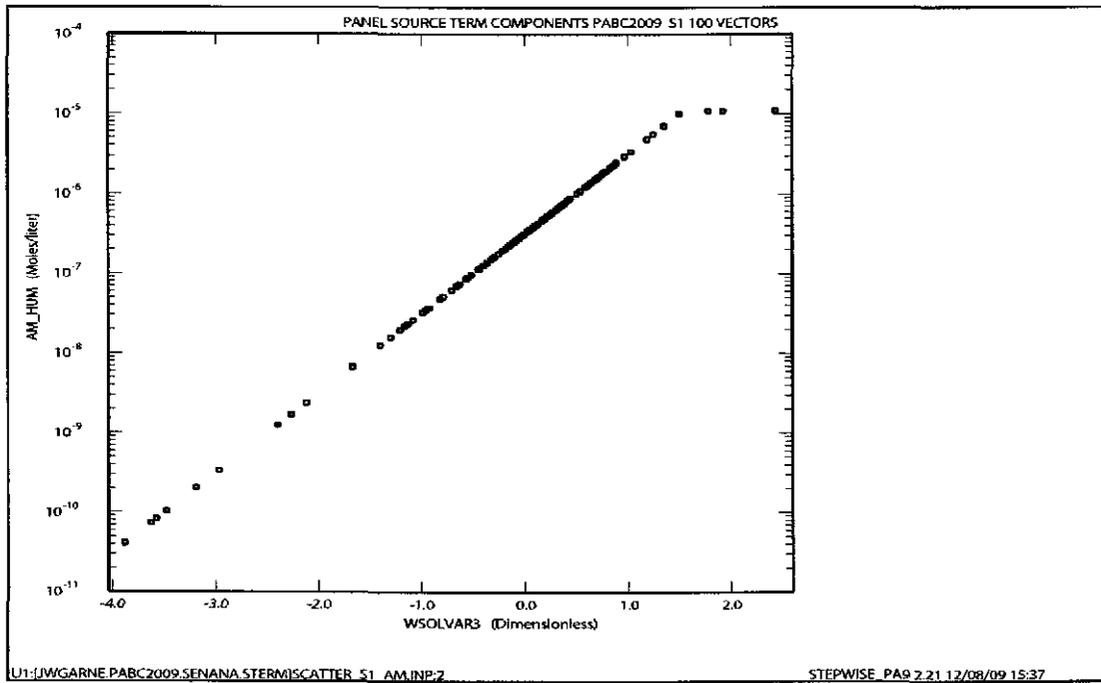
a) CRA-2009 PABC



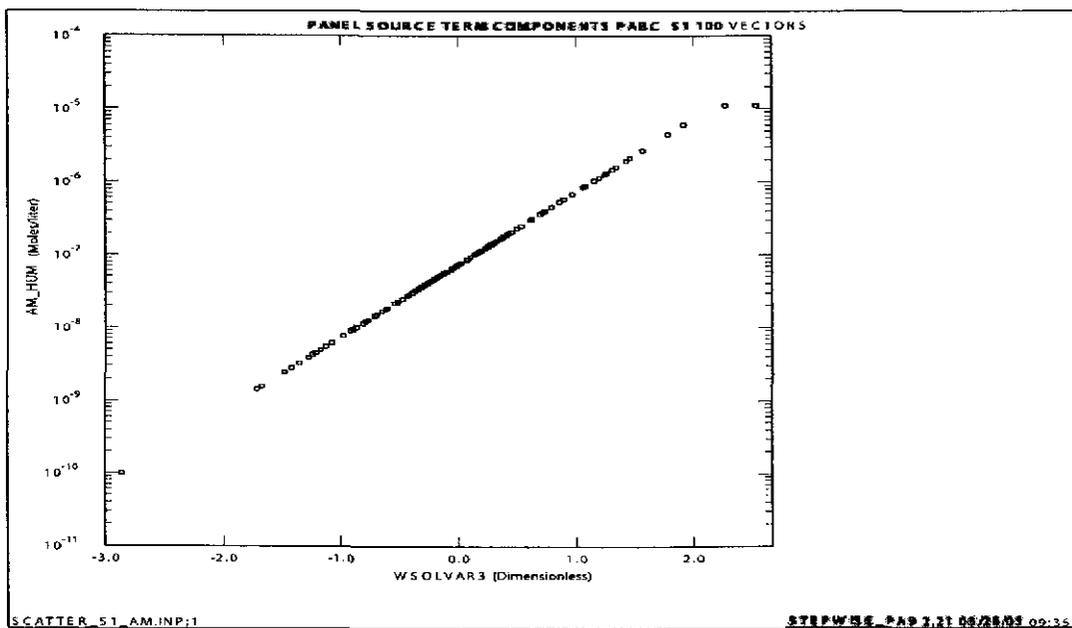
b) CRA-2004 PABC

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-2009 PABC.
Part b) shows results from the CRA-2004 PABC.



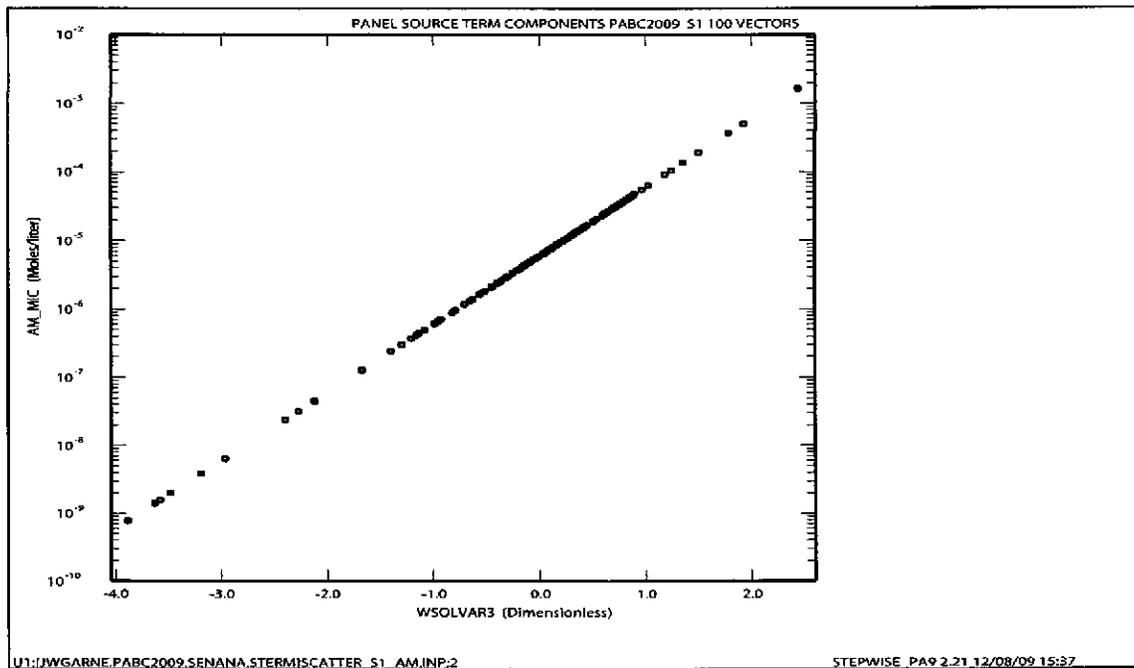
a) CRA-2009 PABC



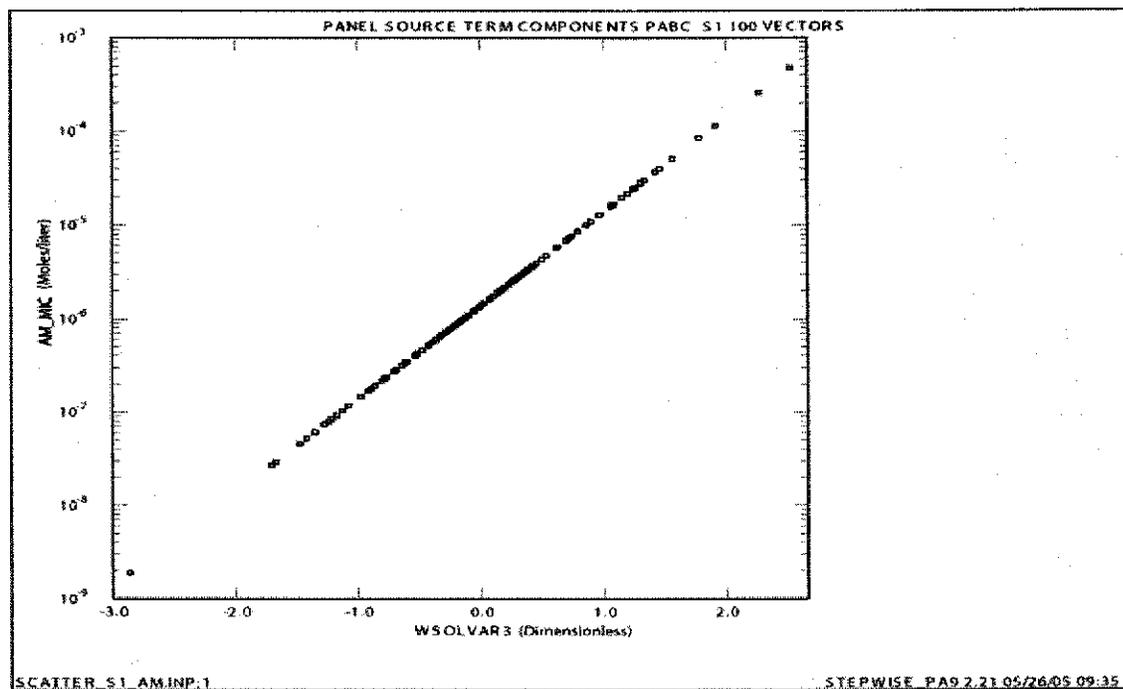
b) CRA-2004 PABC

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

Part a) shows results from the CRA-2009 PABC.
Part b) shows results from the CRA-2004 PABC.



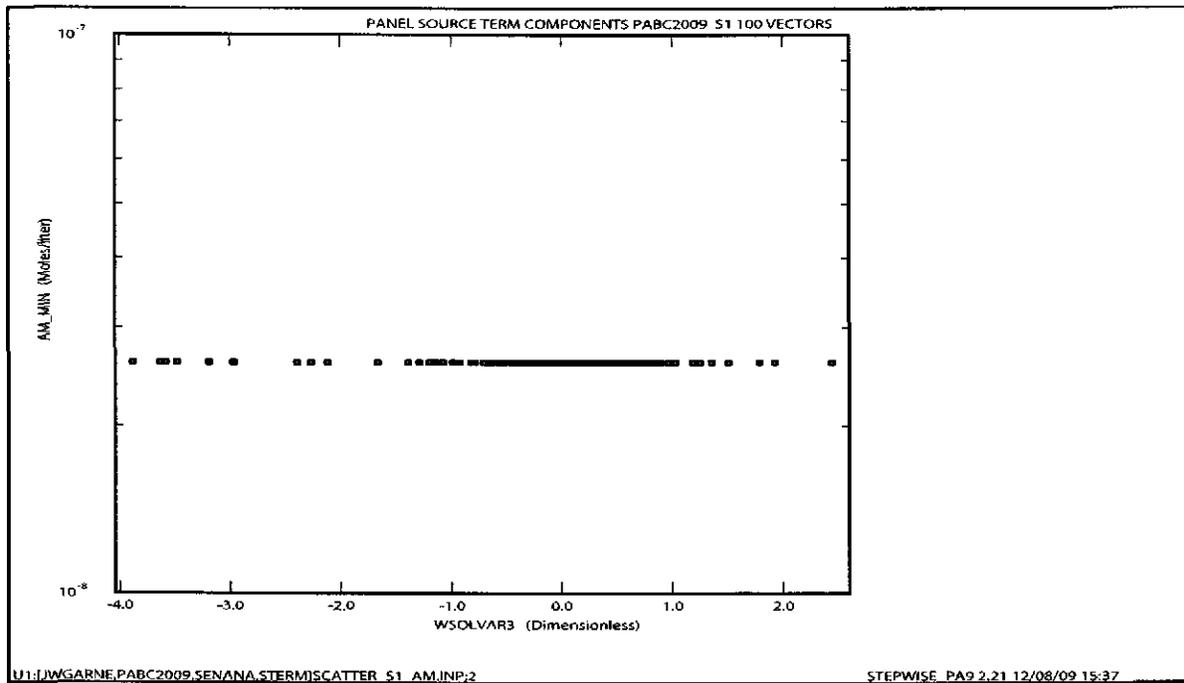
a) CRA-2009 PABC



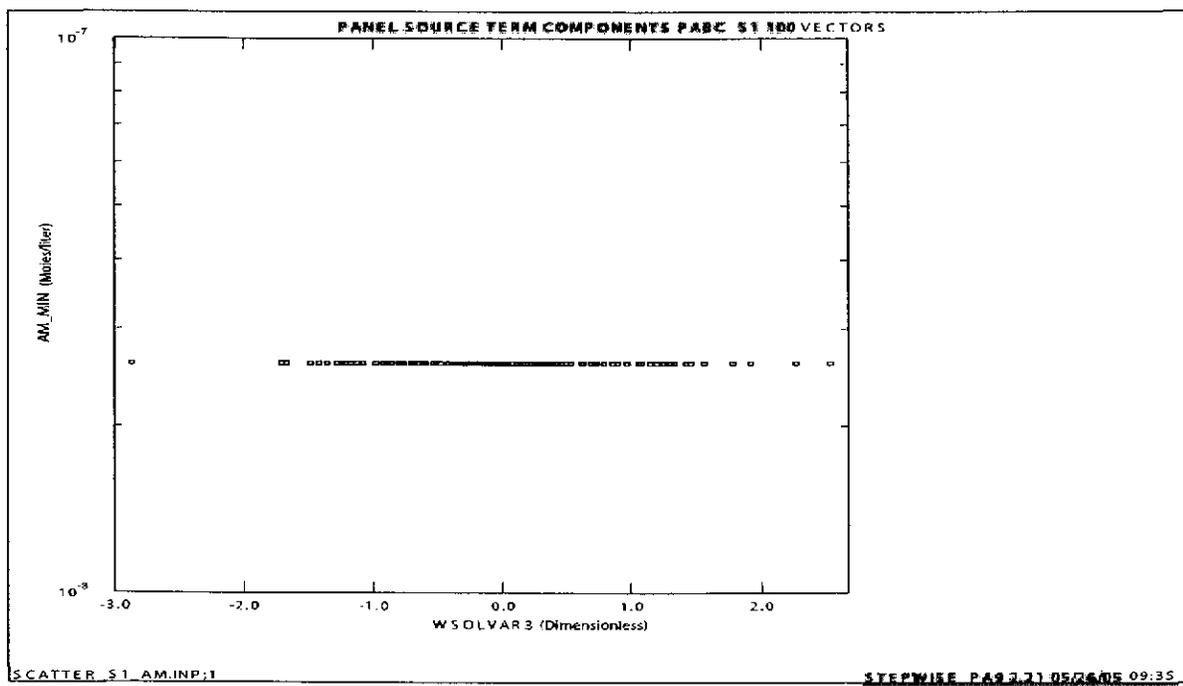
b) CRA-2004 PABC

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-2009 PABC.
Part b) shows results from the CRA-2004 PABC.



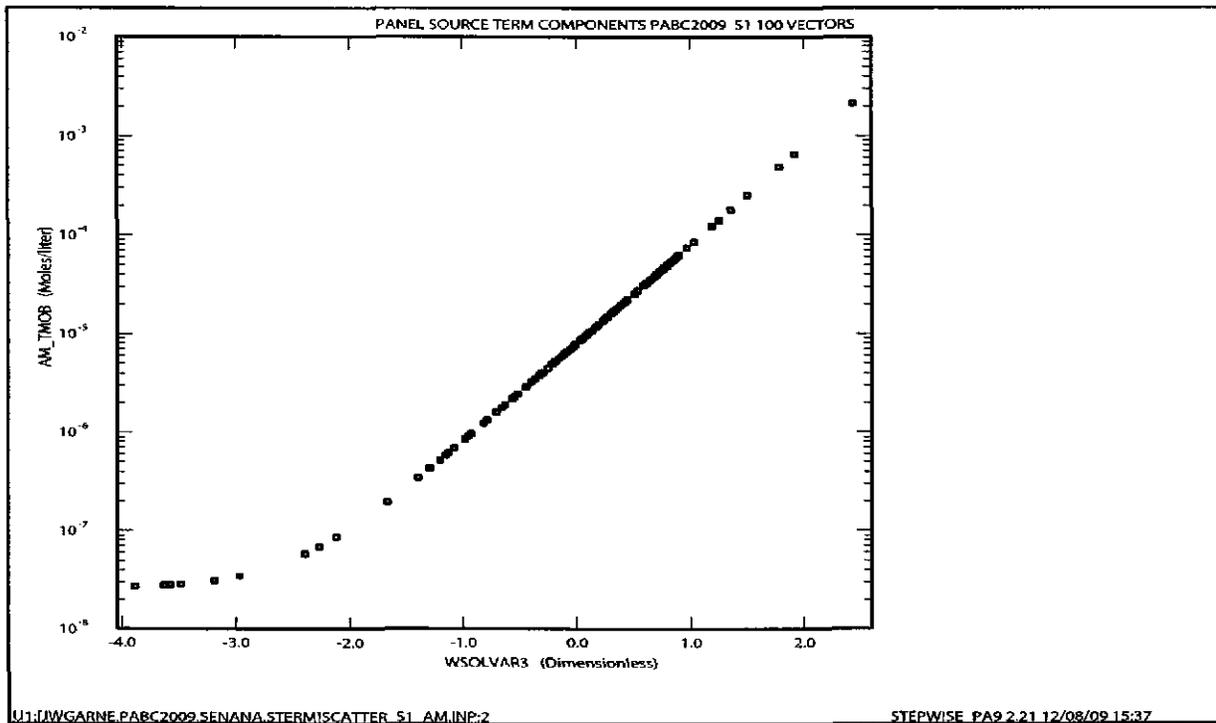
a) CRA-2009 PABC



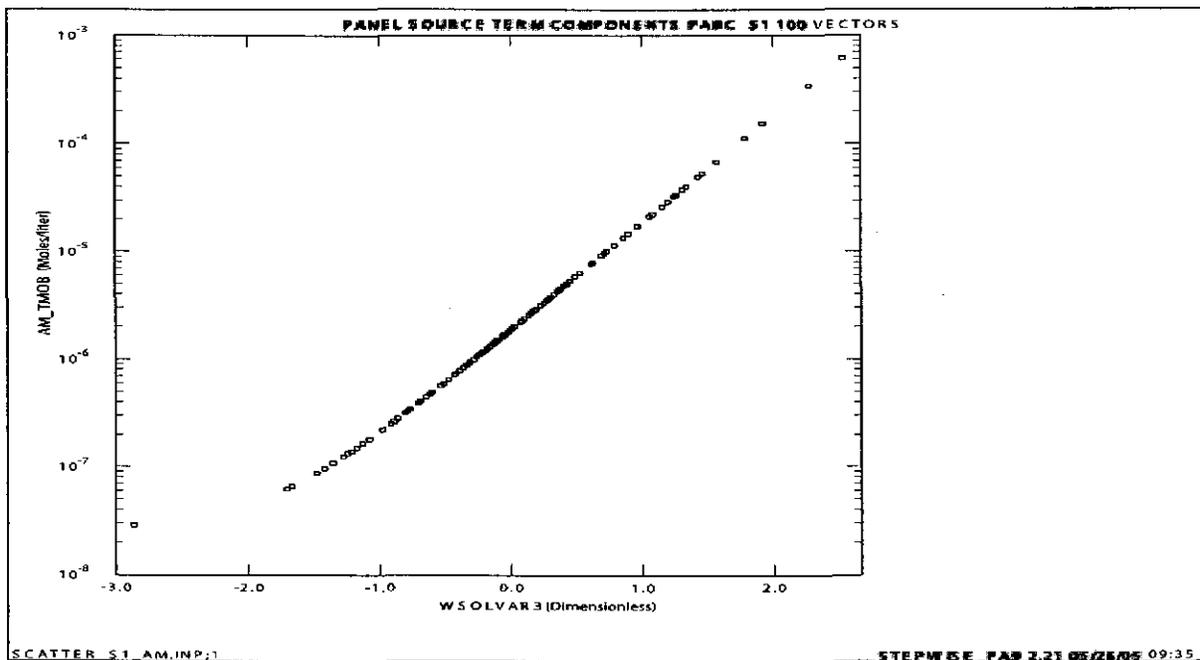
b) CRA-2004 PABC

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-2009 PABC.
Part b) shows results from the CRA-2004 PABC.



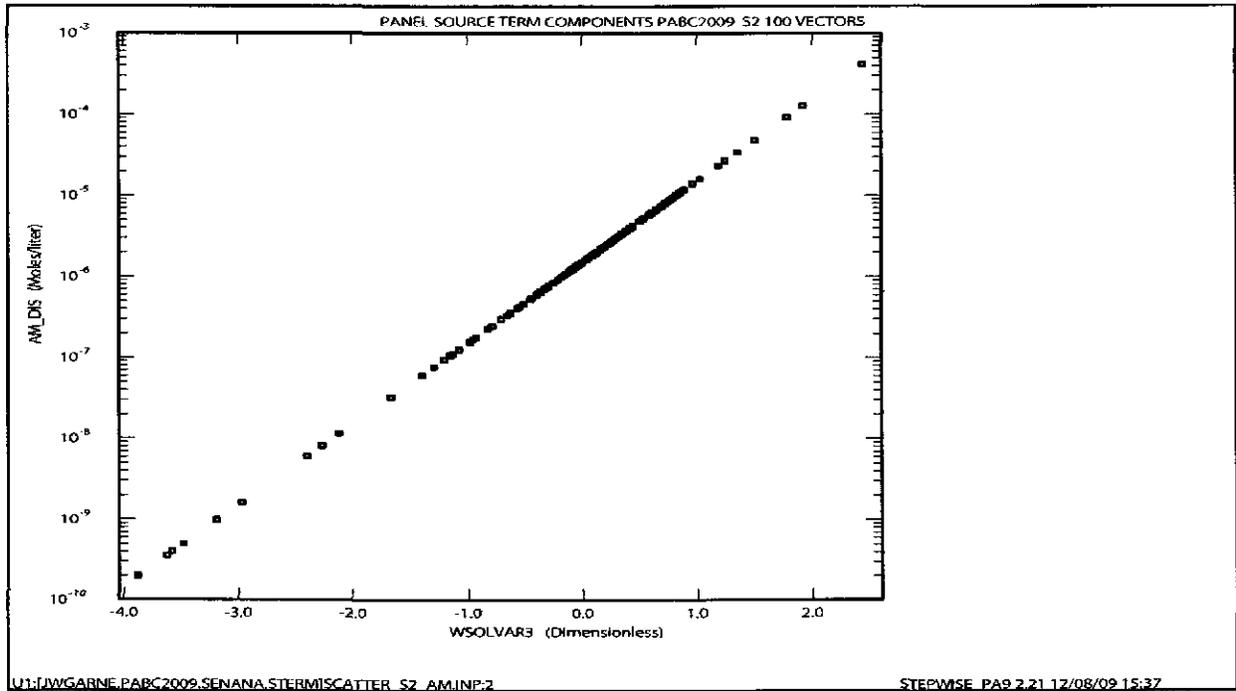
a) CRA-2009 PABC



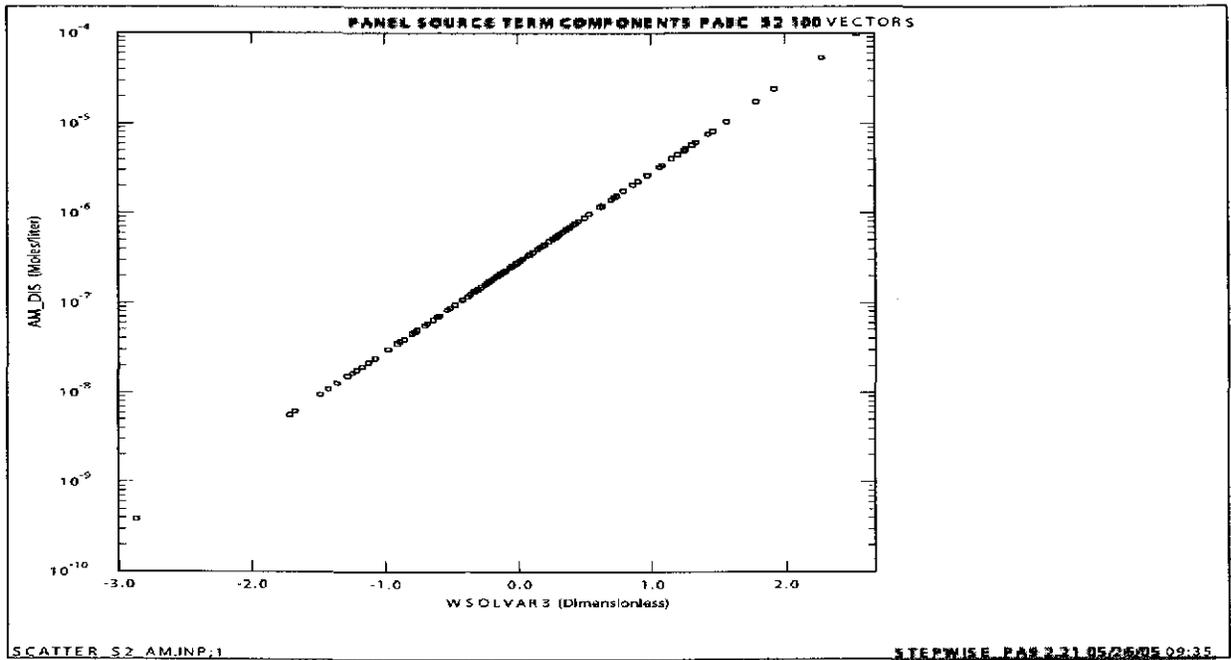
b) CRA-2004 PABC

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

Part a) shows results from the CRA-2009 PABC.
Part b) shows results from the CRA-2004 PABC.



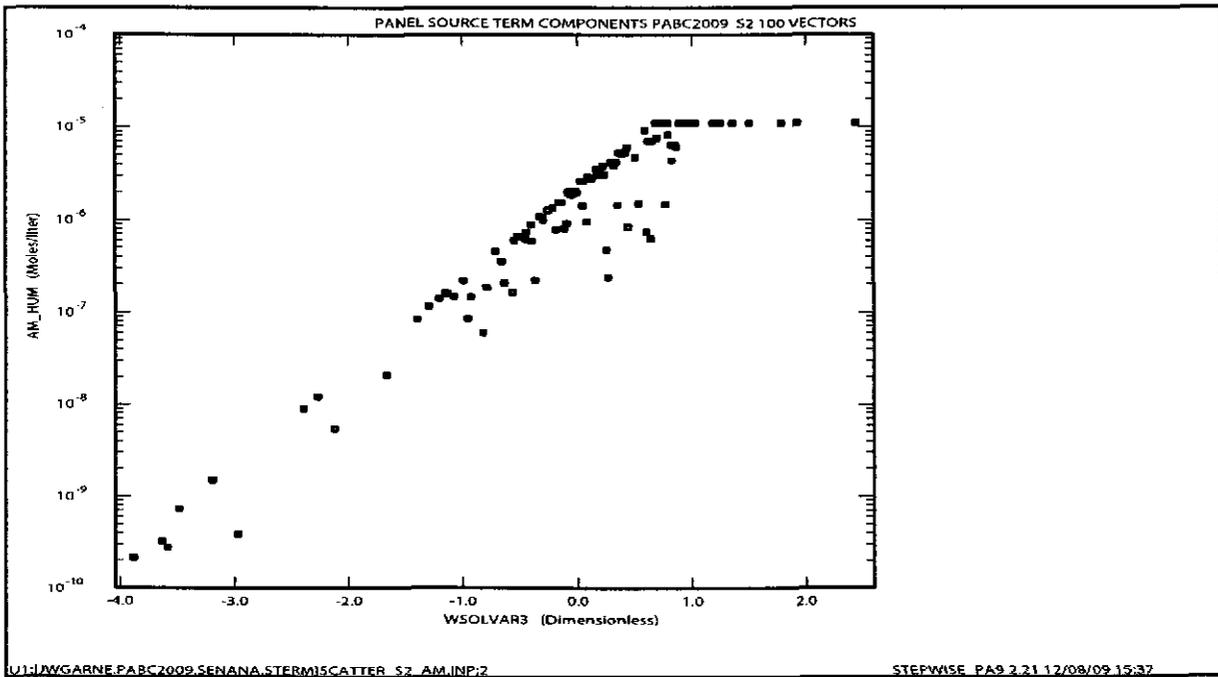
a) CRA-2009 PABC



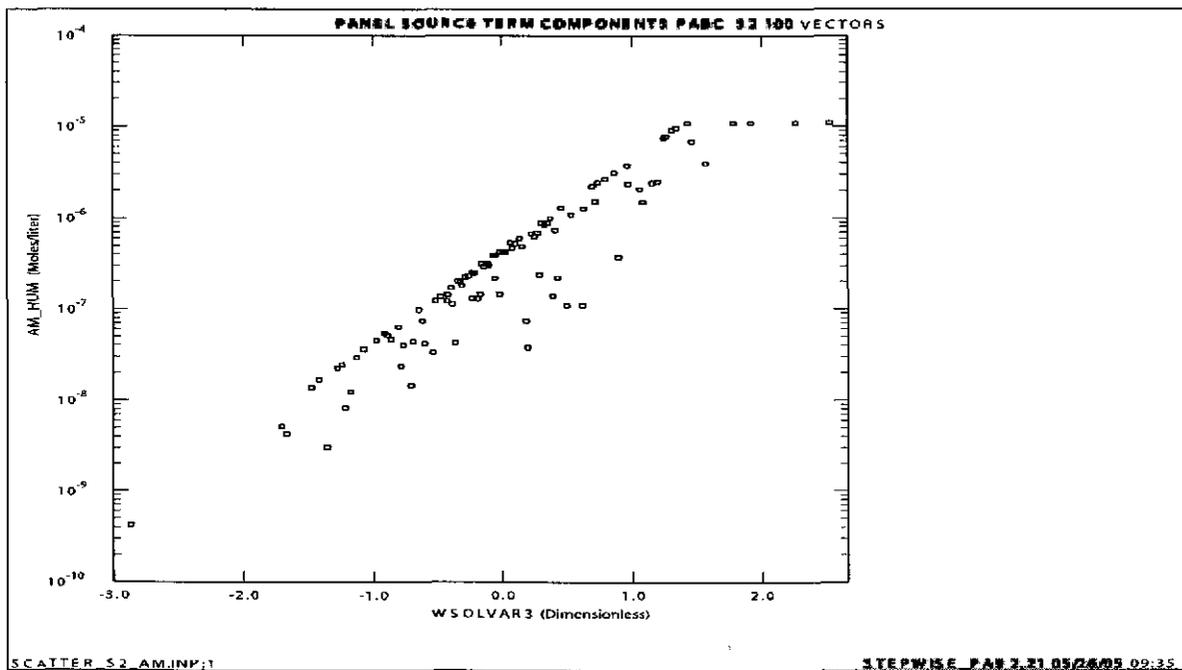
b) CRA-2004 PABC

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-2009 PABC.
Part b) shows results from the CRA-2004 PABC.



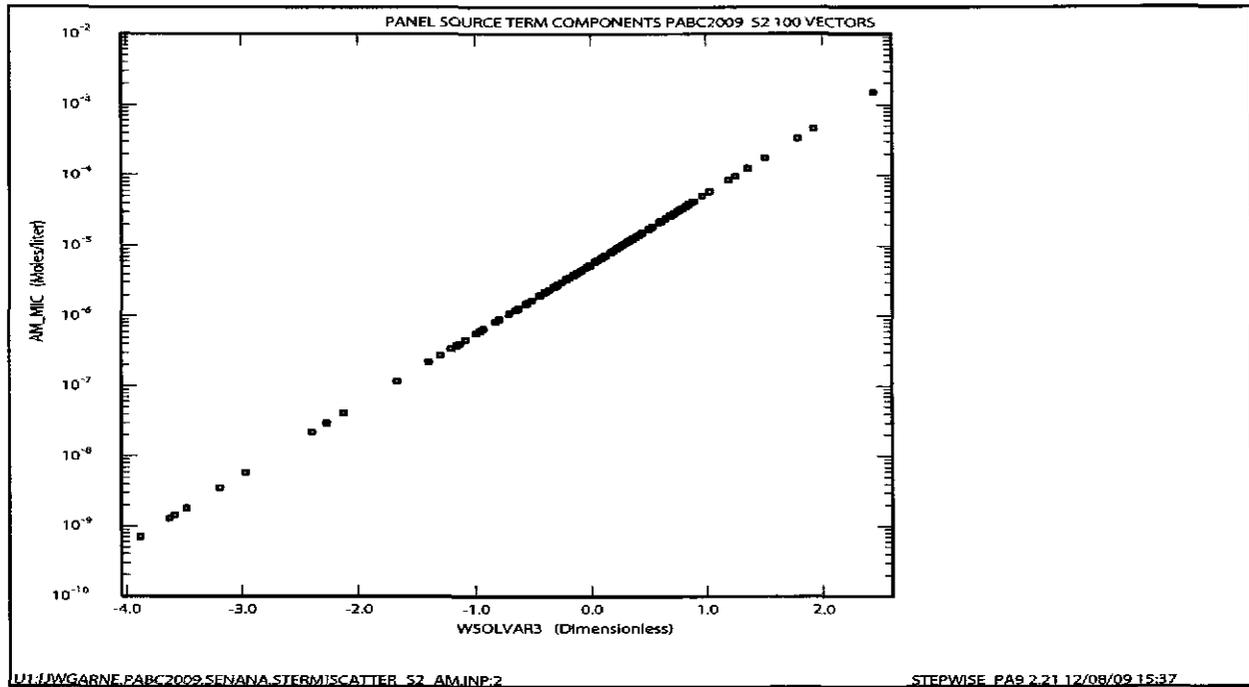
a) CRA-2009 PABC



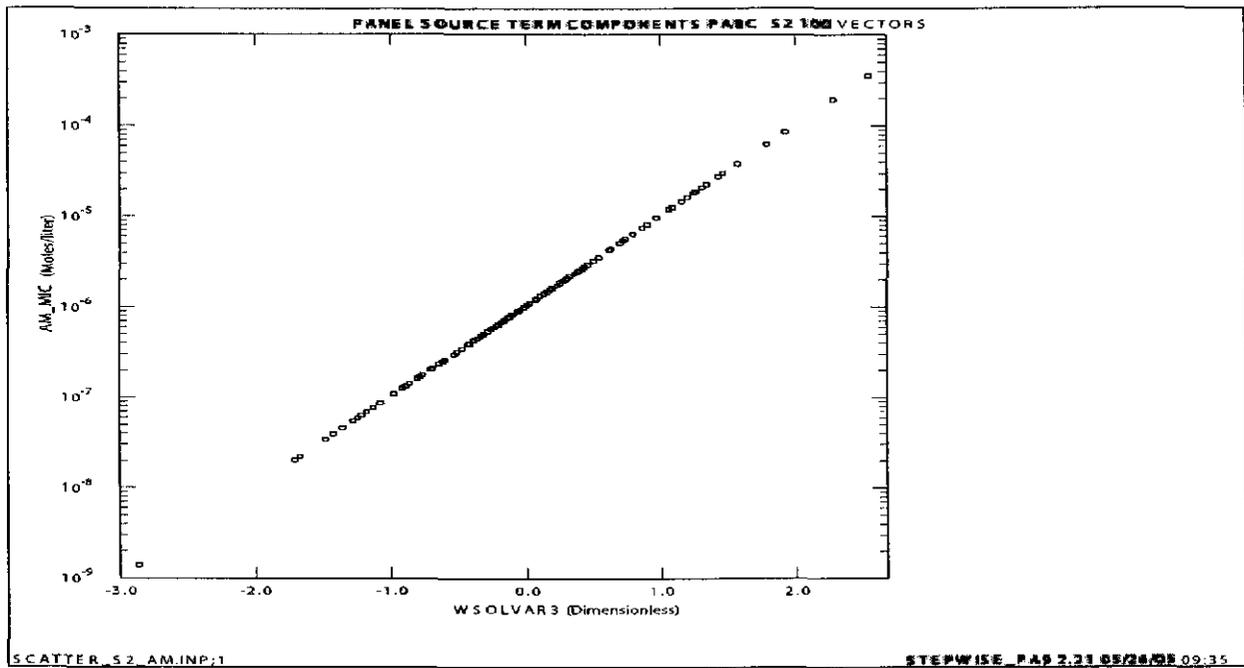
b) CRA-2004 PABC

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-2009 PABC.
Part b) shows results from the CRA-2004 PABC.



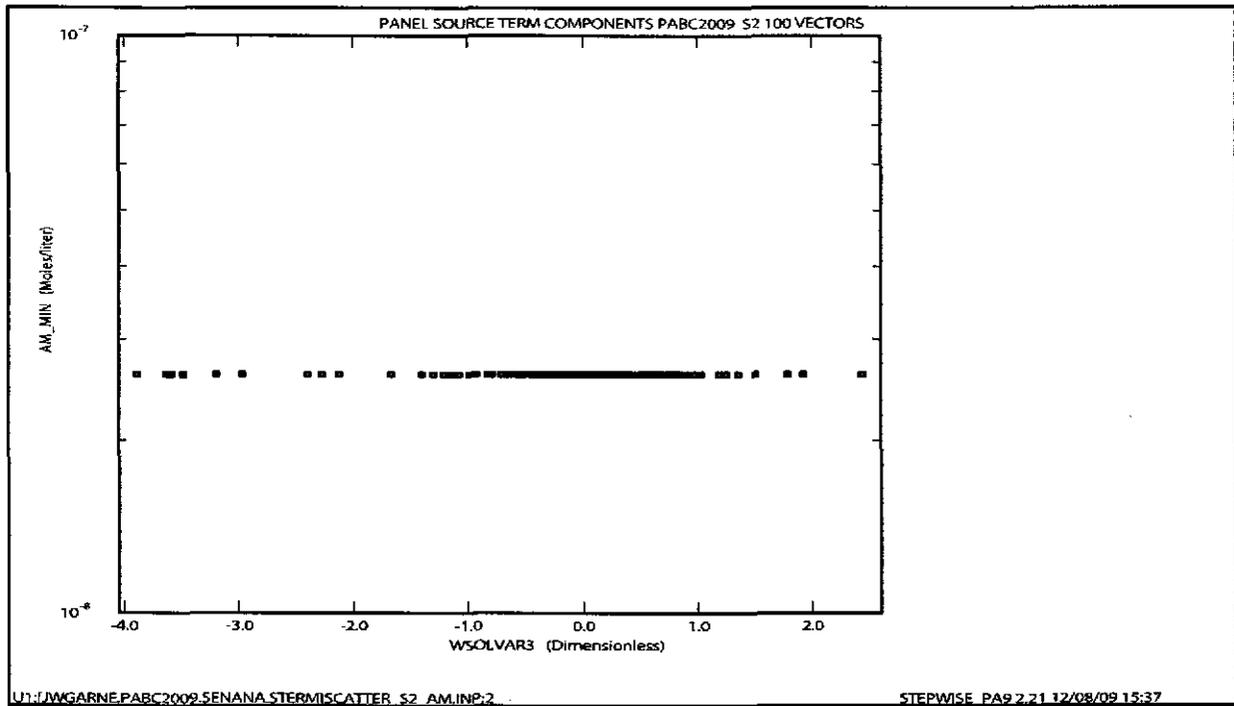
a) CRA-2009 PABC



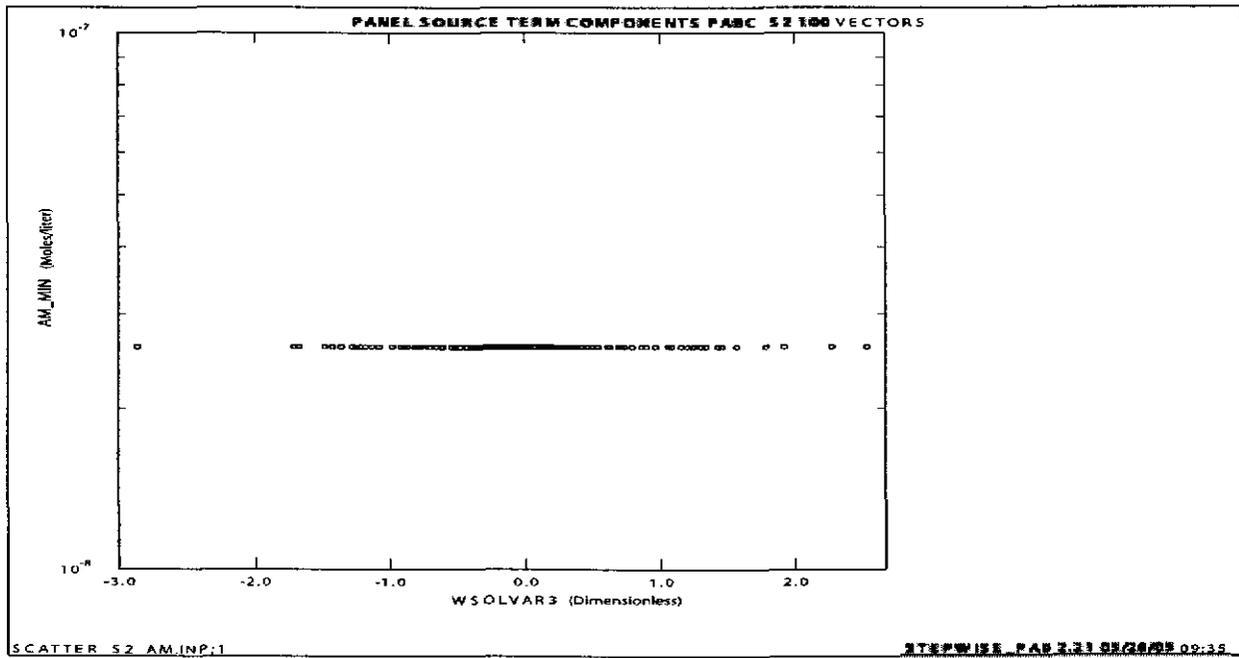
b) CRA-2004 PABC

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-2009 PABC.
Part b) shows results from the CRA-2004 PABC.



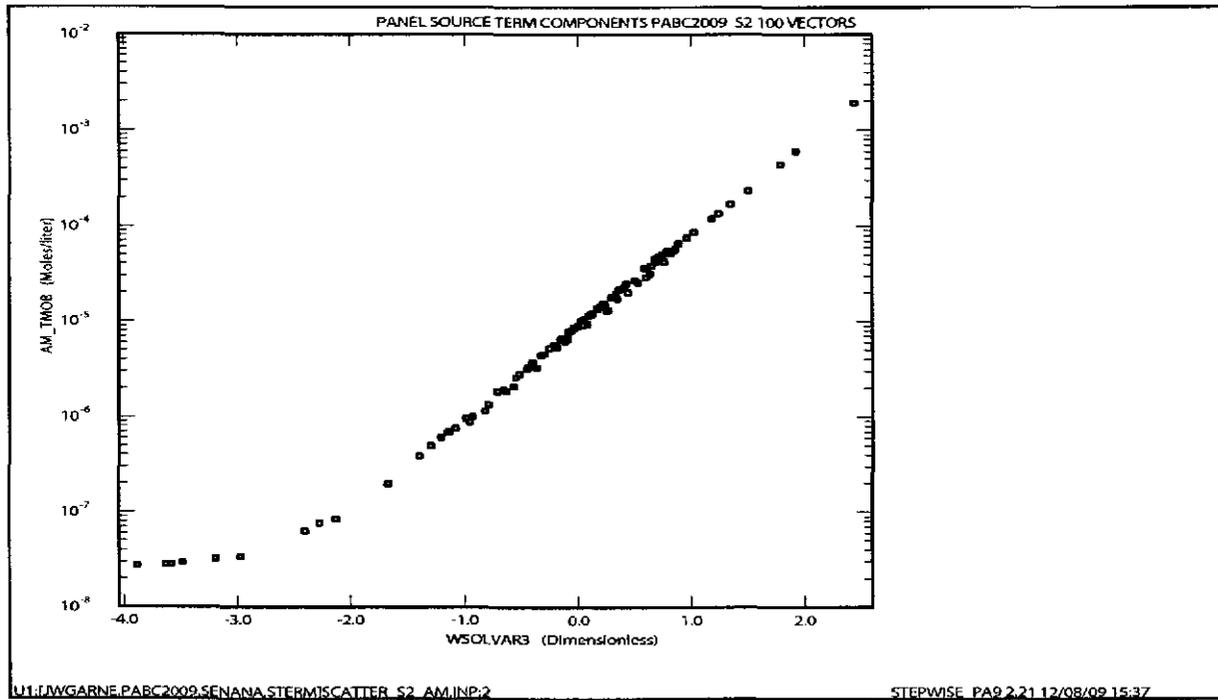
a) CRA-2009 PABC



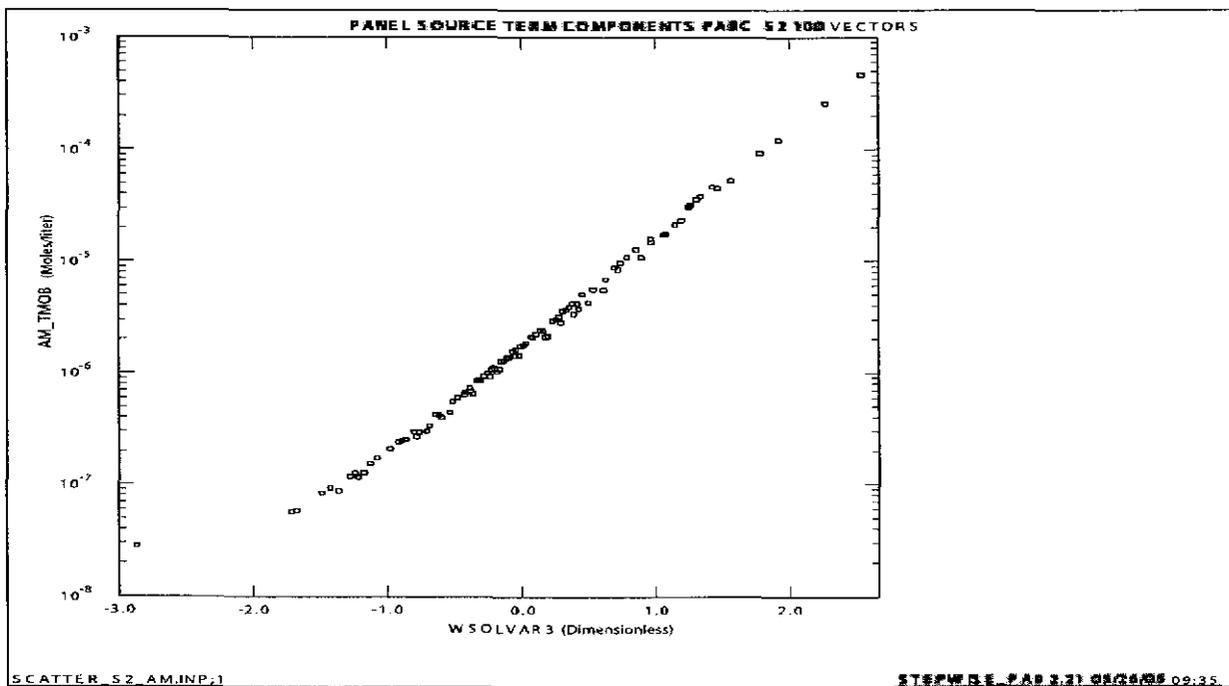
b) CRA-2004 PABC

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-2009 PABC.
Part b) shows results from the CRA-2004 PABC.



a) CRA-2009 PABC



b) CRA-2004 PABC

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

Part a) shows results from the CRA-2009 PABC.
Part b) shows results from the CRA-2004 PABC.

In WIPP PA, Pu can occur in either oxidation state +III or +IV, depending on the value of GLOBAL:OXSTAT (see Table 2) 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.

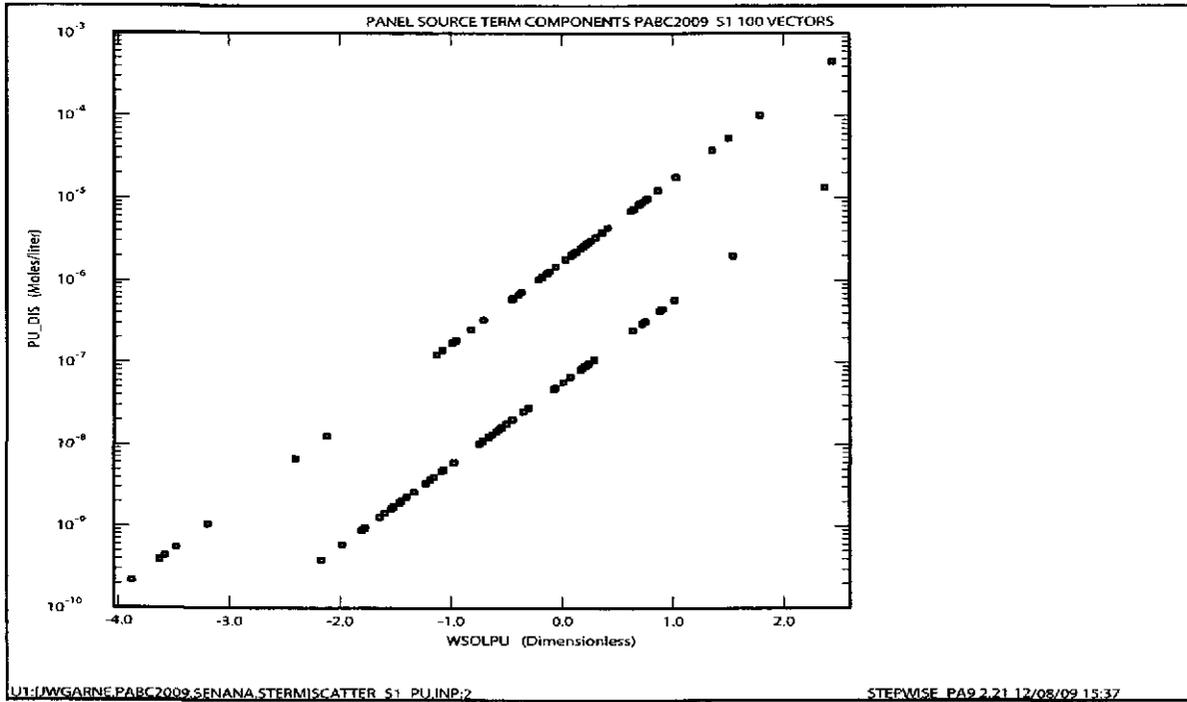
Figure 12 shows the dissolution potential for Pu in Salado brine. Part a (CRA-2009 PABC) has a larger range and the top curve (+III) is greater because of a greater predicted solubility (Table 1).

Figure 18 shows that the dissolution potential for Pu in Castile brine. Part a (CRA-2009 PABC) has a larger range and the top curve (+III) is greater because of a greater predicted solubility (Table 1).

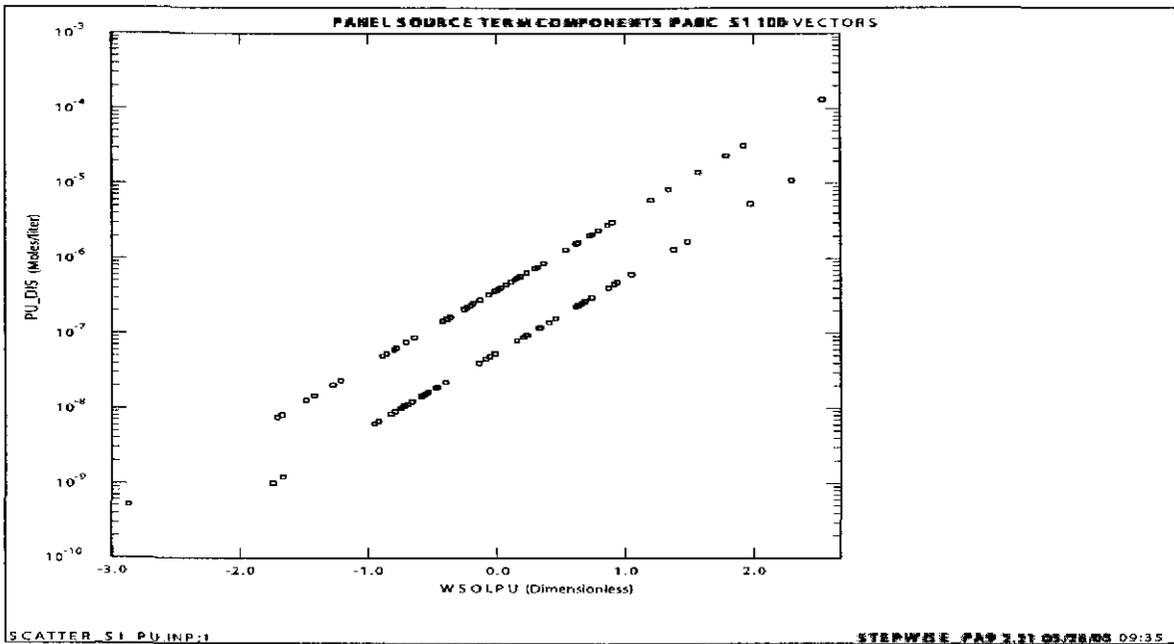
Figure 13 shows that the range of values for the mobilization potential for humic colloids for Pu in Salado brine. Both Part a and Part b reach the maximum value. The CRA-2009 PABC appears as only one line since the +III Salado solubility (Table 1) times the +III Salado humic proportionality constant (Table 6) is approximately equal to the +IV Salado solubility (Table 1) times the +IV Salado humic proportionality constant (Table 6).

Figure 14 shows two sets of data in both Part a (CRA-2009 PABC results) and Part b (the CRA-2004 PABC results). The two sets of data correspond to Pu in the two different oxidation states.

Figure 17 shows the total mobilization potential for Pu in Salado brine. Part a shows the CRA-2009 PABC results and Part b shows the CRA-2004 PABC results. Both show two sets of data corresponding to the two oxidation states for Pu. Figure 23 shows the same trend in the total mobilization potential for Pu in Castile brine. Figure 23 is a bit noisier because of the sampled portionality factor in the +III oxidation state.



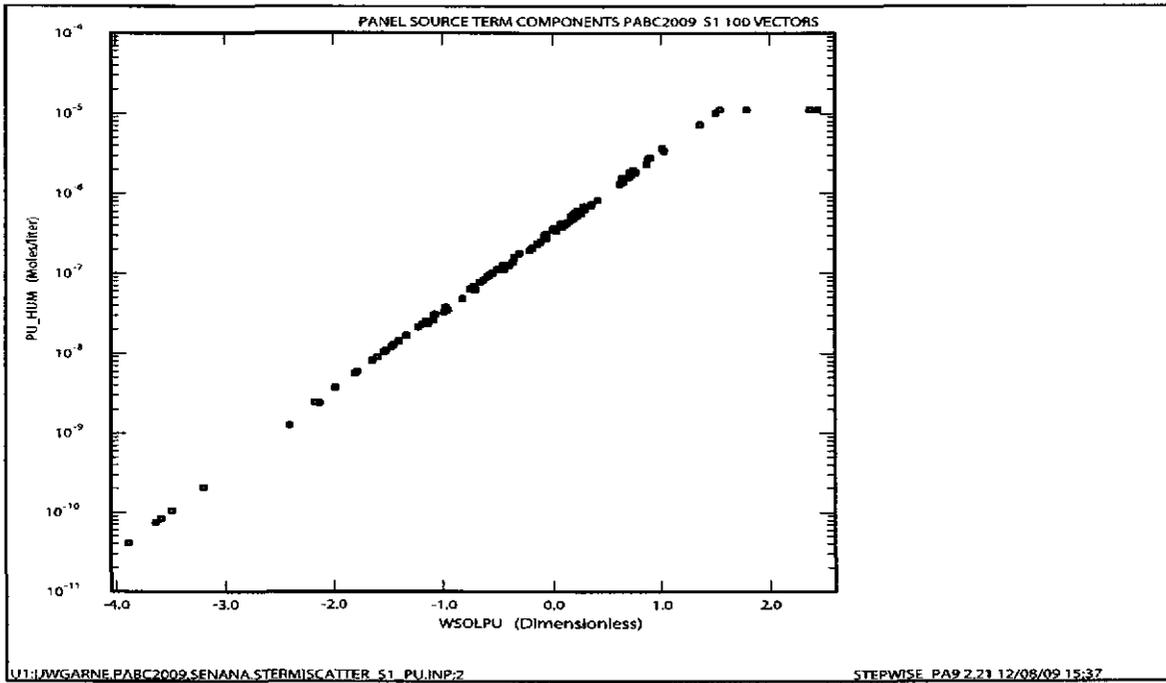
a) CRA-2009 PABC



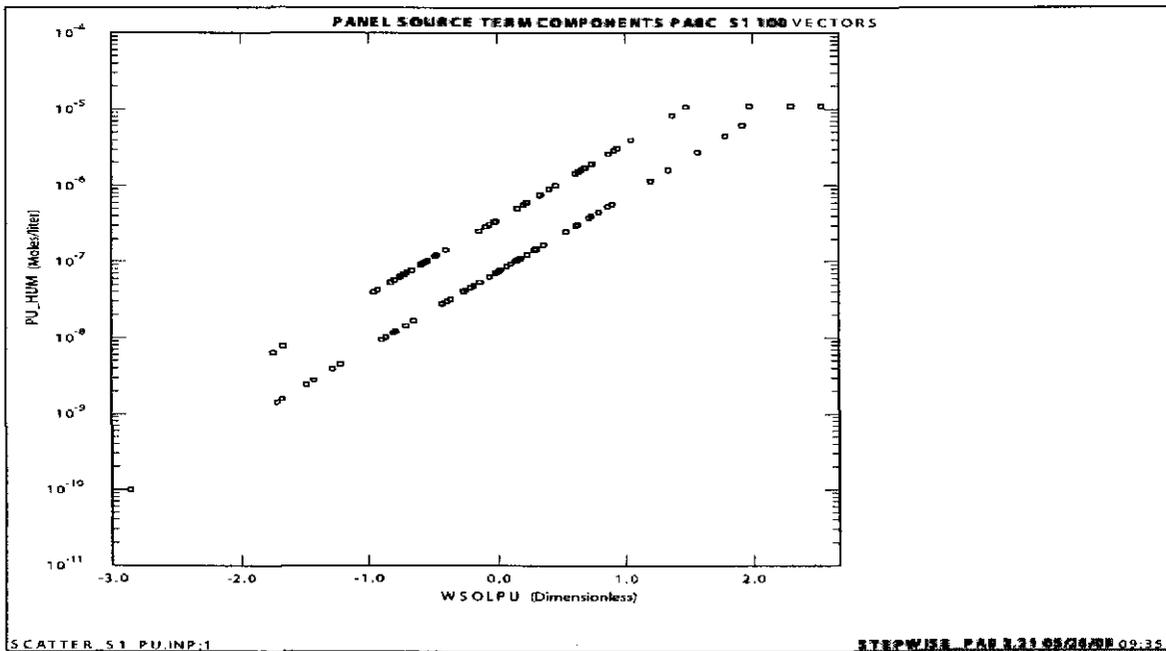
b) CRA-2004 PABC

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-2009 PABC.
Part b) shows results from the CRA-2004 PABC.



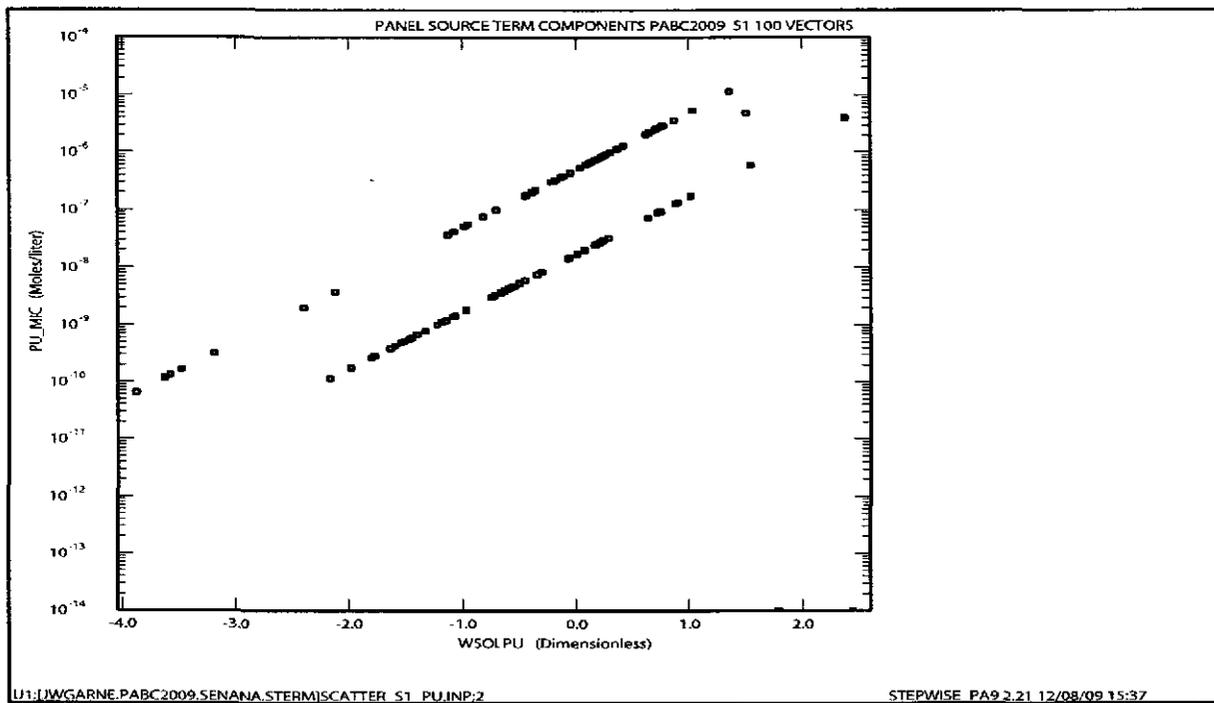
a) CRA-2009 PABC



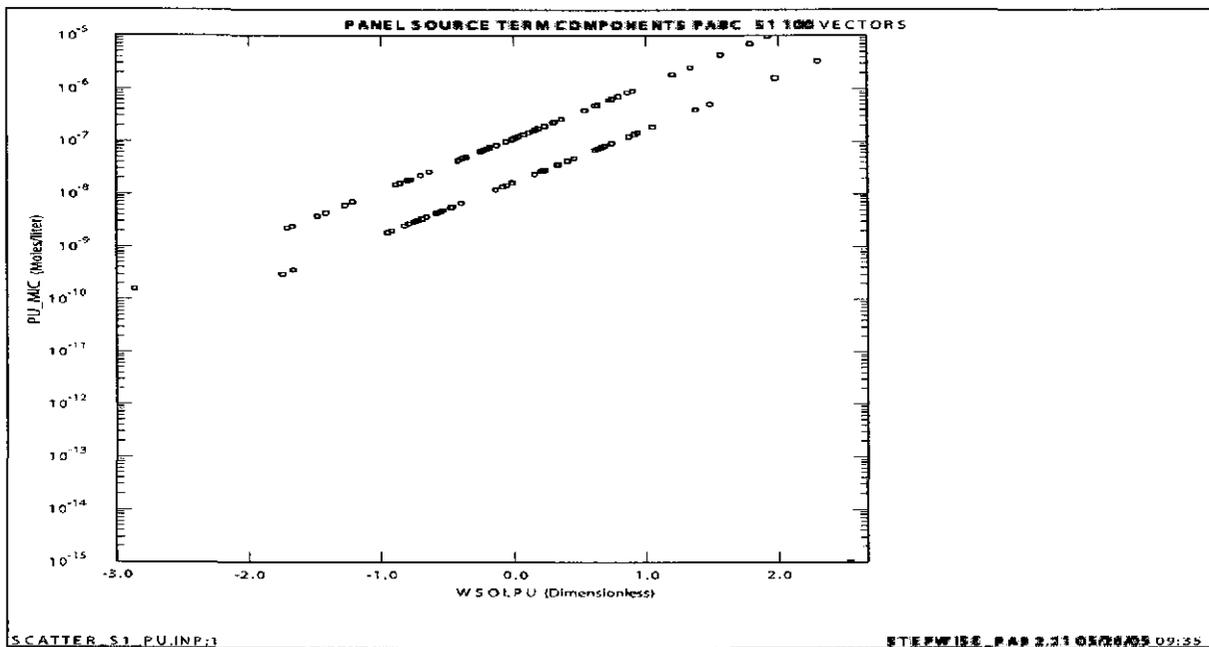
b) CRA-2004 PABC

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-2009 PABC.
Part b) shows results from the CRA-2004 PABC.



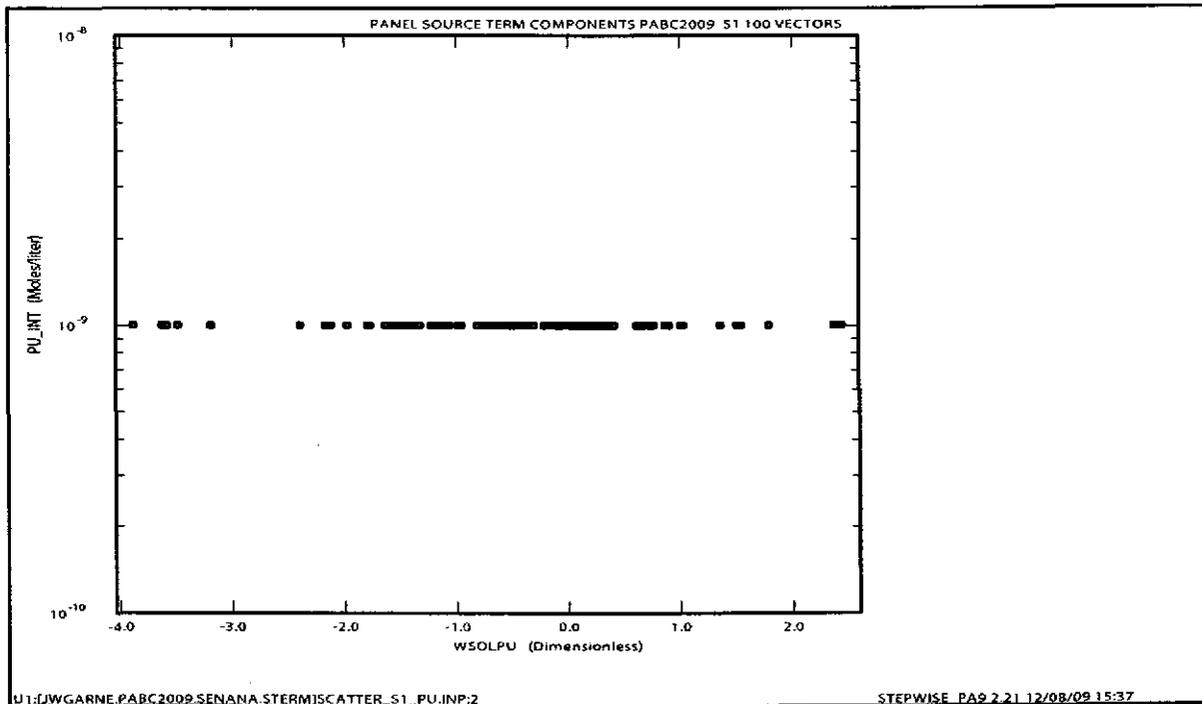
a) CRA-2009 PABC



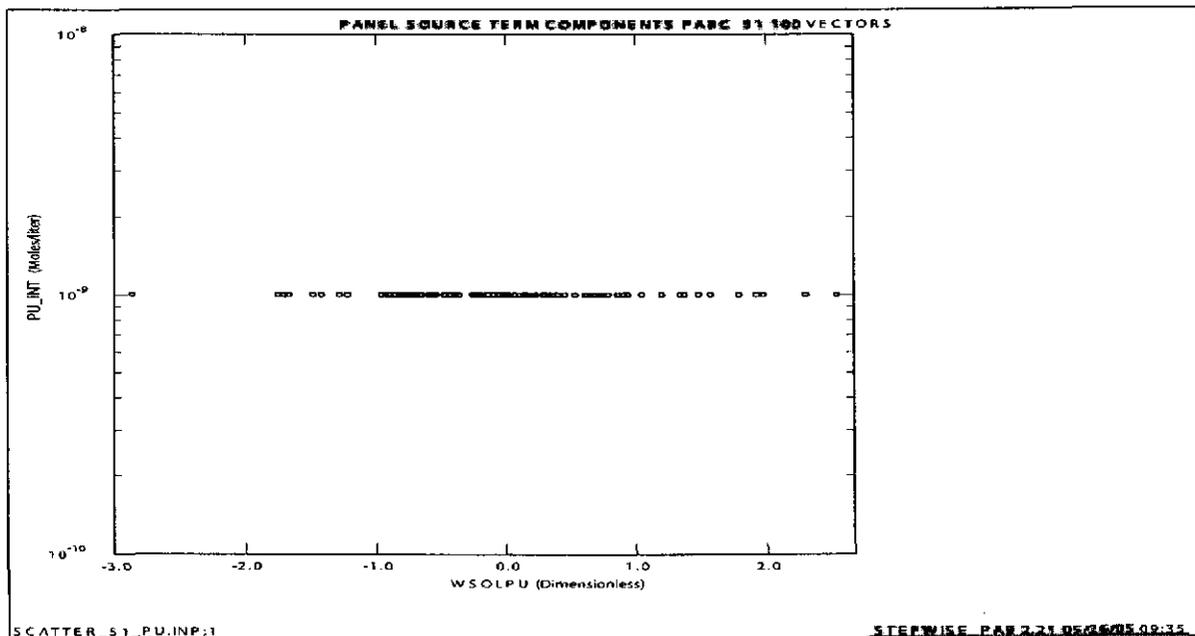
b) CRA-2004 PABC

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-2009 PABC.
Part b) shows results from the CRA-2004 PABC.



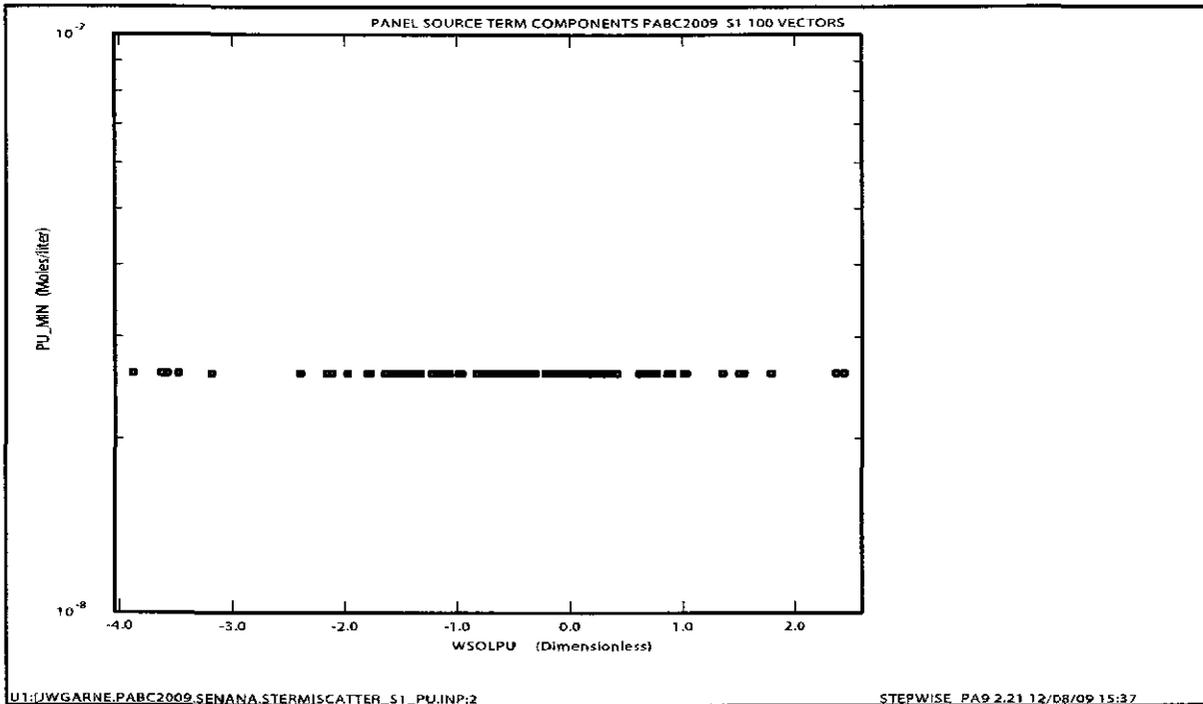
a) CRA-2009 PABC



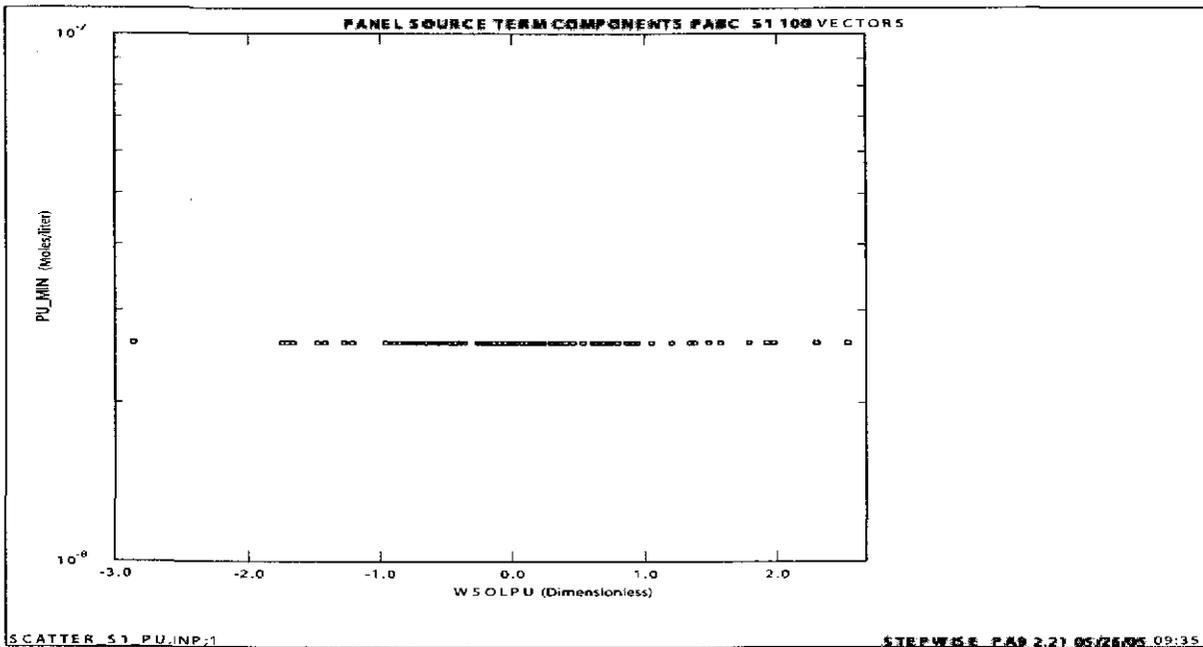
b) CRA-2004 PABC

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-2009 PABC.
Part b) shows results from the CRA-2004 PABC.



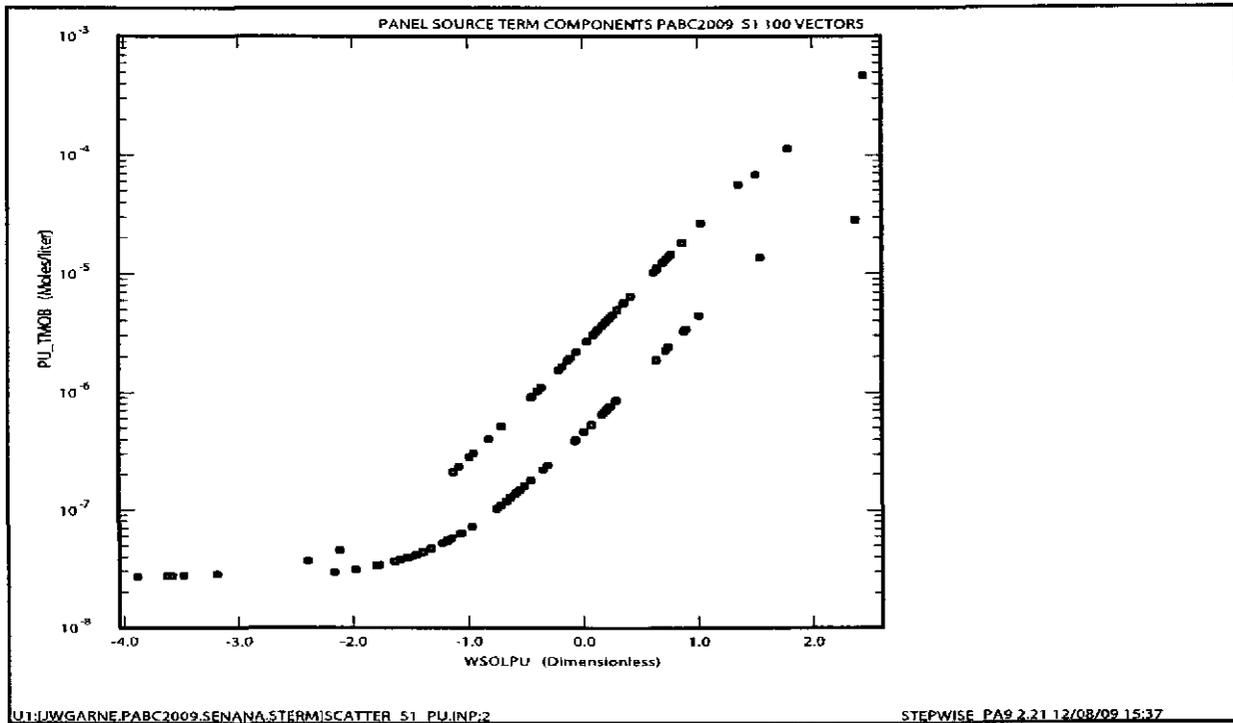
a) CRA-2009 PABC



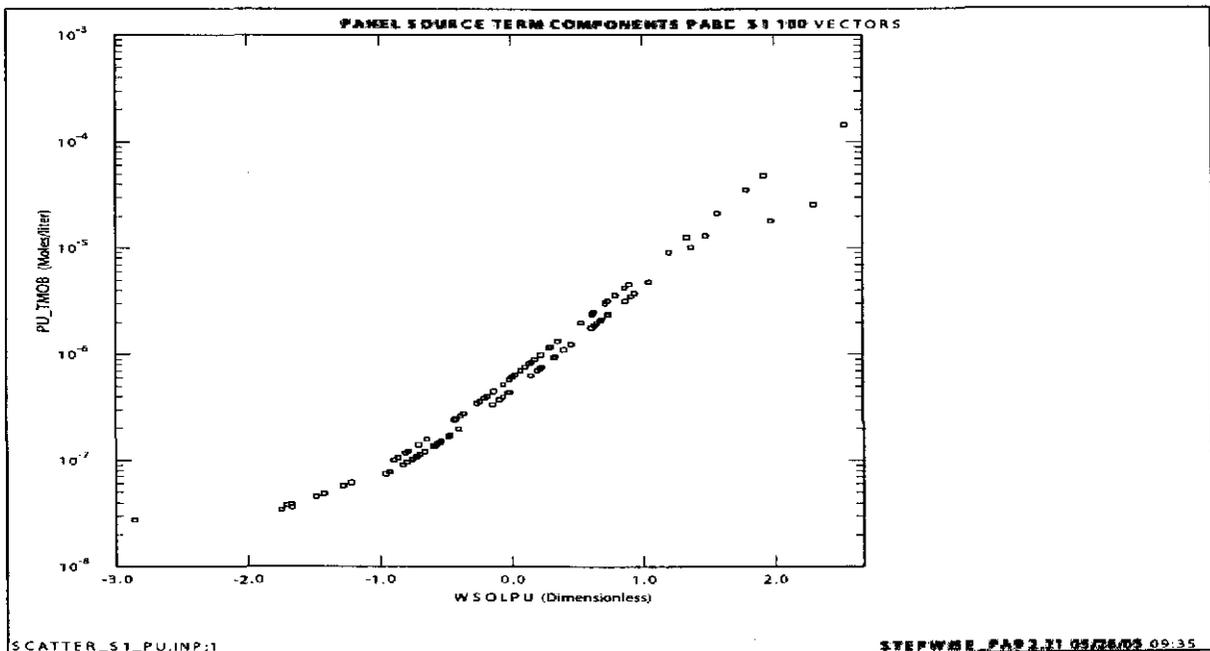
b) CRA-2004 PABC

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-2009 PABC.
Part b) shows results from the CRA-2004 PABC.



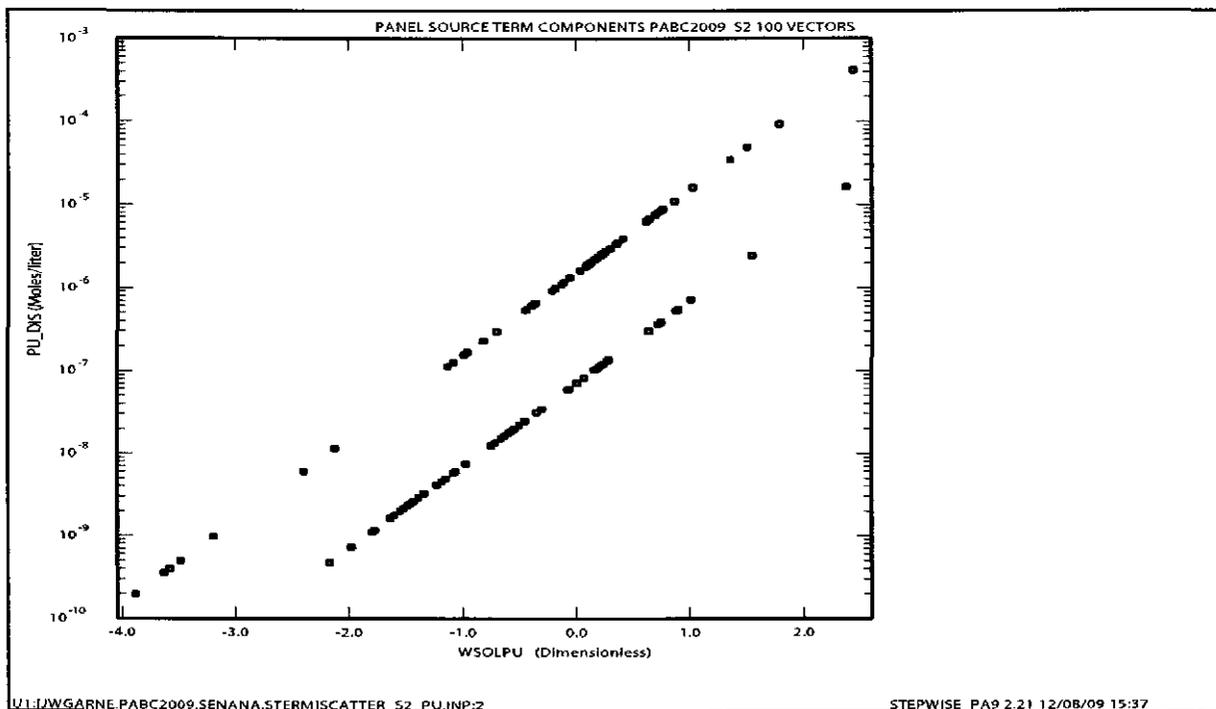
a) CRA-2009 PABC



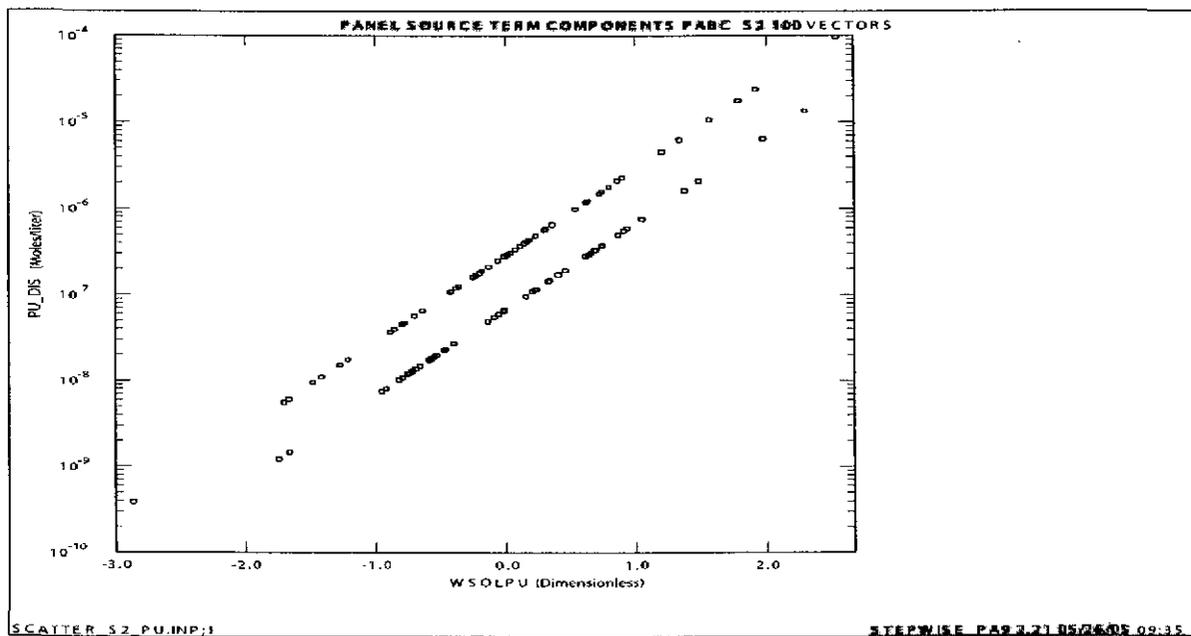
b) CRA-2004 PABC

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

Part a) shows results from the CRA-2009 PABC.
Part b) shows results from the CRA-2004 PABC.



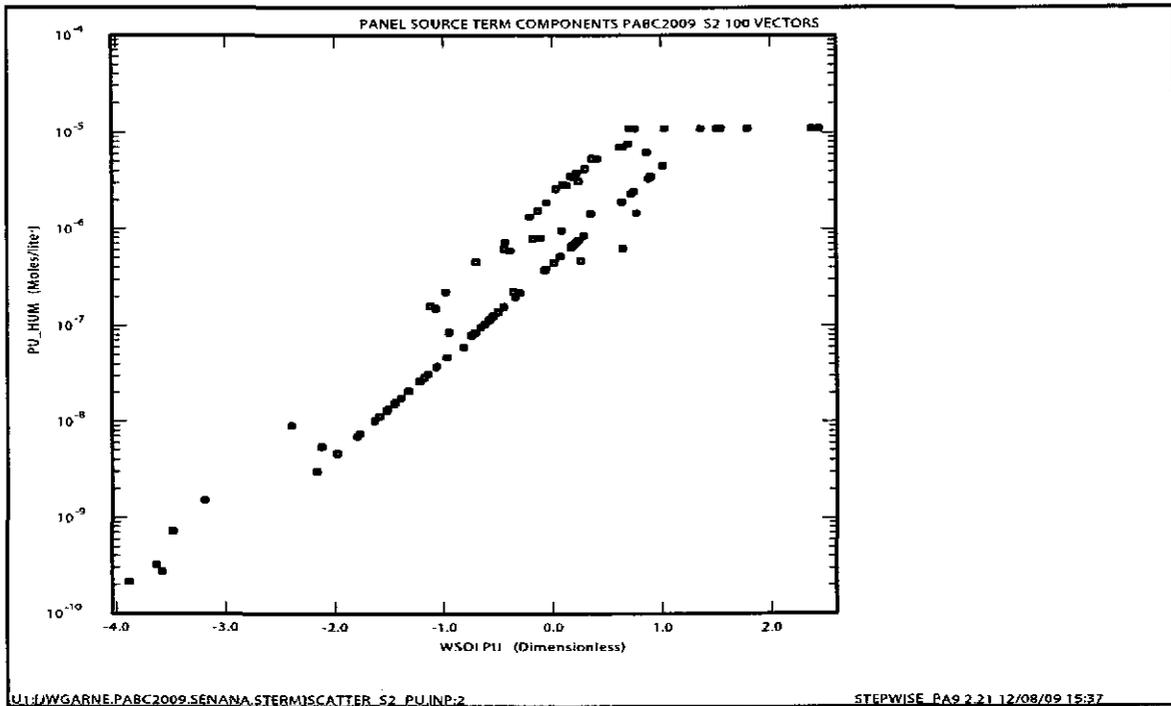
a) CRA-2009 PABC



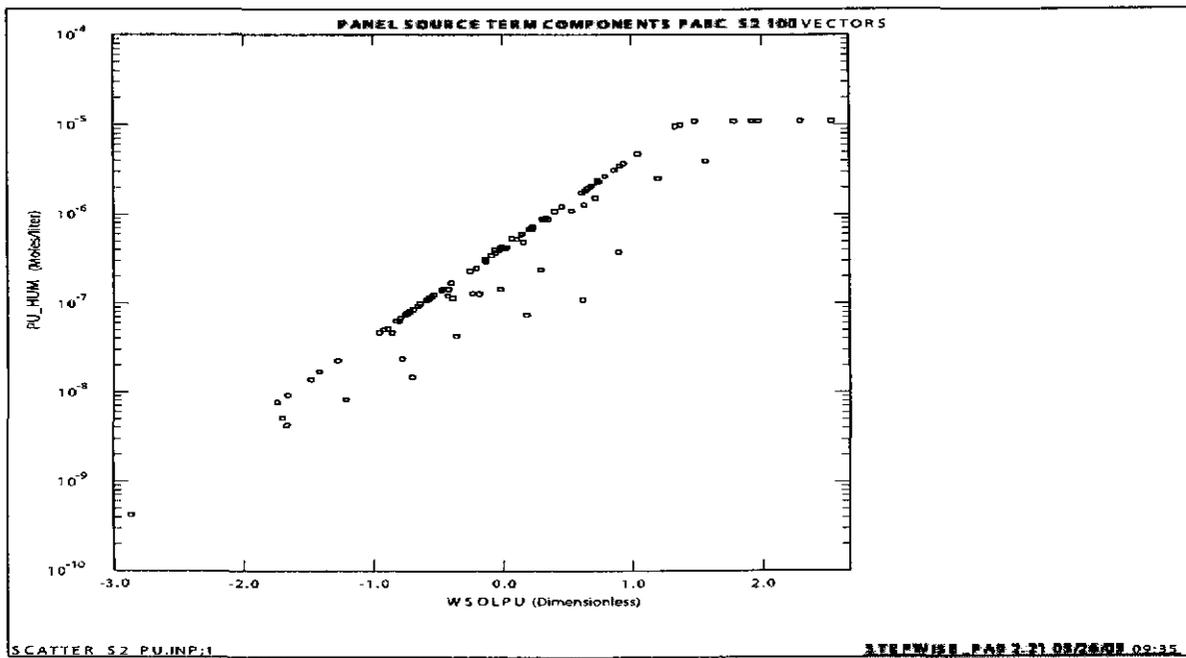
b) CRA-2004 PABC

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-2009 PABC.
Part b) shows results from the CRA-2004 PABC.



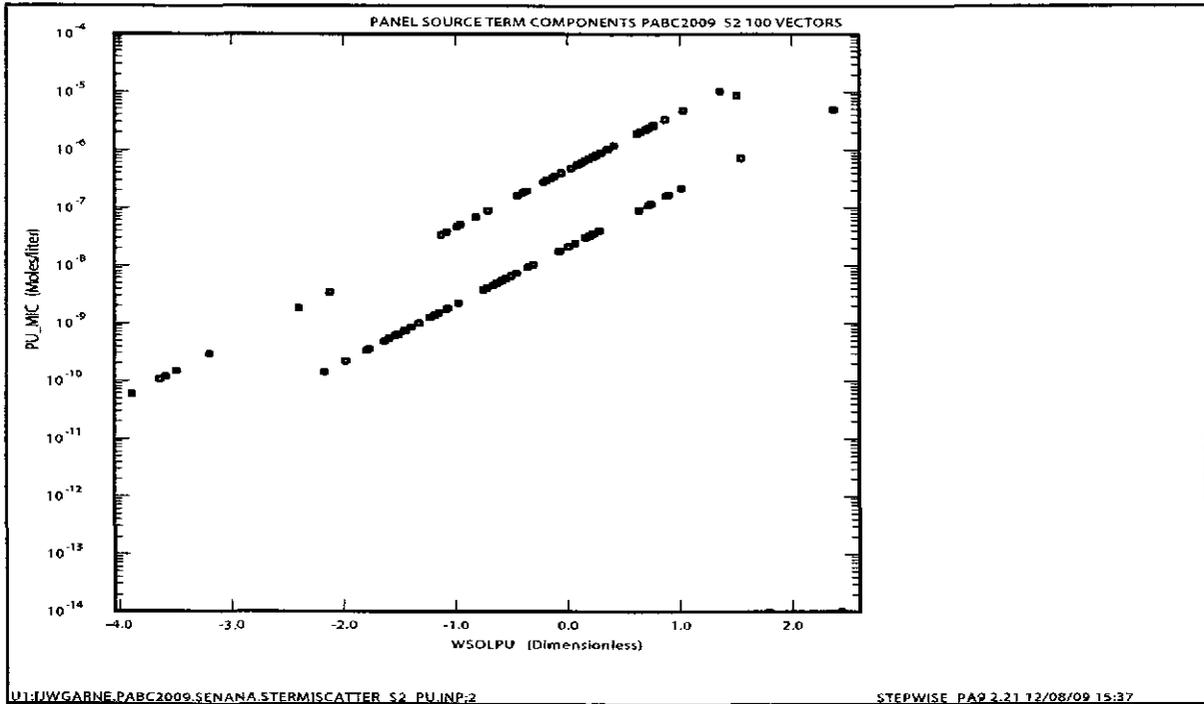
a) CRA-2009 PABC



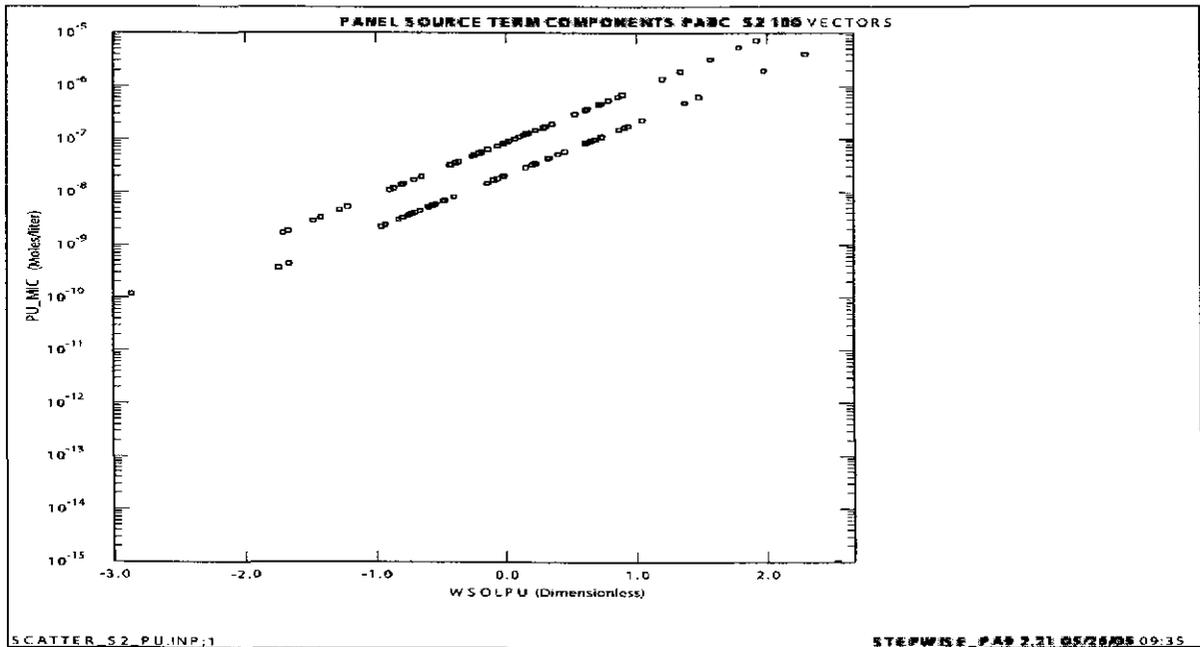
b) CRA-2004 PABC

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-2009 PABC.
Part b) shows results from the CRA-2004 PABC.



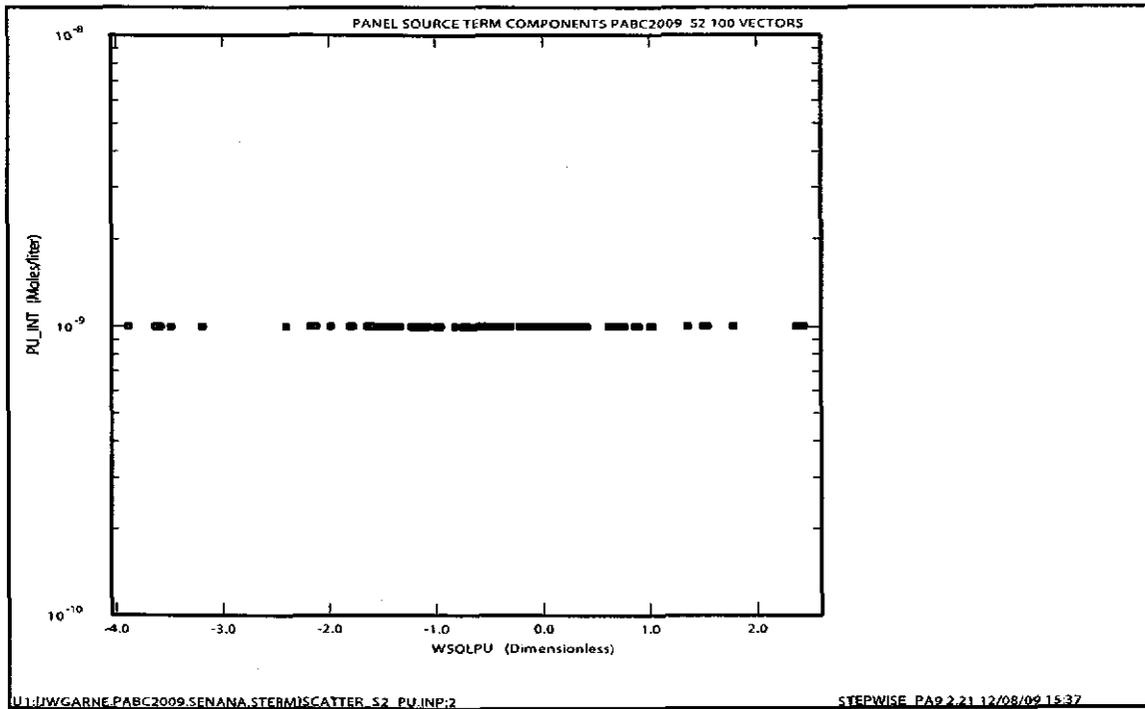
a) CRA-2009 PABC



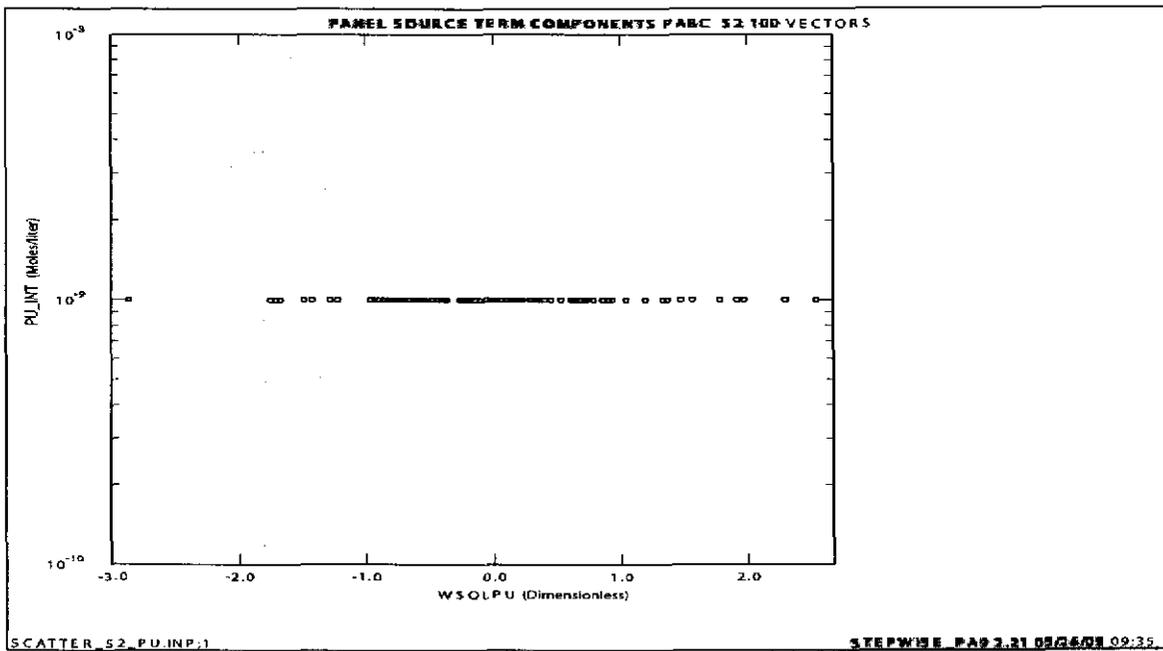
b) CRA-2004 PABC

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-2009 PABC.
Part b) shows results from the CRA-2004 PABC.



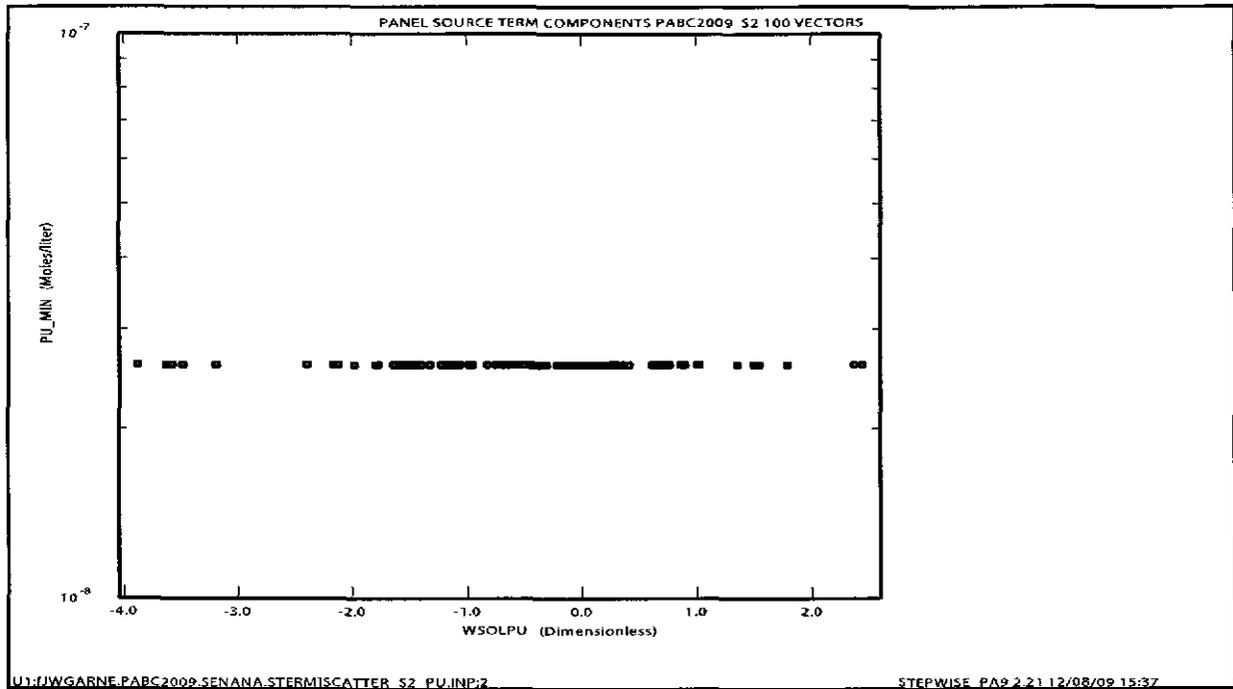
a) CRA-2009 PABC



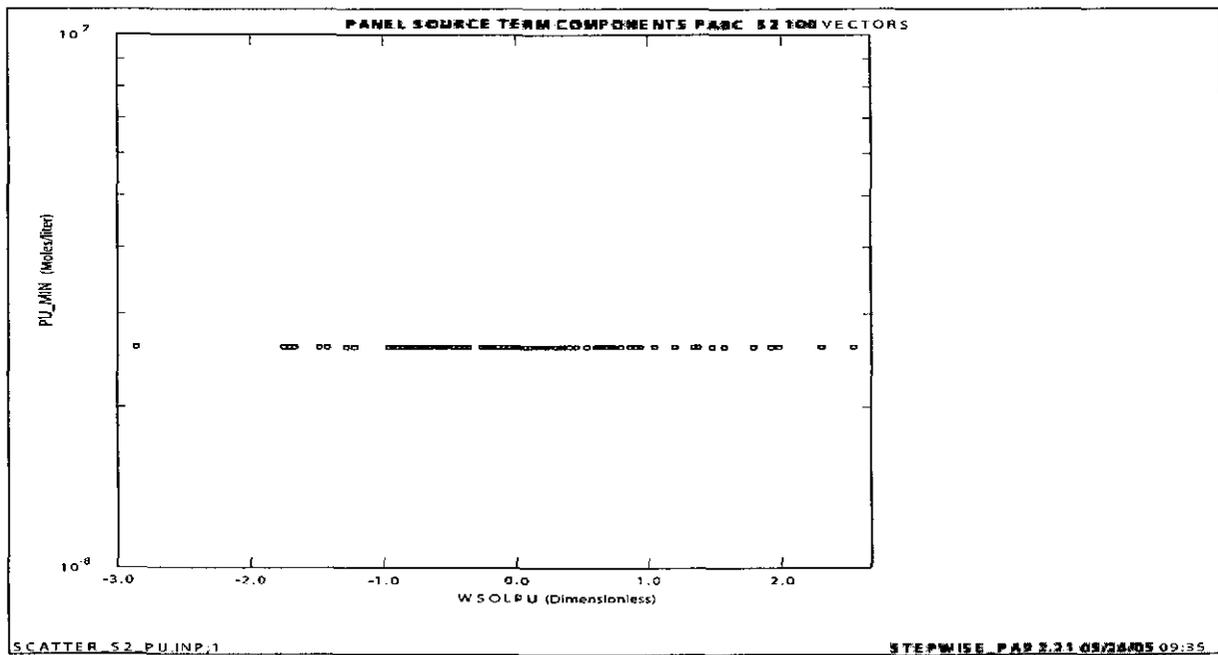
b) CRA-2004 PABC

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-2009 PABC.
Part b) shows results from the CRA-2004 PABC.



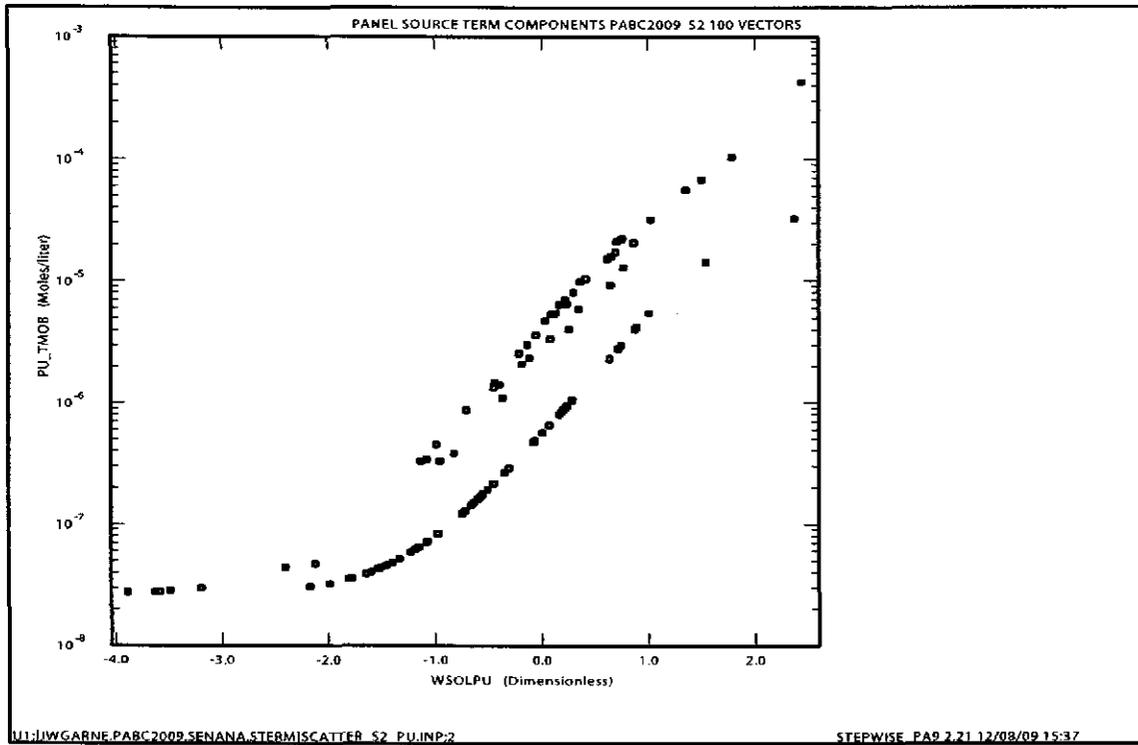
a) CRA-2009 PABC



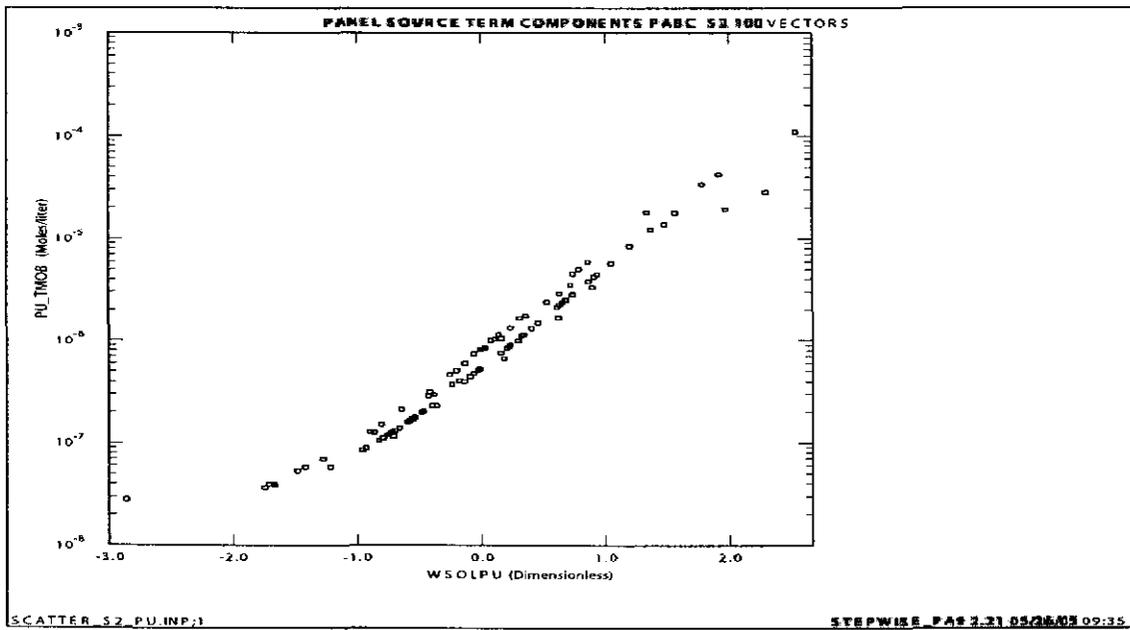
b) CRA-2004 PABC

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-2009 PABC.
Part b) shows results from the CRA-2004 PABC.



a) CRA-2009 PABC



b) CRA-2004 PABC

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

Part a) shows results from the CRA-2009 PABC.
Part b) shows results from the CRA-2004 PABC.

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 PABC results (Part b in each figure) and the CRA-2009 PABC results (Part a in each figure) presented. There were no changes that affected PANEL Decay type runs between CRA-2004 PABC and CRA-2009 PA. This is why we compare the CRA-2009 PABC results and the CRA-2004 PABC results. 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 14 provides definitions for the variables plotted in Figures 24 through 29.

Table 14. Definitions of Variables Plotted in Figures 24 through 29

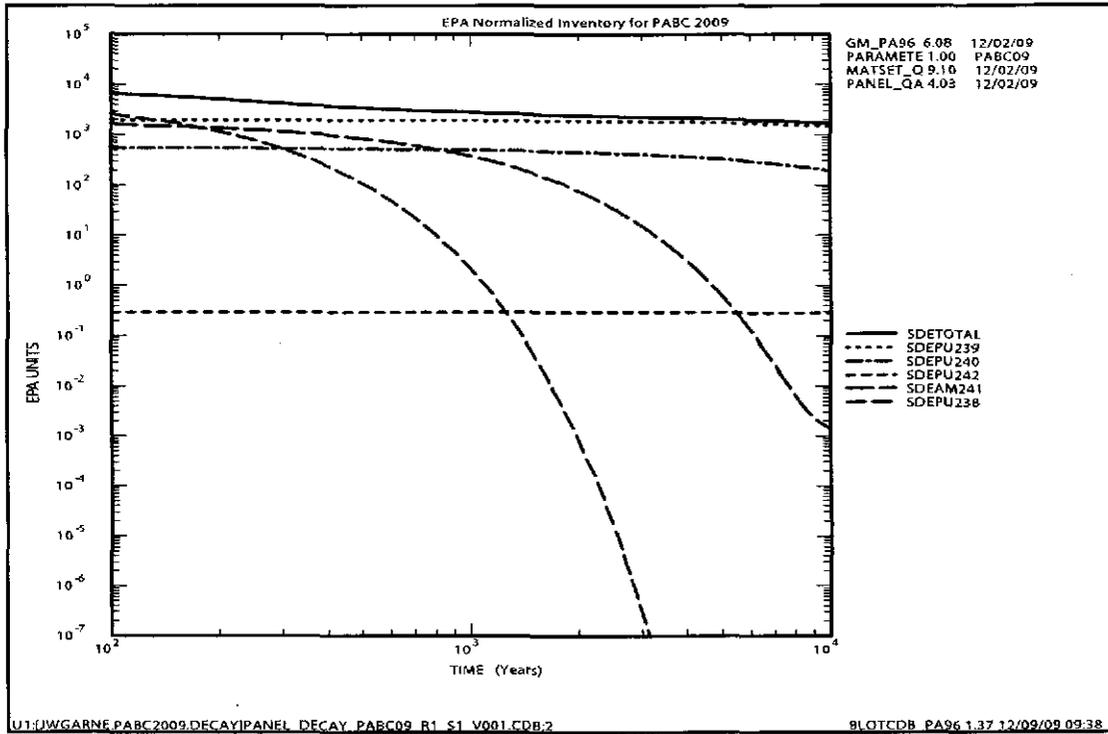
Name	Type/Units	Description
SDETOTAL	EPA Units	Total Activity
SDEPU239	EPA Units	Activity of PU239
SDEPU240	EPA Units	Activity of PU240
SDEPU242	EPA Units	Activity of PU242
SDEAM241	EPA Units	Activity of AM241
SDEPU238	EPA Units	Activity of PU238
SDEU233	EPA Units	Activity of U233
SDEU234	EPA Units	Activity 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

Figures 24 through 29 indicate that while the radionuclide inventory increased in CRA-2009 PABC, the overall differences were minor since EPA Units are normalized by f_w .

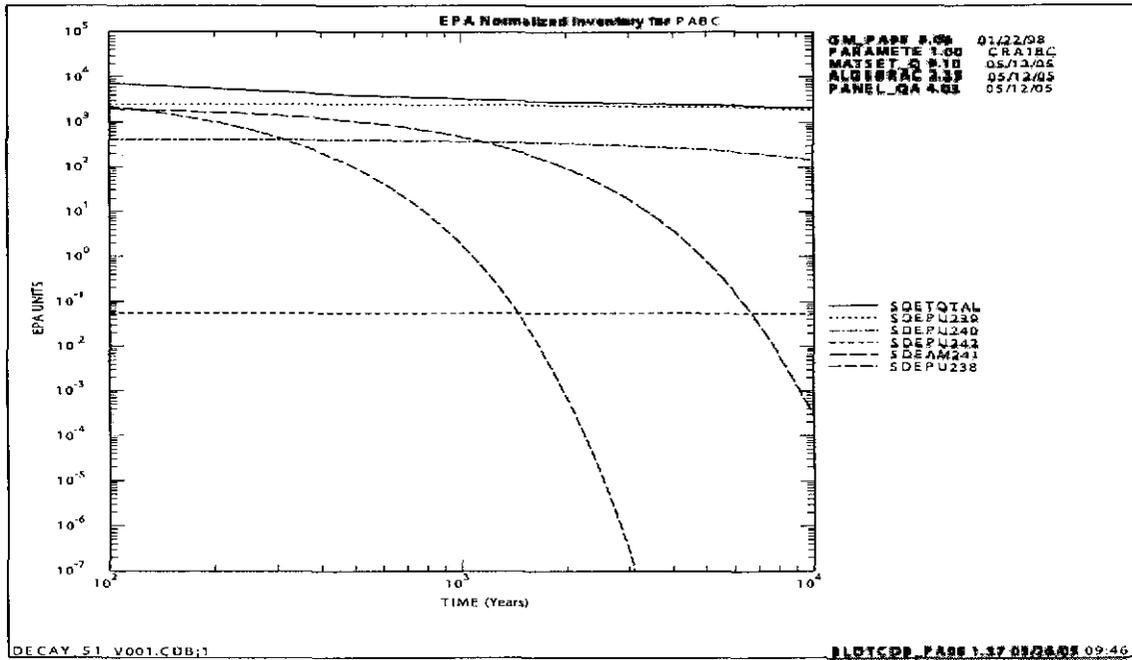
Figure 24 shows the decay behavior for the Am and Pu isotopes over time. In general, the Pu isotopic inventory is steady over time with the exception of Pu238 which decays away by about 2000 years. In addition, Am241 decays away over time with the final inventory of Am241 at 10,000 years about 10^{-7}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



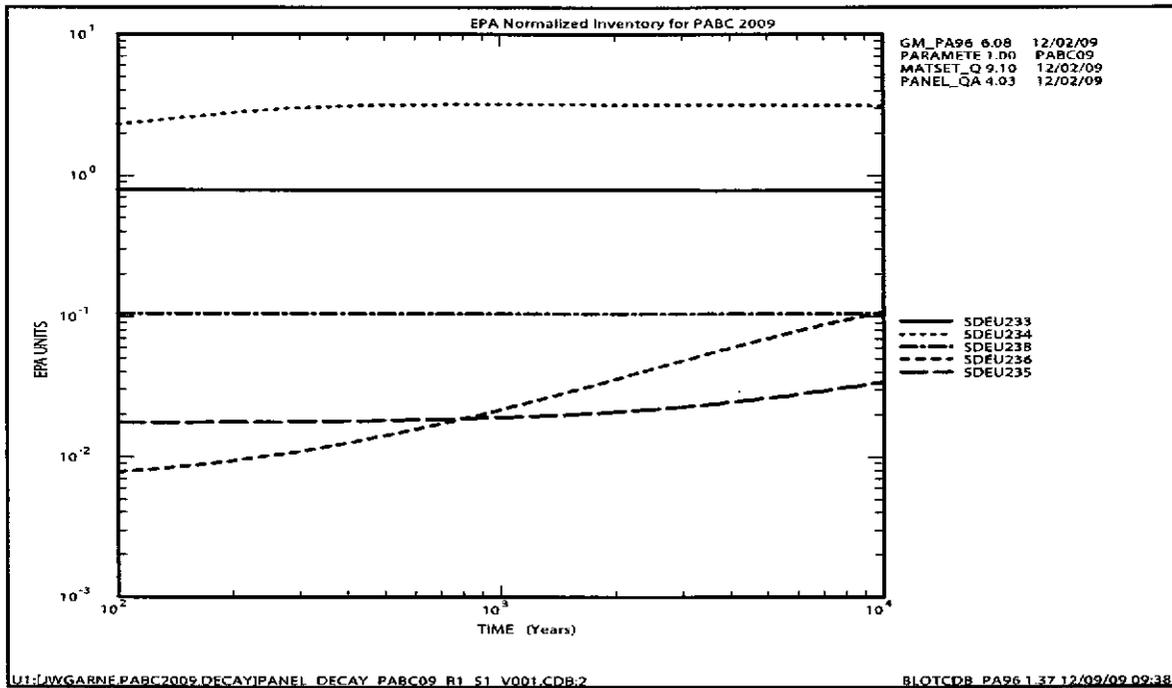
a) CRA-2009 PABC



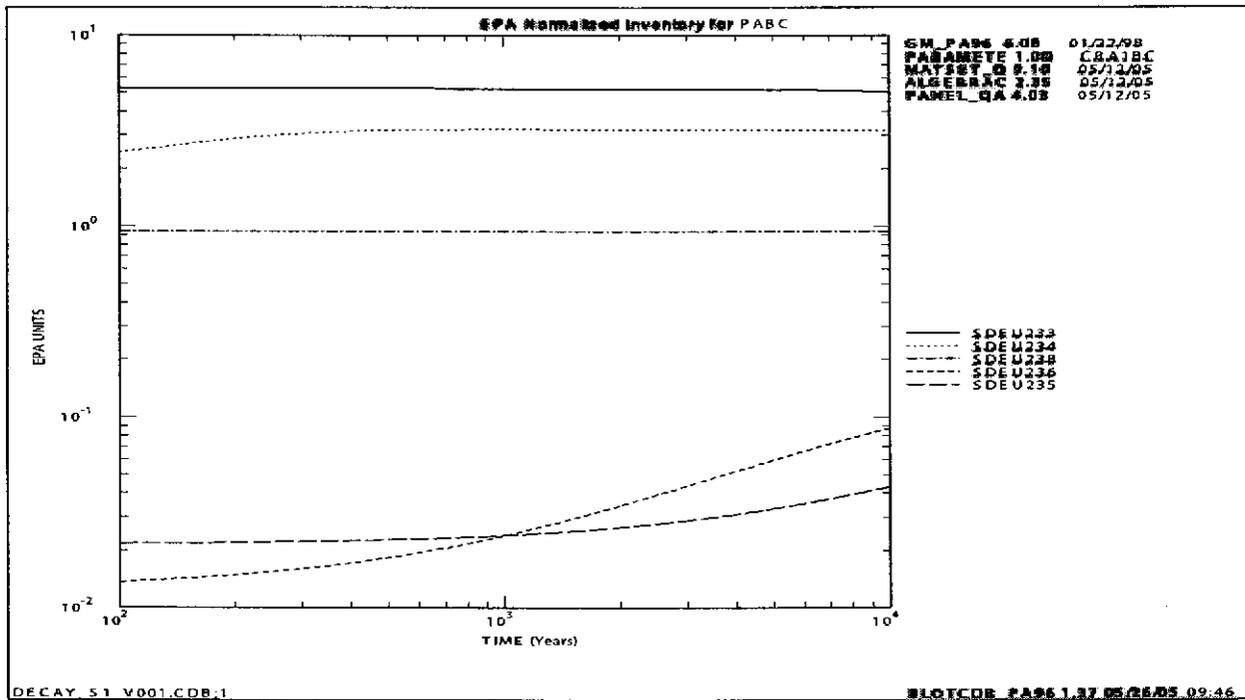
b) CRA-2004 PABC

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

Part a) shows results from the CRA-2009 PABC.
 Part b) shows results from the CRA-2004 PABC.



a) CRA-2009 PABC

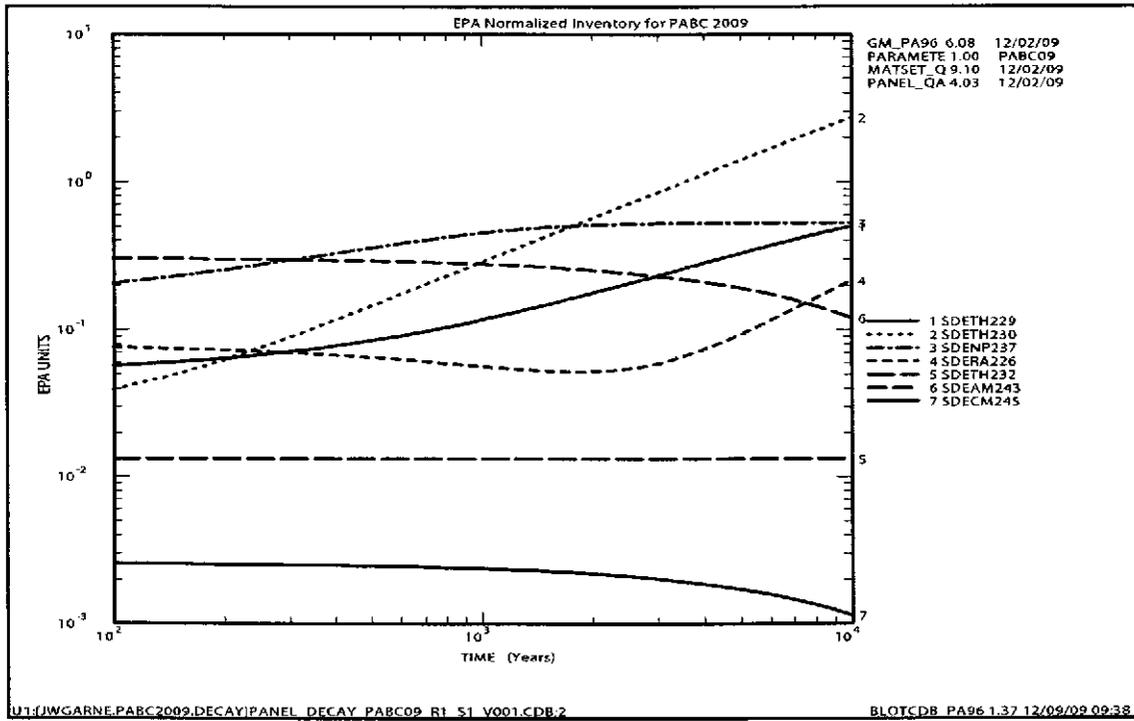


b) CRA-2004 PABC

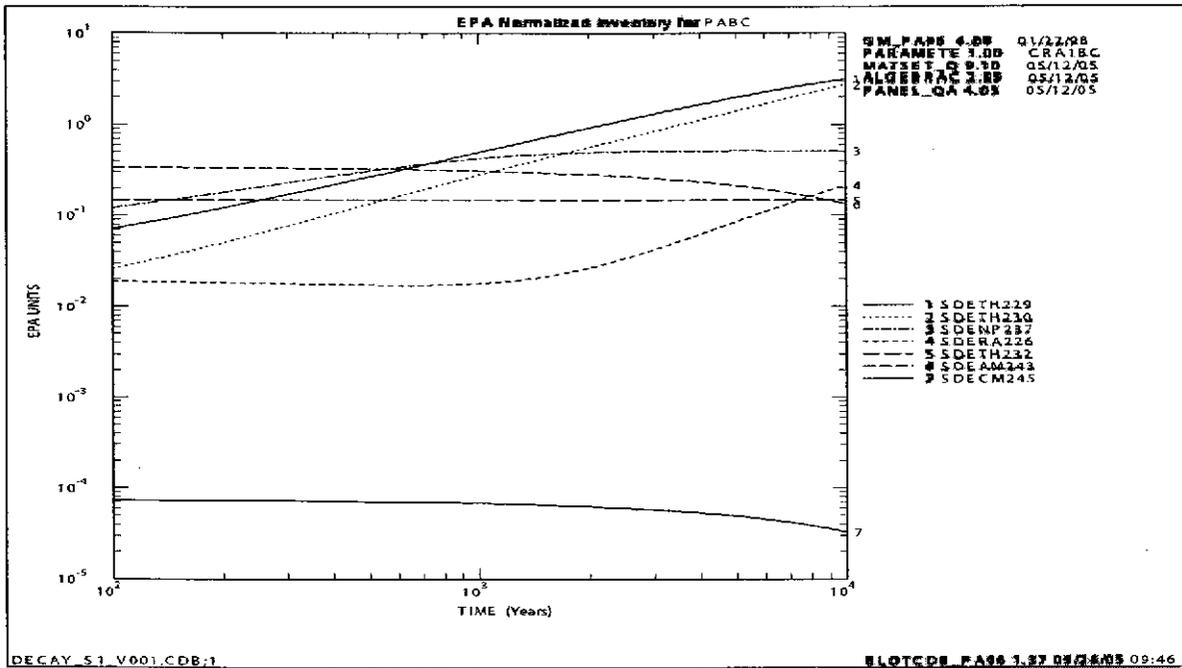
Figure 25. Time dependent inventories of U isotopes.

Part a) shows results from the CRA-2009 PABC.

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



a) CRA-2009 PABC

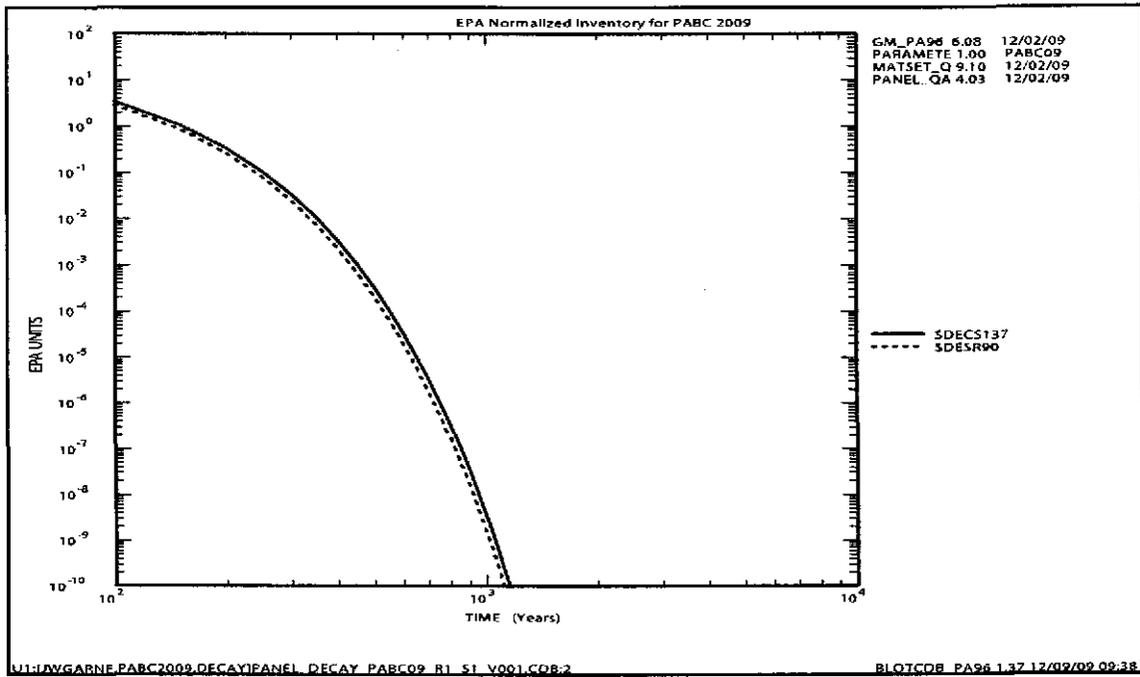


b) CRA-2004 PABC

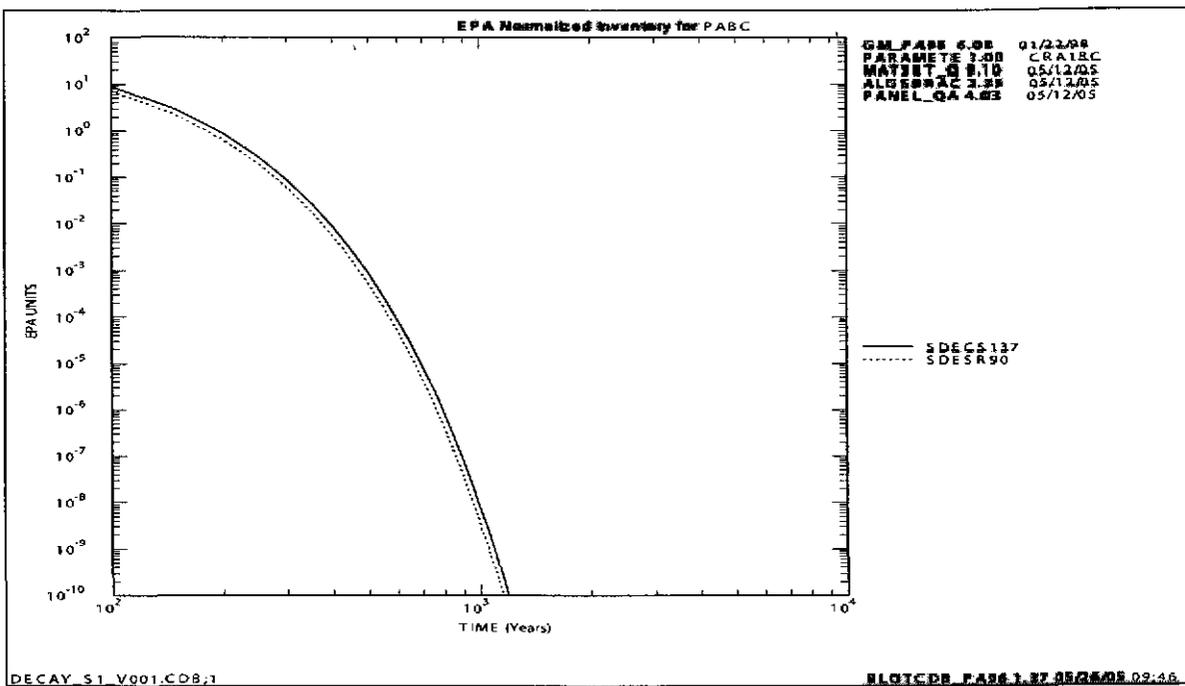
Figure 26. Time dependent inventories of various isotopes.

Part a) shows results from the CRA-2009 PABC.

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



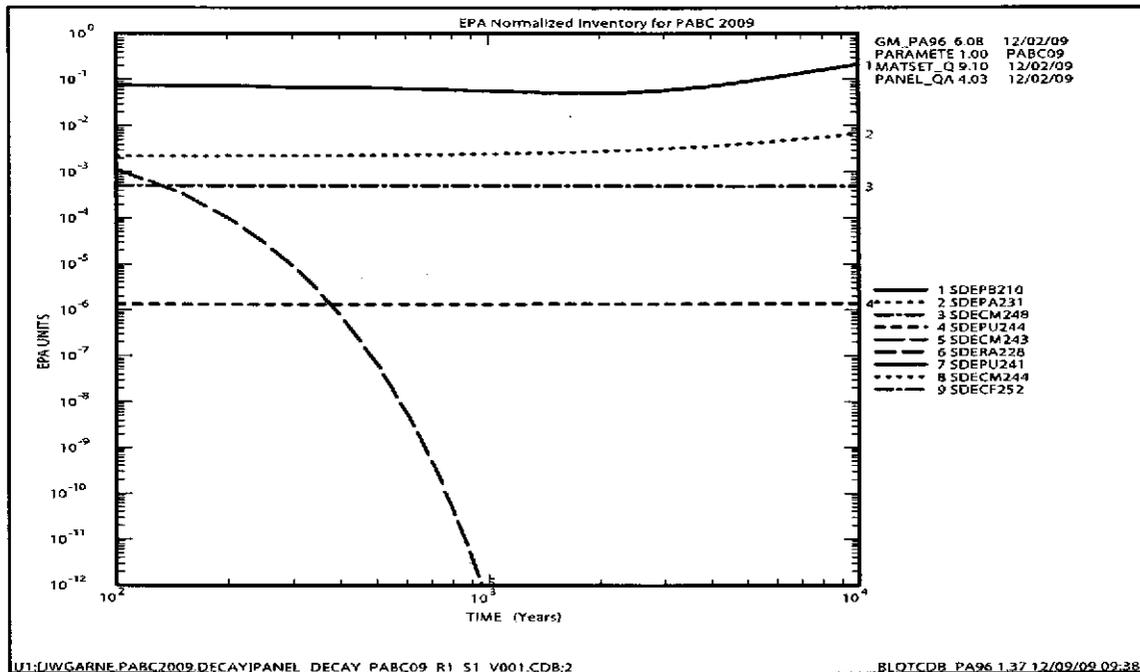
a) CRA-2009 PABC



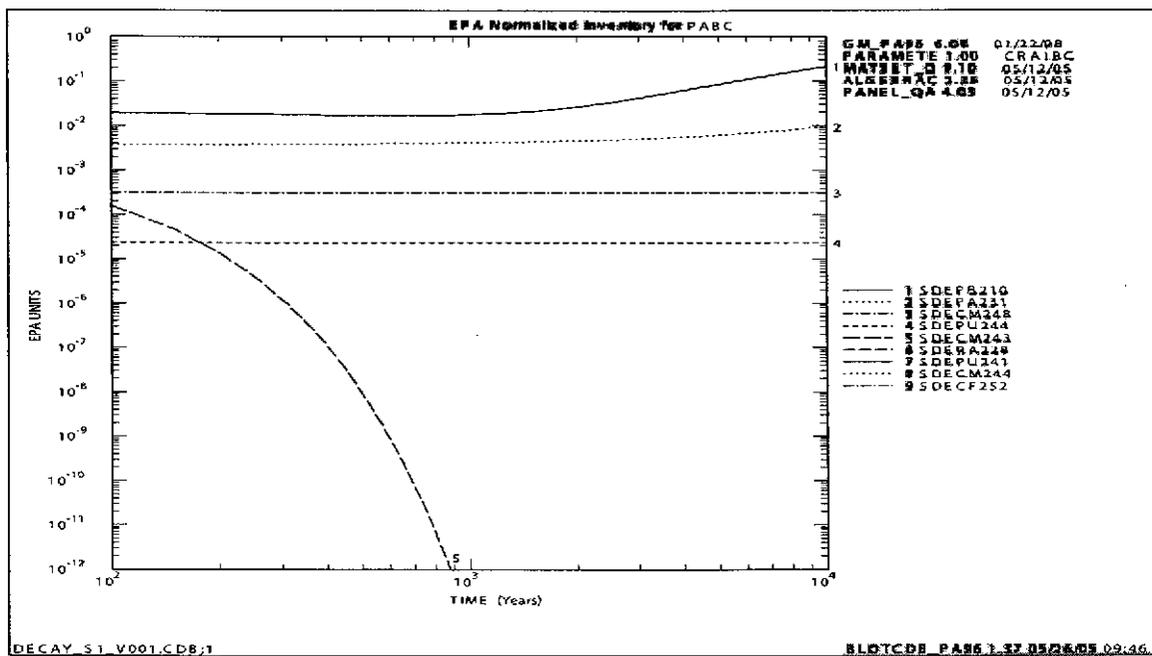
b) CRA-2004 PABC

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

Part a) shows results from the CRA-2009 PABC.
Part b) shows results from the CRA-2004 PABC.



a) CRA-2009 PABC

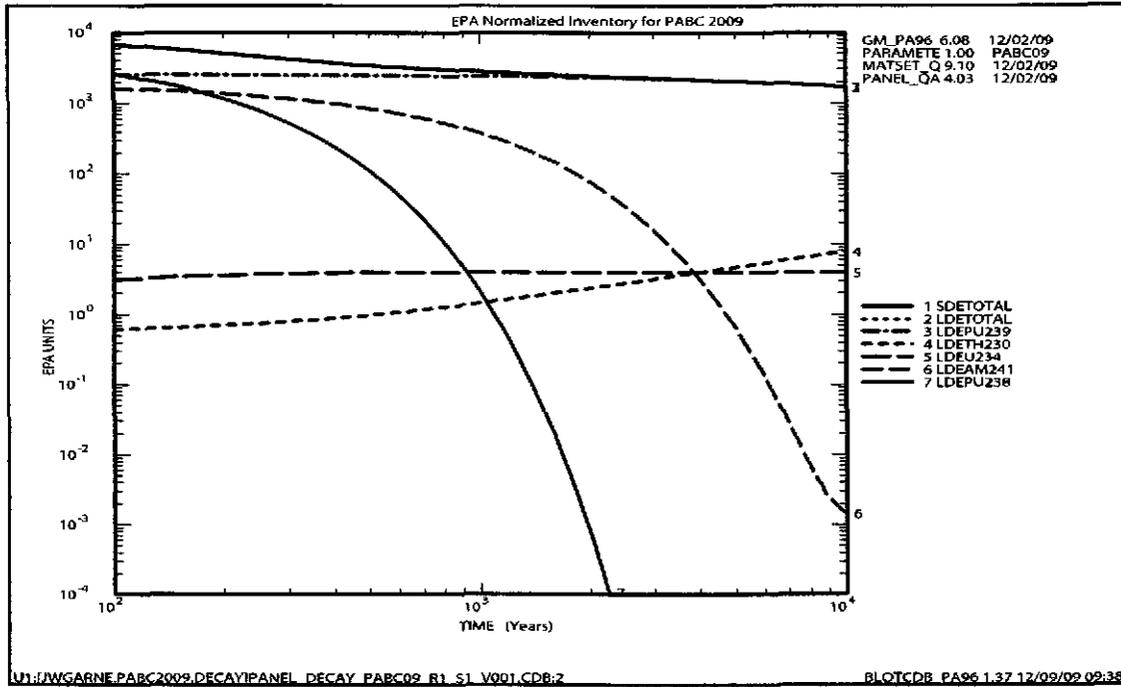


b) CRA-2004 PABC

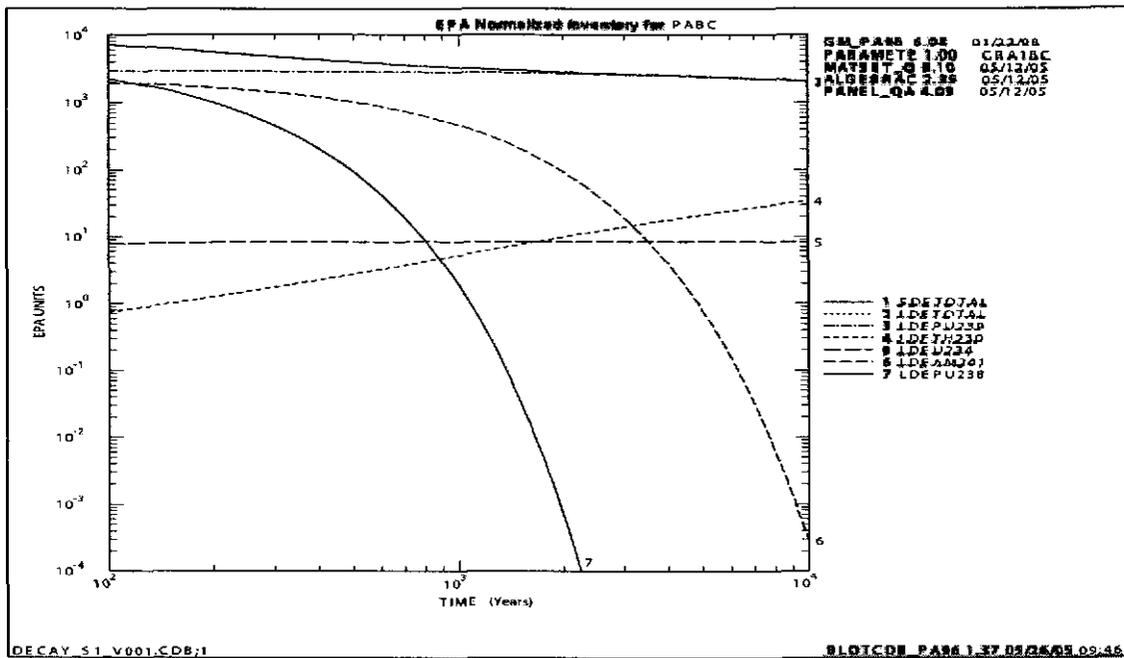
Figure 28. Time dependent inventories of various minor isotopes.

Part a) shows results from the CRA-2009 PABC.

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



a) CRA-2009 PABC



b) CRA-2004 PABC

Figure 29. Time dependent inventories of lumped isotopes.

Part a) shows results from the CRA-2009 PABC.
 Part b) shows results from the CRA-2004 PABC.

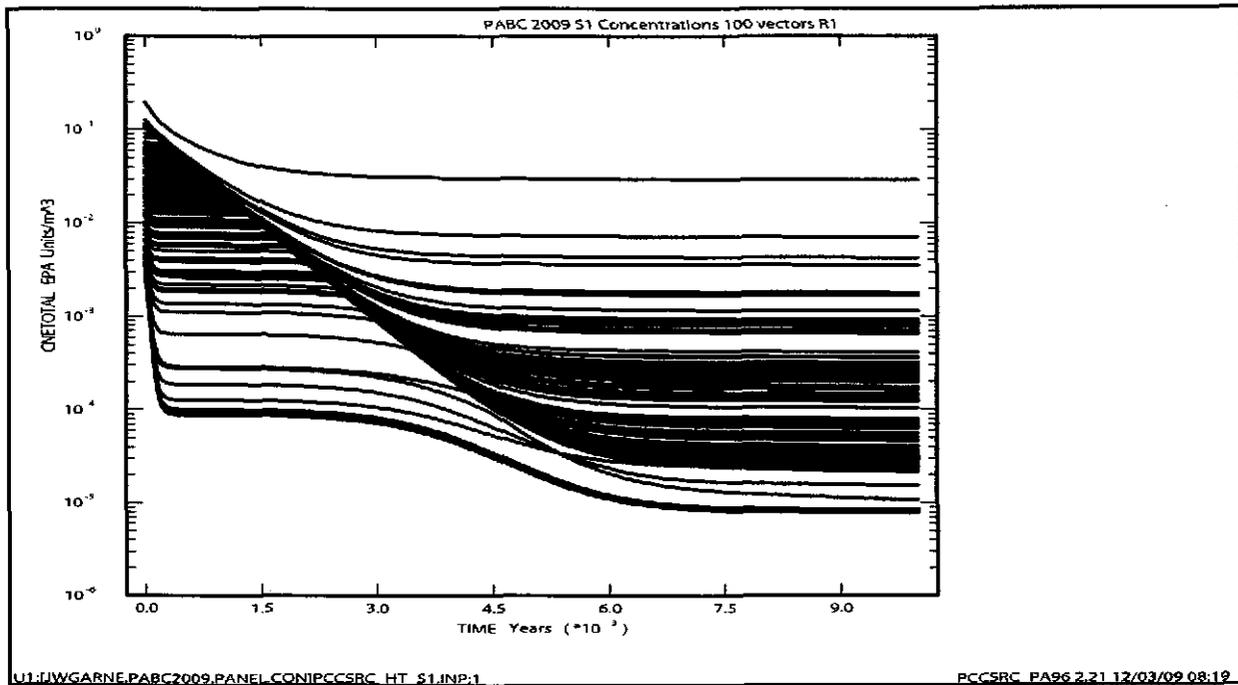
5.3 PANEL CONCENTRATIONS

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.

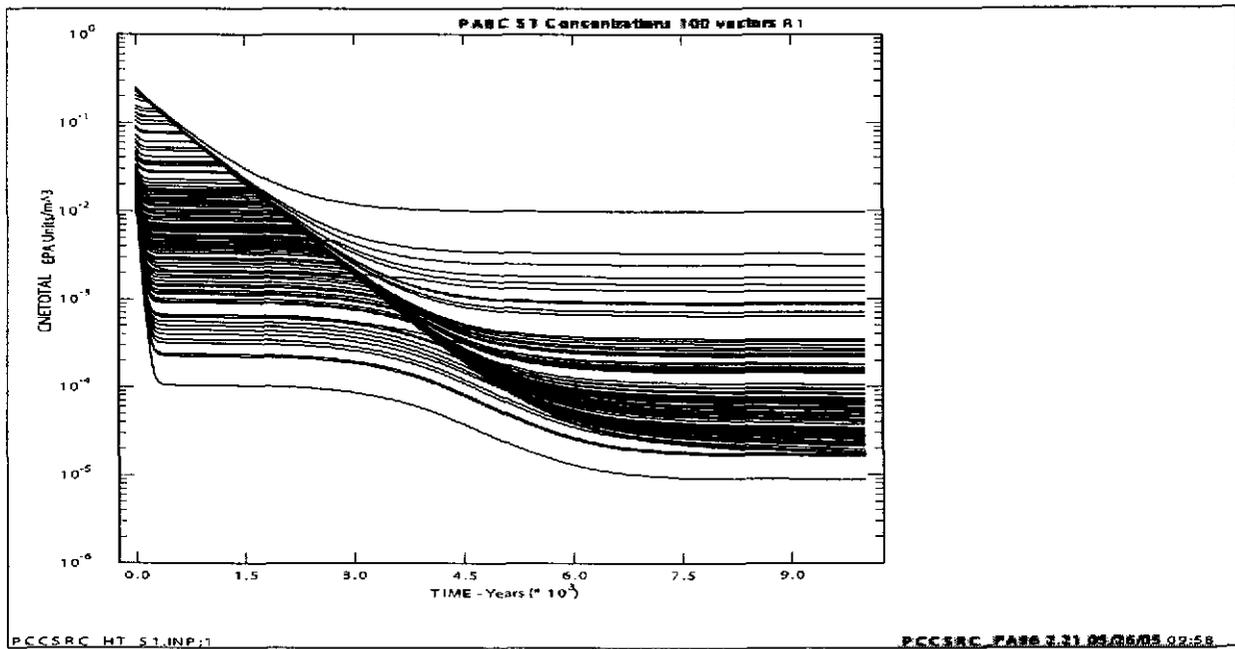
Figure 30 shows the total mobilized concentration (summed for the individual radionuclides from Table 11) in Salado brine in EPA units per cubic meter. Figure 35 shows the total mobilized concentration in Castile brine in EPA units per cubic meter. These concentration values are supplied to CCDFGF to 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 2000 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 35). 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-2009 PABC results for total mobilized concentrations show more variability (more spread in the curves) and greater values than seen in the CRA-2004 PABC results. More variability in the CRA-2009 PABC results is understandable because in general the variability in solubility was increased for the CRA-2009 PABC. The greater values in the CRA-2009 PABC are because of the increased solubility of the +III oxidation state.



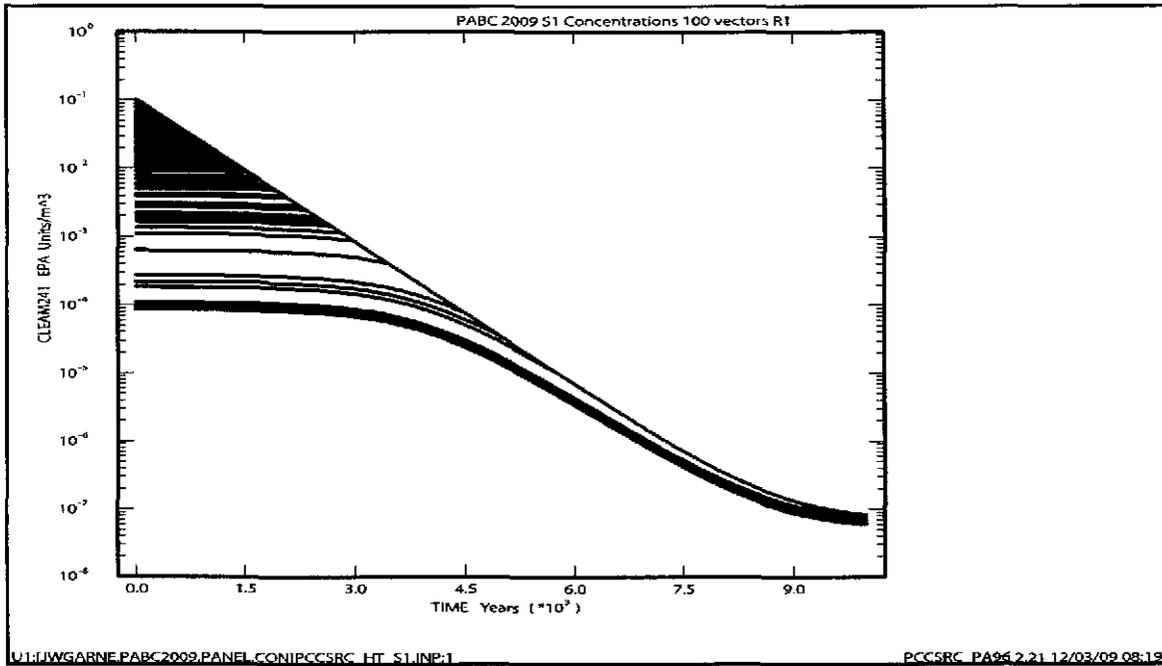
a) CRA-2009 PABC



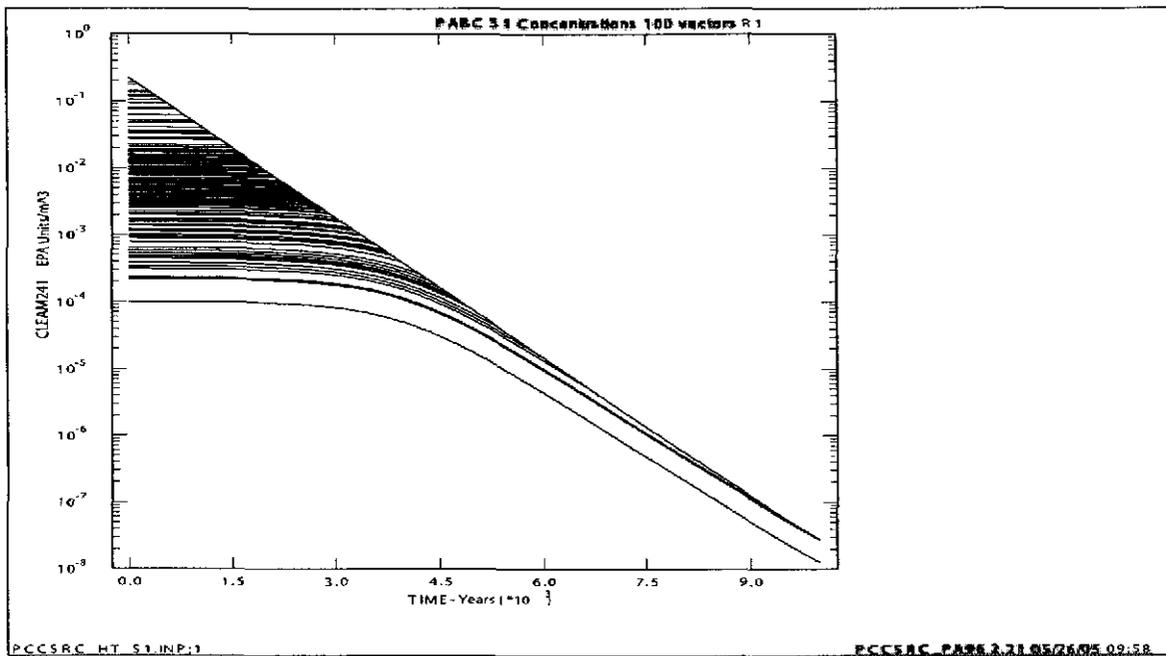
b) CRA-2004 PABC

Figure 30. Time dependent total concentrations in Salado brine.

Part a) shows results from the CRA-2009 PABC.
Part b) shows results from the CRA-2004 PABC.



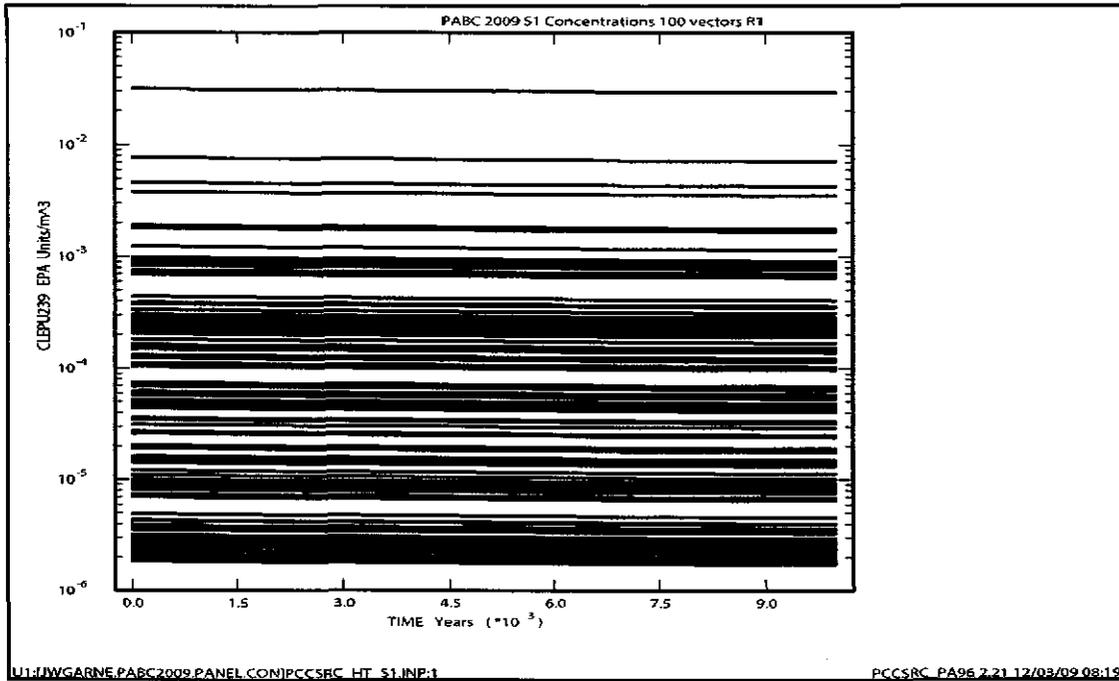
a) CRA-2009 PABC



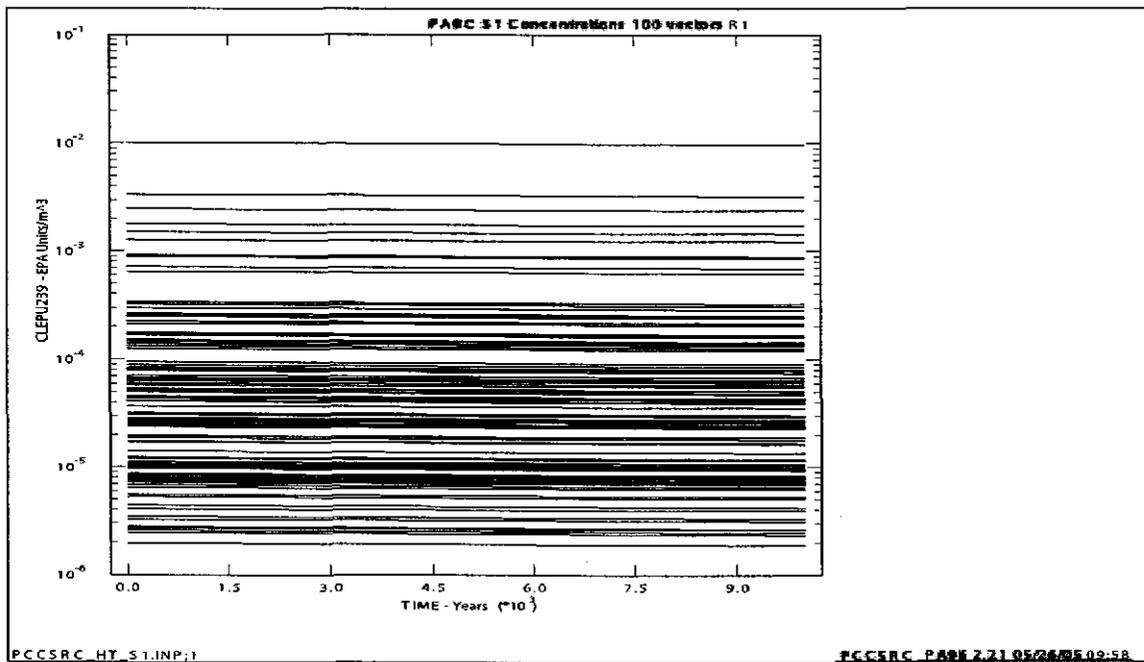
b) CRA-2004 PABC

Figure 31. Time dependent AM241L concentration in Salado brine.

Part a) shows results from the CRA-2009 PABC.
Part b) shows results from the CRA-2004 PABC.



a) CRA-2009 PABC

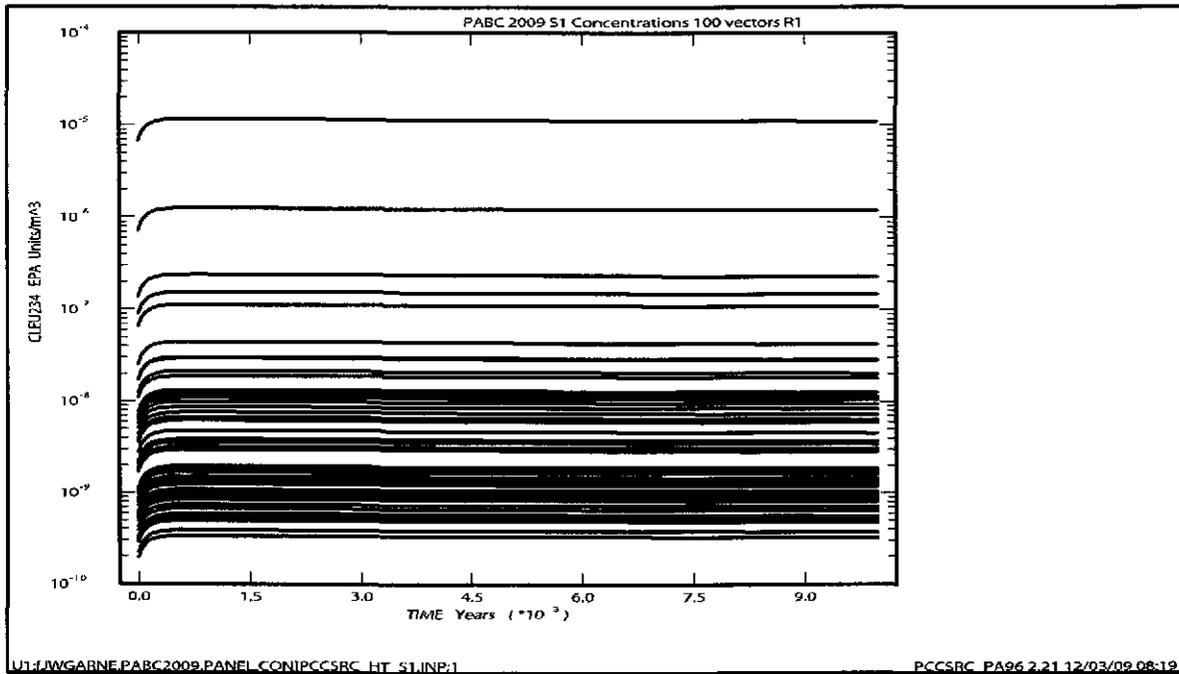


b) CRA-2004 PABC

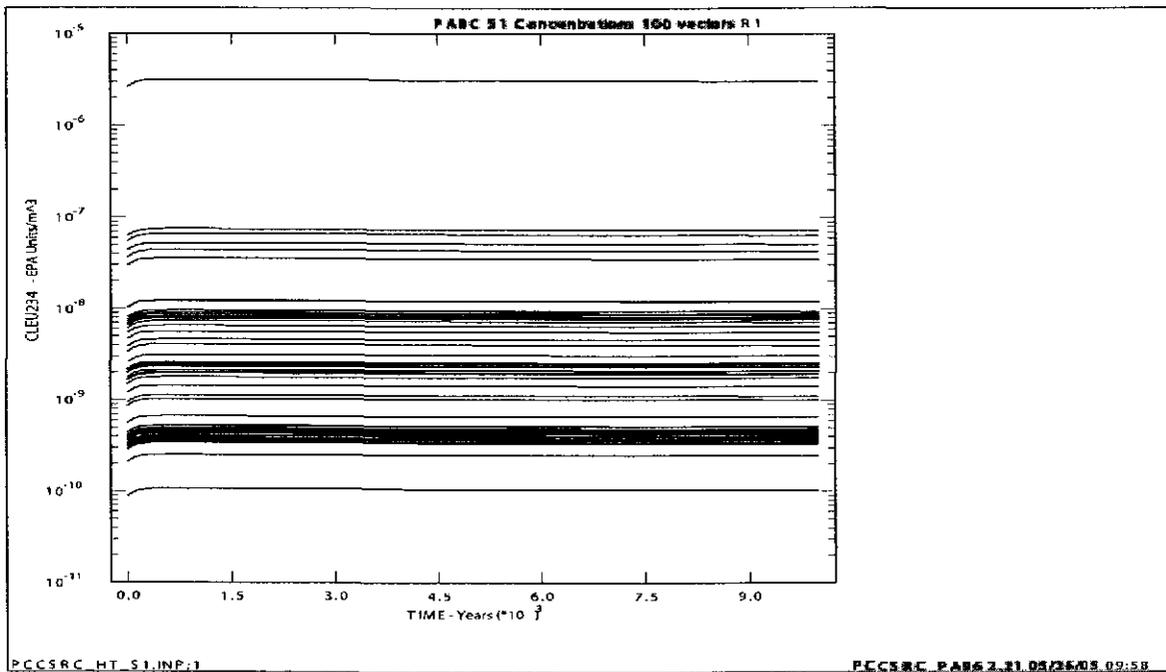
Figure 32. Time dependent PU239L concentration in Salado brine.

Part a) shows results from the CRA-2009 PABC.

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



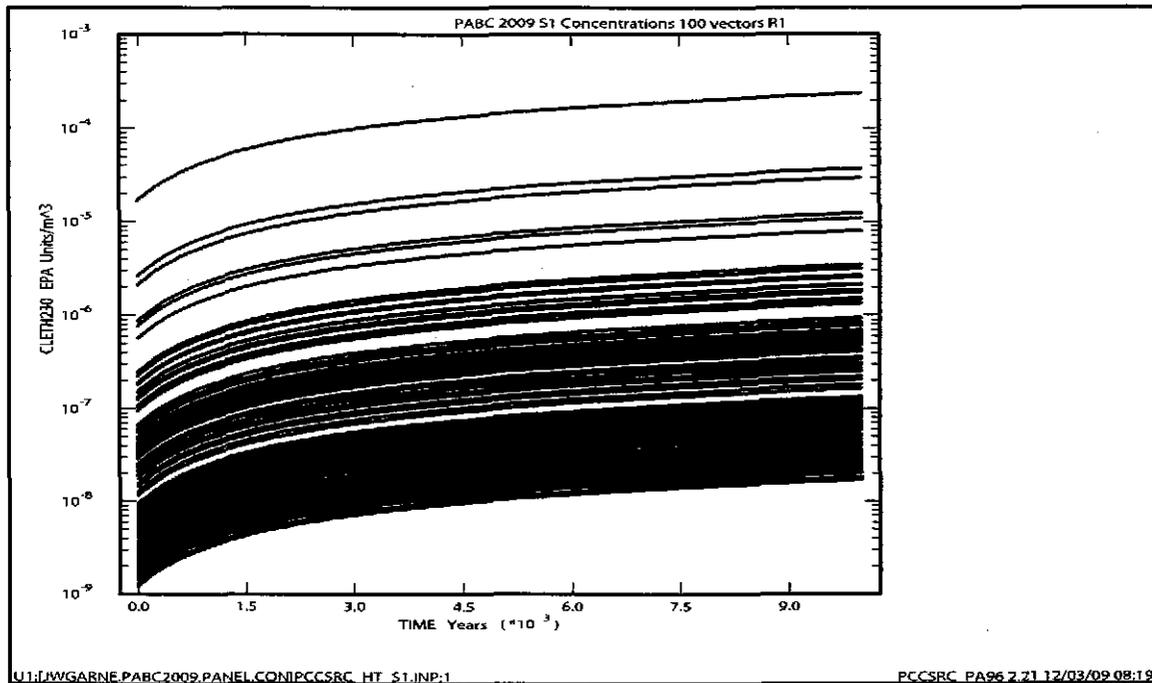
a) CRA-2009 PABC



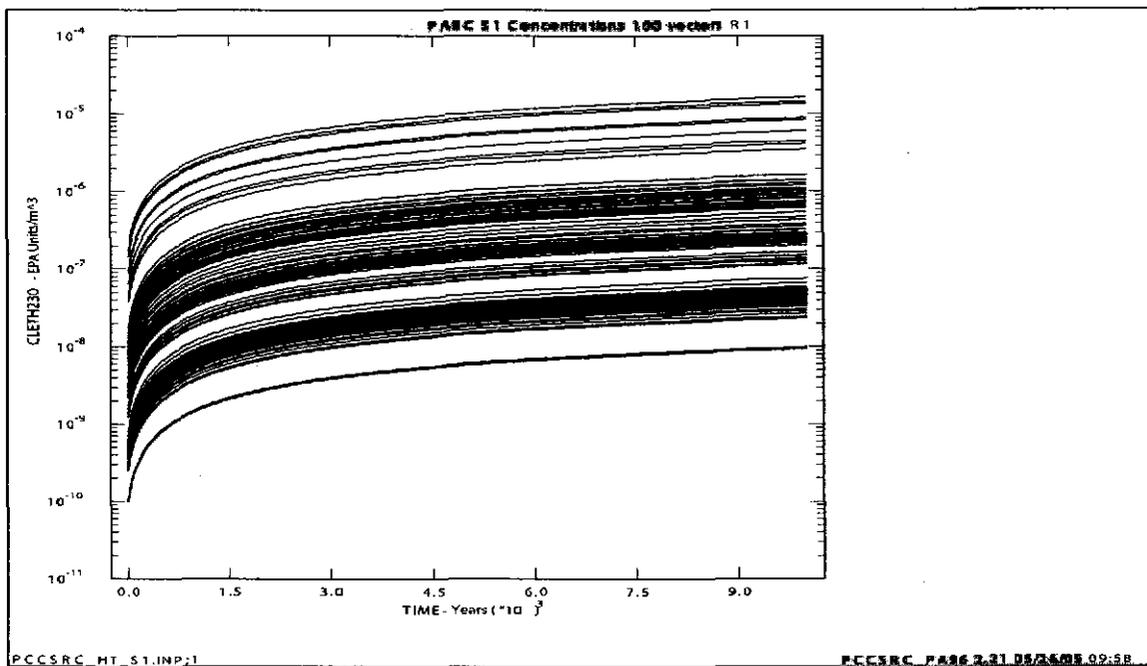
b) CRA-2004 PABC

Figure 33. Time dependent U234L concentration in Salado brine.

Part a) shows results from the CRA-2009 PABC.
Part b) shows results from the CRA-2004 PABC.



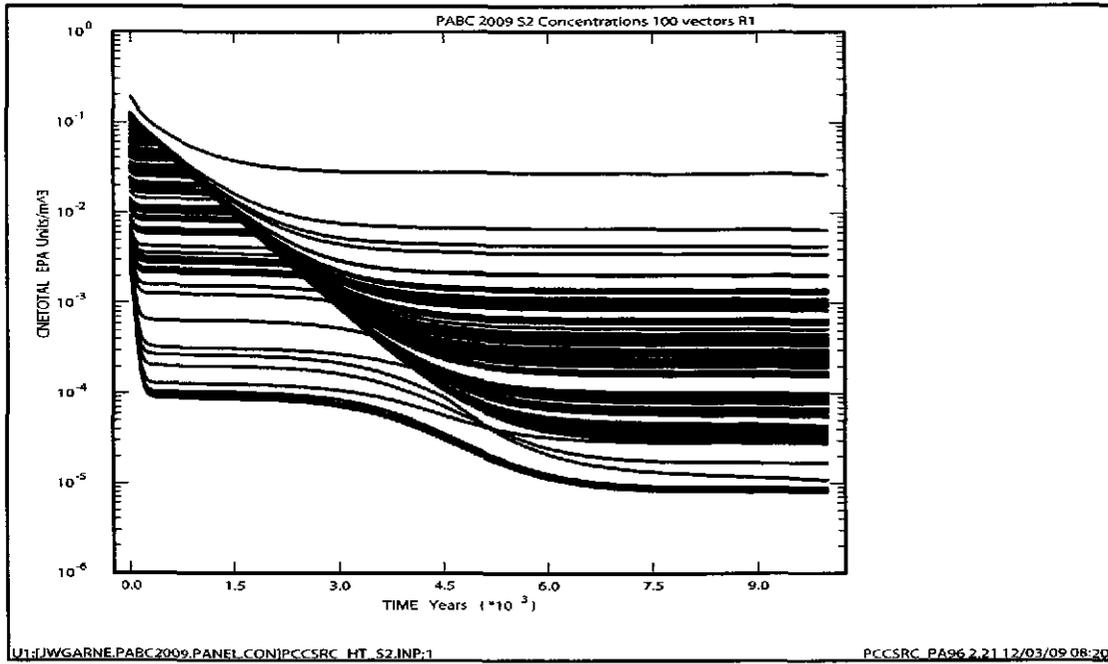
a) CRA-2009 PABC



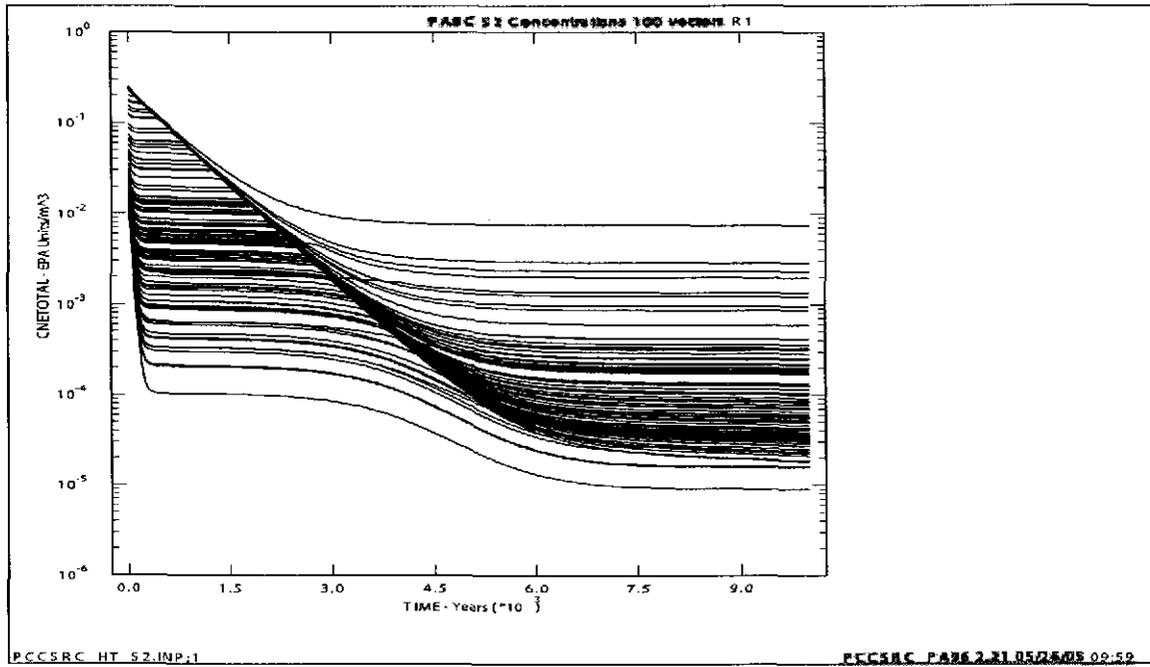
b) CRA-2004 PABC

Figure 34. Time dependent TH230L concentration in Salado brine.

Part a) shows results from the CRA-2009 PABC.
Part b) shows results from the CRA-2004 PABC.



a) CRA-2009 PABC

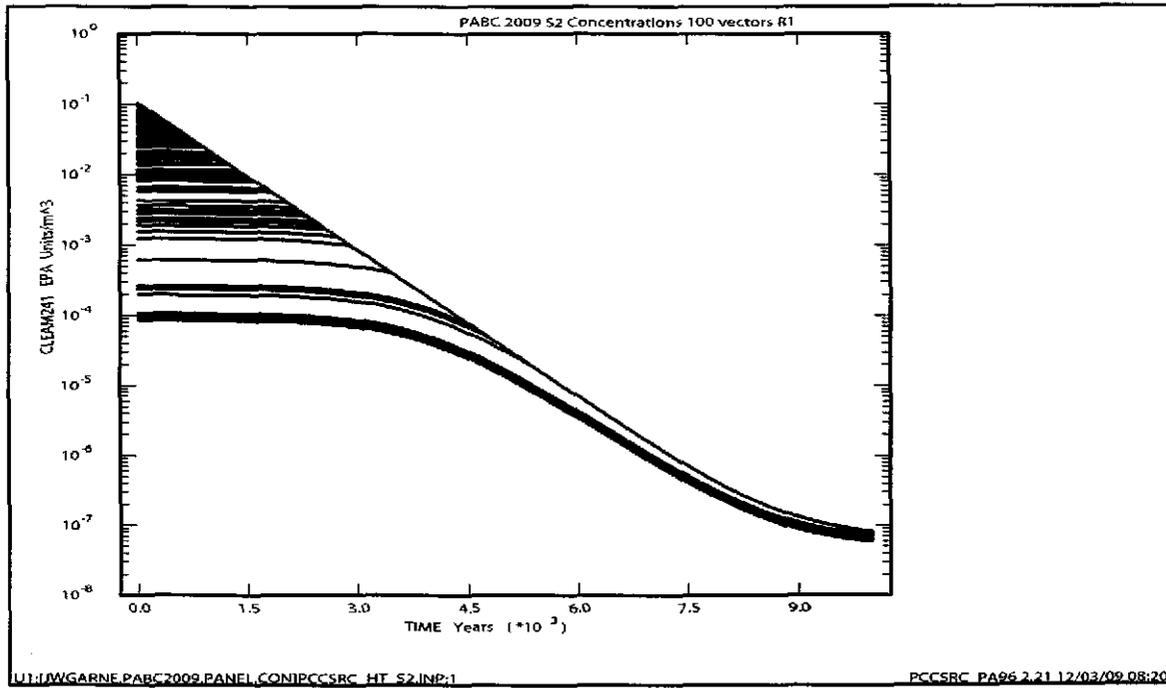


b) CRA-2004 PABC

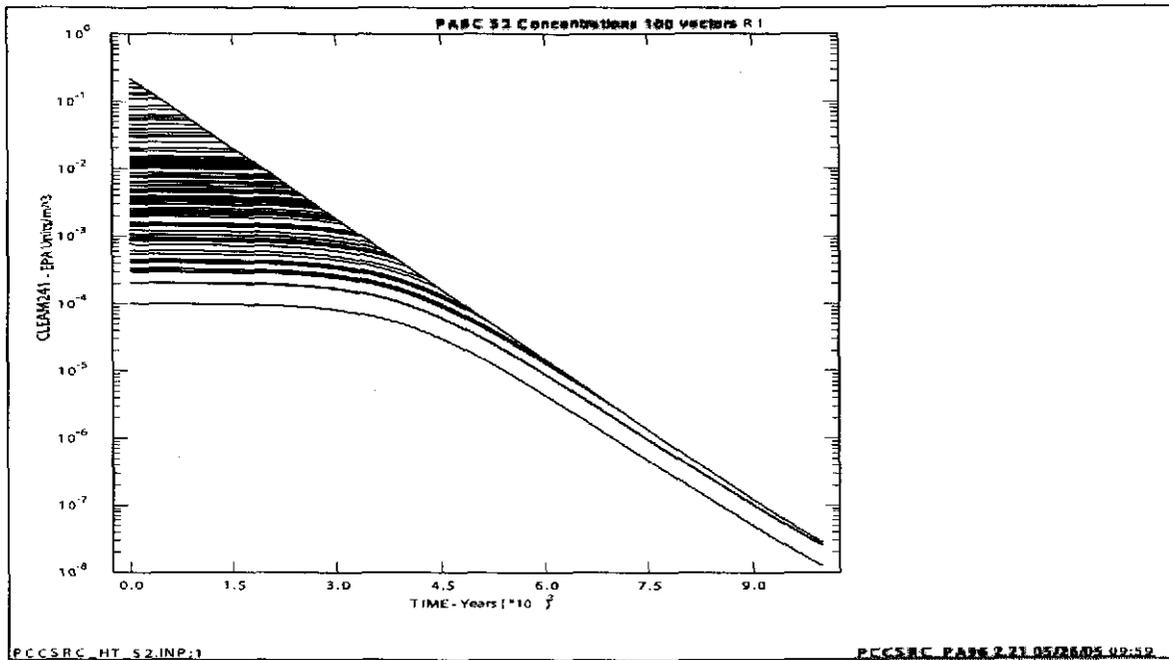
Figure 35. Time dependent total concentrations in Castile brine.

Part a) shows results from the CRA-2009 PABC.

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



a) CRA-2009 PABC

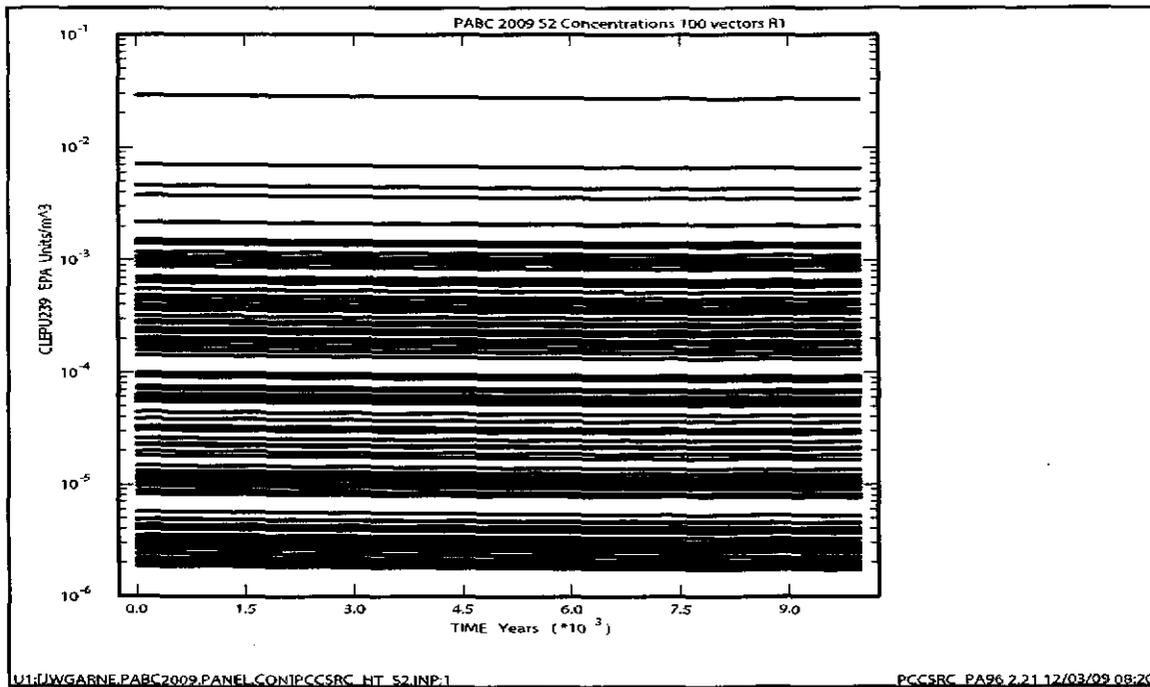


b) CRA-2004 PABC

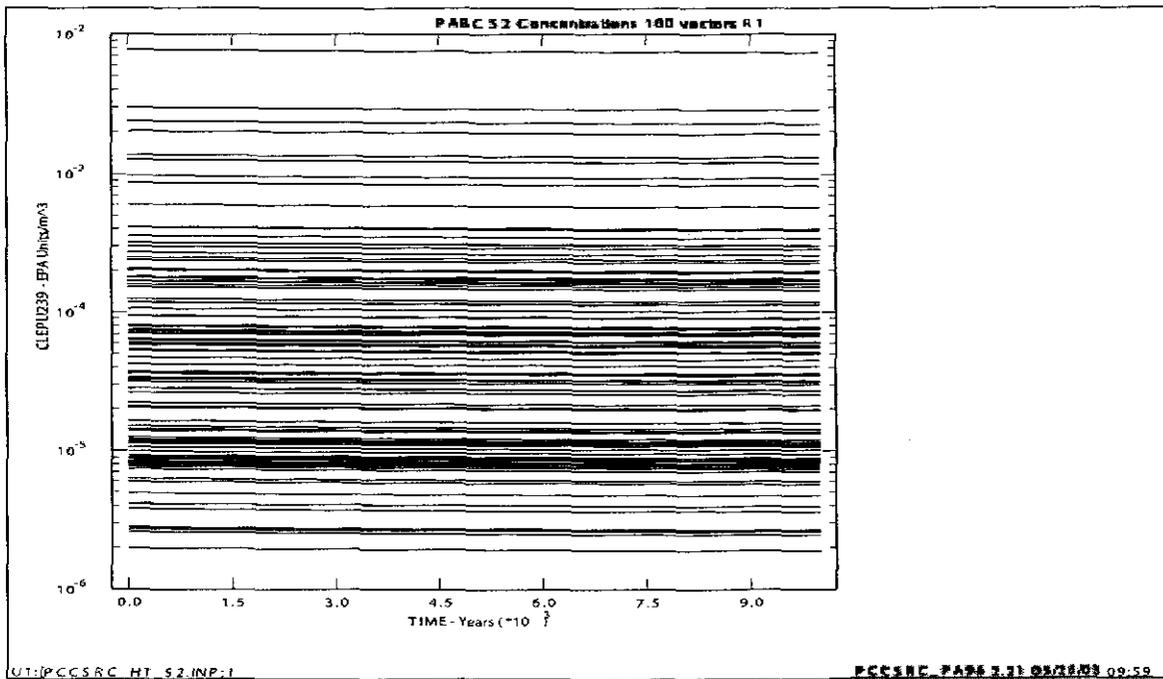
Figure 36. Time dependent AM241L concentration in Castile brine.

Part a) shows results from the CRA-2009 PABC.

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



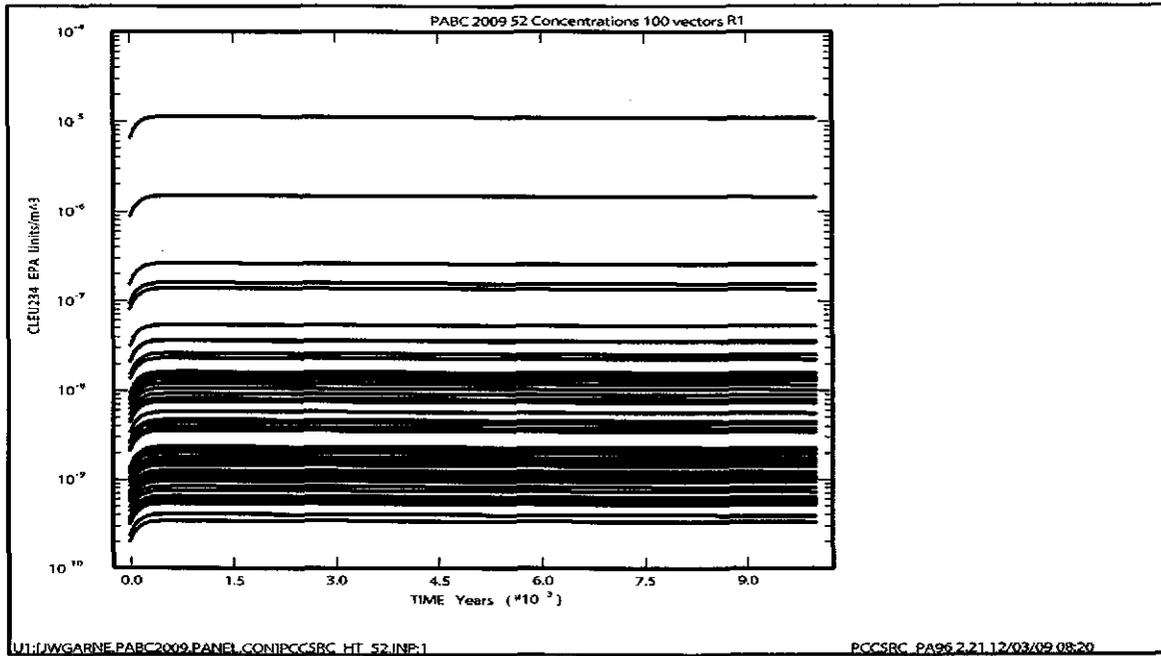
a) CRA-2009 PABC



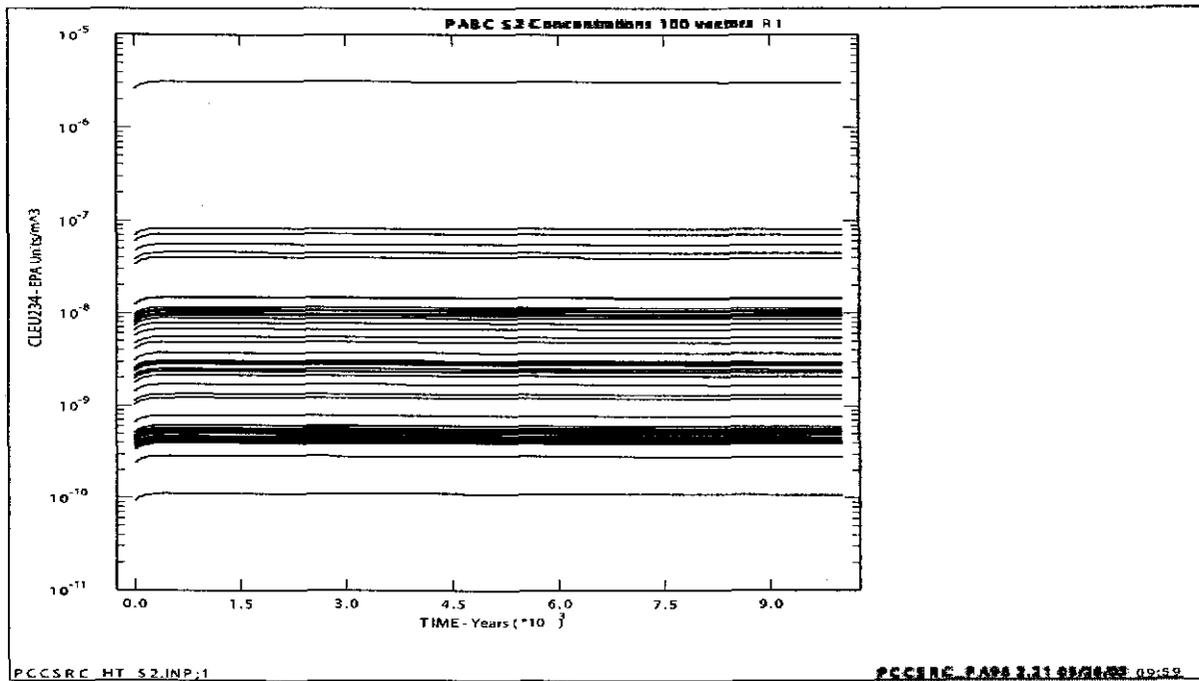
b) CRA-2004 PABC

Figure 37. Time dependent PU239L concentration in Castile brine.

Part a) shows results from the CRA-2009 PABC.
Part b) shows results from the CRA-2004 PABC.



a) CRA-2009 PABC

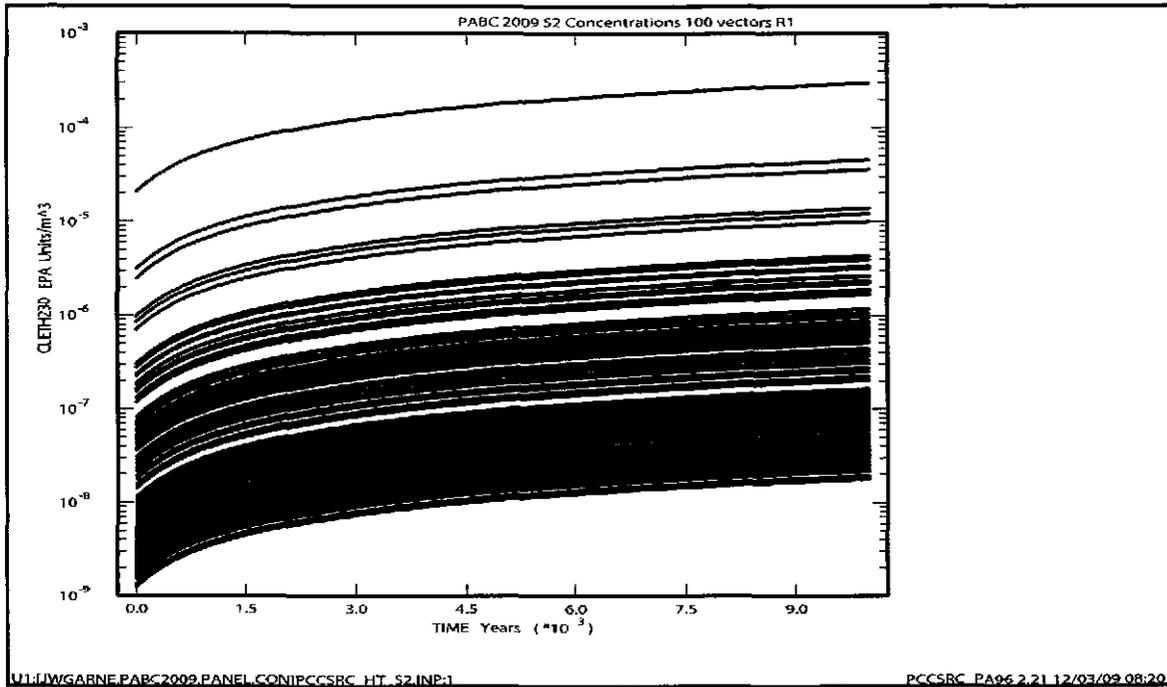


b) CRA-2004 PABC

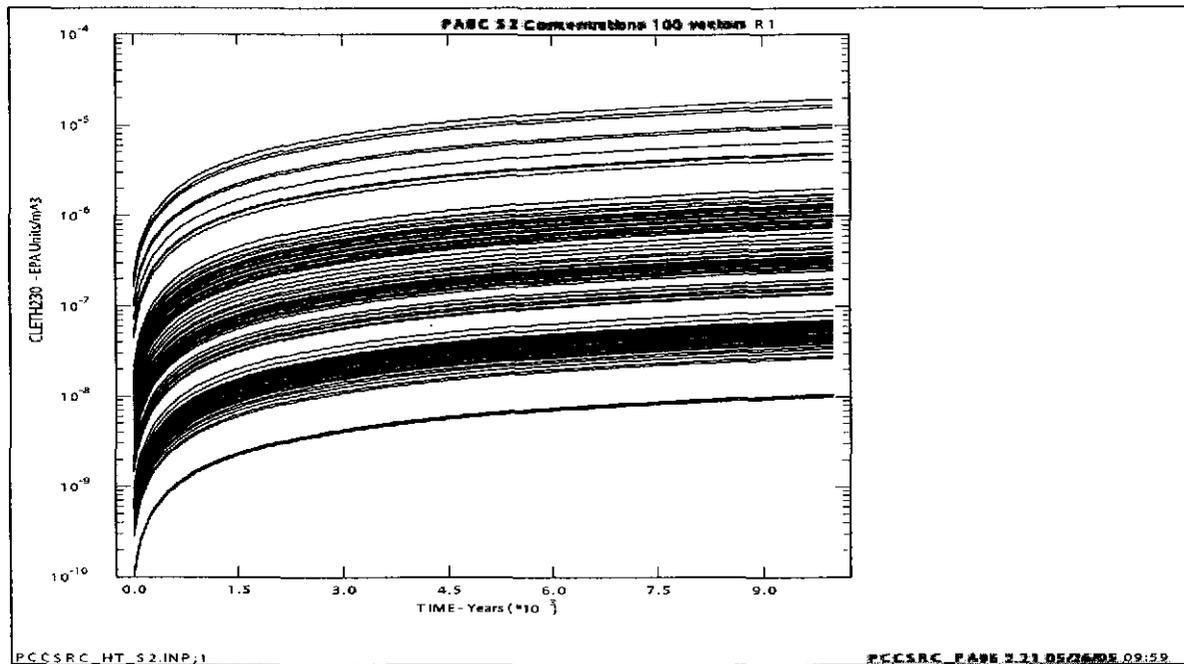
Figure 38. Time dependent U234L concentration in Castile brine.

Part a) shows results from the CRA-2009 PABC.

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



a) CRA-2009 PABC



b) CRA-2004 PABC

Figure 39. Time dependent TH230L concentration in Castile brine.

Part a) shows results from the CRA-2009 PABC.
Part b) shows results from the CRA-2004 PABC.

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 not included in this document. They are listed in the NUTS/PANEL 2009 (Ismail and Garner 2010).

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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).

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

Where $\left\{ TC_{brine}^{red/ox} \right\}_{NUTS}$ is the potential moles per liter mobilized for the lumped isotopes in Table 11 (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:

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

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:

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

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

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

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:

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

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:

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

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 for the CRA-2004 PABC. For the CRA-2009 PABC, these values are computed in the run scripts with the inclusion of a PANEL decay run and two ALGEBRA runs (Clayton 2009a).

APPENDIX B: INPUT FILES USED FOR PANEL CRA-2009 PABC CALCULATIONS

B.1 GM_PANEL_PABC09.INP

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

```
-----
! Analysis      : CRA-2009 PA Baseline Calculation (PABC) AP-145
! 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_PABC09.INP

The following MATSET input file is used to set the values needed for PANEL for the CRA-2009 PABC run for concentration and standard type runs.

```
!=====
! TITLE:      MATSET input file for PANEL (PABC09 for SOURCE term in PANEL runs)
! This input file is for the 2009 CRA Baseline Calculation (AP-145)
! ANALYSTS: J. W. GARNER
! CREATED:   June 24, 2009
! A modification of the 2004 PABC 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=BORRHOLE, &
              65=WAS_AREA

!MATERIALS 59-63 ARE LUMPED PARAMETERS FOR NUTS
!
PROPERTY MATERIAL=WAS_AREA, NAMES =PROBDEG
PROPERTY MATERIAL=Global,  NAMES =OKSTAT, DBRMINBV
PROPERTY MATERIAL=REFCON,  NAMES =YRSEC, VPANLEX, VREPOS
!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
PROPERTY MATERIAL=PU239L,  NAMES =InvCHD, InvRHD
PROPERTY MATERIAL=TH230L,  NAMES =InvCHD, InvRHD
PROPERTY MATERIAL=U234L,   NAMES =InvCHD, InvRHD
!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
!=====
*END
```

B.3 ALG1_PANEL_PABC09.INP

The First ALGEBRA file is for computing the mole fractions for lumped isotopes.

```
!
! This input file is for the PABC09 calculation, AP-145
! This file calculates the total moles of U,Pu, and Th and the mole fractions
! of U233+U234, PU238, and TH229+TH230, as well as the maximum mole fractions
!
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

LSD_U = -LOG10(ENVMAX(MF_U))
LSD_PU = -LOG10(ENVMAX(MF_PU))
LSD_TH = -LOG10(ENVMAX(MF_TH))

EXIT
```

B.4 ALG2_PANEL_PABC09.INP

The second ALGEBRA file is for cleaning up the mole fraction runs and setting property variables for LSOLDIFF and defining the reference volume for one panel.

```
! This input file is for the PABC09 Calculation, AP-145
! Sets the maximum over time of the Log Sol Difference
!
STEP 201

DELETE HISTORY

LIMIT BLOCK 60
LSOLDIFF = MAKEPROP(LSD_PU[T:1])

LIMIT BLOCK 62
LSOLDIFF = MAKEPROP(LSD_TH[T:1])

LIMIT BLOCK 63
LSOLDIFF = MAKEPROP(LSD_U[T:1])

! COMPUTE SCALEING FOR ONE PANEL AND PANEL MIN BRINE VOLUME
LIMIT BLOCK 2
INVSCALE=MAKEPROP(VPANLEX/VREPOS)
PANDEFVOL=MAKEPROP(DBRMINBV[B:1]*INVSCALE)
EXIT
```

B.5 ALG3_PANEL_PABC09.INP

The third ALGEBRA input file is used for all PANEL runs for the CRA-2009 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 PABC09 Calculations, AP-145  
!  
!  
! 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
```

B.6 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

MATERIAL	PROPERTY	VALUE	
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	1.6600E-03	SDB: SOLMOD3, SOLSOH
SOLMOD3	SOLCOH	1.5100E-06	SDB: SOLMOD3, SOLCOH
SOLMOD3	SOLVAR	7.2000E-02	SDB: SOLMOD3, SOLVAR
SOLMOD4	SOLSOH	5.6300E-08	SDB: SOLMOD4, SOLSOH
SOLMOD4	SOLCOH	6.9800E-08	SDB: SOLMOD4, SOLCOH
SOLMOD4	SOLVAR	-5.2000E-02	SDB: SOLMOD4, SOLVAR
SOLMOD5	SOLSOH	3.9000E-07	SDB: SOLMOD5, SOLSOH
SOLMOD5	SOLCOH	8.7500E-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	2.6000E+00	SDB: BOREHOLE, WUF
GLOBAL	OXSTAT	5.0000E-01	SDB: GLOBAL, OXSTAT
WAS_AREA	PROBDEG	1.2500E+00	SDB: WAS_AREA, PROBDEG

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