

Are the following appropriately defined and documented in the DD?

1. Software Name: PANEL
 2. Software Version ID (proposed): 4.0
 3. Document Version ID: 4:00
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|--|-------------------------------------|-----|--------------------------|----|-------------------------------------|-----|--------------------------|-----|
| 5. Major Software Components | <input checked="" type="checkbox"/> | Yes | <input type="checkbox"/> | No | <input type="checkbox"/> | N/A | <input type="checkbox"/> | N/R |
| 6. Theoretical Basis | <input checked="" type="checkbox"/> | Yes | <input type="checkbox"/> | No | <input type="checkbox"/> | N/A | <input type="checkbox"/> | N/R |
| 7. Embodied Mathematical Model | <input checked="" type="checkbox"/> | Yes | <input type="checkbox"/> | No | <input type="checkbox"/> | N/A | <input type="checkbox"/> | N/R |
| 8. Major Control Flow | <input checked="" type="checkbox"/> | Yes | <input type="checkbox"/> | No | <input type="checkbox"/> | N/A | <input type="checkbox"/> | N/R |
| 9. Control Logic | <input checked="" type="checkbox"/> | Yes | <input type="checkbox"/> | No | <input type="checkbox"/> | N/A | <input type="checkbox"/> | N/R |
| 10. Data Structures | <input checked="" type="checkbox"/> | Yes | <input type="checkbox"/> | No | <input type="checkbox"/> | N/A | <input type="checkbox"/> | N/R |
| 11. Allowable or Prescribed Ranges for Inputs and Outputs | <input type="checkbox"/> | Yes | <input type="checkbox"/> | No | <input checked="" type="checkbox"/> | N/A | <input type="checkbox"/> | N/R |
| 12. Verifiability
Is the design verifiable through testing or other means? | <input checked="" type="checkbox"/> | Yes | <input type="checkbox"/> | No | <input type="checkbox"/> | N/A | <input type="checkbox"/> | N/R |
| 13. Consistency and Traceability
Is the design consistent with and traceable to the software's requirements? | <input checked="" type="checkbox"/> | Yes | <input type="checkbox"/> | No | <input type="checkbox"/> | N/A | <input type="checkbox"/> | N/R |
| 14. Technical Feasibility
Is the design technically feasible? | <input checked="" type="checkbox"/> | Yes | <input type="checkbox"/> | No | <input type="checkbox"/> | N/A | <input type="checkbox"/> | N/R |
| 15. Implementation
Is the design presented in sufficient detail to allow for implementation as computer software? | <input checked="" type="checkbox"/> | Yes | <input type="checkbox"/> | No | <input type="checkbox"/> | N/A | <input type="checkbox"/> | N/R |

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WIPP PA
Design Document

for

PANEL (Version 4.00)

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1.0 INTRODUCTION

The Waste Isolation Pilot Plant (WIPP) located in southeastern New Mexico is being developed by the U.S. Department of Energy (DOE) as a disposal facility for transuranic (TRU) waste. The WIPP must comply with various environmental regulations, including 40 CFR 191, Subpart B, "Environmental Radiation Protection Standards for the Management and Disposal of Spent Nuclear Fuel, High-Level and Transuranic Radioactive Wastes," and 40 CFR 268.6, "Petitions to Allow Land Disposal of a Waste Prohibited Under Subpart C of Part 268." As part of the development process for the WIPP, a sequence of Performance Assessments (PAs) has been carried out by Sandia National Laboratories (SNL) to organize knowledge currently available about the WIPP and to provide guidance for future research and development efforts.

An important part of the 1996 Compliance Certification Application (CCA) for the WIPP is the complementary cumulative distribution function (CCDF) for comparison with the release limits specified in 40 CFR 191.13. In the 1991 and 1992 WIPP PAs, this CCDF was constructed with a procedure based on importance sampling. To provide greater flexibility and improved use of available information, the CCA used a Monte Carlo procedure for the CCDF construction program (CDFGF).

The PANEL program was used in the 1996 CCA and the 1997 Performance Assessment Verification Test (PAVT) calculations. Before these calculations were performed, it was necessary to run the Source Term ALGEBRA file to calculate the solubility information needed for PANEL and NUTS. It was also necessary to complete an ALGEBRA run after each PANEL run to convert to the lumped isotopes needed for input to CCDFGF. A separate ALGEBRA run was needed to convert a different type of PANEL run to concentration calculations. These concentration calculations were also needed for CCDFGF.

A criticism of PANEL was that the half-lives and atomic weights were hard-wired in PANEL and not obtained from the WIPP database. Another criticism was that strontium and cesium were not considered for mobilization.

In order to eliminate these criticisms and also eliminate the ALGEBRA runs that followed each PANEL run, it was necessary to modify PANEL. At the same time, the source term calculations that were done with ALGEBRA were to be added to PANEL. The solubility source term theory and ALGEBRA implementation are described in *Analysis Package for Salado Transport* (Stockman 1996).

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In PANEL, the source term calculations will be performed first. These values are output to the Computational Data Base (CDB) as Property values. Property values are part of the header section of the CDB and must be added before any time-dependent values are written to the CDB. Then, PANEL will run as before, outputting history variables. All isotope output will be in three different units: cumulative discharged mass in kg; cumulative discharge in curies; and cumulative discharge in EPA units. Lumped isotope output (i.e., Am241L, Pu239L, Pu238L, U234L, and Th230L) are also output in the three different units.

In the run sequence, PANEL will have to be run before NUTS. This is because NUTS needs the Source Term variables added by PANEL.

Parts of the analysis package for Salado transport calculations for the CCA are included here for completeness as Chapter 2 and Appendixes A through E. Appendix D and Appendix F are ALGEBRA files that were run after previous versions of PANEL; these files are not used with PANEL 4.0. Appendix B is the ALGEBRA file for the CCA Source Term; it is also not used with PANEL 4.0.

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2.0 ANALYSIS PACKAGE FOR SALADO TRANSPORT

2.1 The Types of Data Required by NUTS and PANEL

In the 1996 CCA PA, both NUTS and PANEL assumed, at each timestep, instant mobilization of radioisotopes (1) up to their mobilization limits if inventory was sufficient, or (2) up to their inventory limits if inventory was insufficient (below effective solubility limits). NUTS applied the rules within each grid block, whereas PANEL applied them within the single waste panel it considered. The total inventory contained within the repository was assumed to be homogeneously and uniformly distributed throughout. NUTS assigned portions of the inventory to each grid block on the basis of that block's volume fraction of the repository as a whole. PANEL did the same, but it treated an entire waste panel as its one and only grid block. Since PANEL now takes the place of the Source Term ALGEBRA CDB, it will provide NUTS with (1) the total inventory of all its lumped equivalent isotopes, the half-lives and atomic weights of those isotopes, so NUTS could perform its decay calculations and (2) the elemental effective solubility data required to mobilize the lumped equivalent isotopes.

2.2 "Effective Solubility"—Combining Dissolution and Colloidal Mobilization

In addition to dissolution, the Actinide Source Term Program determined that actinides may mobilize within or on colloids (Papenguth 1996 a, b, c, d). In general, dissolved and colloidal species may transport at different rates because of differences in their molecular-diffusion, sorption, and size-exclusion effects (filtration and hydrodynamic chromatography¹). Filtration was not included in either NUTS or PANEL, although its effects could have been approximated using NUTS' sorption models. However, sorption to fixed surfaces, molecular diffusion, and dispersion options were all intentionally omitted from the 1996 CCA mobilization codes. Hydrodynamic chromatography may increase colloid transport rates over dissolved transport rates by factors up to two for theoretically perfect colloid-transport conditions. However, in practice, observed increases are usually much less, and well within the uncertainty of the WIPP calculated flow fields. Therefore, this minor increase in transport rate of colloids over dissolved species was not modeled. Because the mechanisms that differentiate the transport of dissolved and colloidal species were turned off in the CCA calculations, these species were combined for transport within the Salado Formation. The combined mobilized actinide was assigned an

¹ Hydrodynamic chromatography refers to the tendency of small suspended particles to migrate transversely within an advective current so as to congregate in the high-speed core of the flow field, which is usually near the center of a conduit. As a result, they travel not at the average speed, which is the advective speed, but rather at speeds approximating the maximum speed that occurs in the cross-sectional profile.

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“effective solubility,” which is equal to the sum of the maximum dissolved concentration plus the maximum mobilized concentration of the actinide on each of four colloid types: humic, microbe, mineral fragment, and actinide intrinsic.

2.3 The Effects of Brine Composition on Solubility

The Actinide Source Term Program found that actinide solubility and maximum actinide concentrations on humic colloids may vary significantly with oxidation state, pH, carbonate concentration, and brine composition. The pH and carbonate concentration within the repository was expected to be well controlled by the MgO backfill (Wang 1996), leaving brine composition and oxidation state as the major determinants of solubility. Brine composition is described in the following paragraphs; oxidation state is described in Section 2.4.

Depending on the nature of future human intrusions, brine may enter the repository from three sources. The six human-intrusion scenarios considered in the calculations can be categorized into three groups: (1) no human intrusion, (2) intrusion through the repository and into the Castile Formation intersecting a pressurized brine pocket, and (3) intrusion through the repository but not into a pressurized brine pocket. Under all scenarios, brine will flow from the surrounding Salado Formation, through the disturbed rock zone (DRZ), and into the repository in response to the pressure difference between the repository at closure and the surrounding formation. In scenarios where a borehole is drilled into the repository but not into an underlying brine pocket, brine may flow down the borehole from the Rustler and Dewey Lake Formations. In scenarios where a pressurized Castile brine pocket is penetrated, brine from the Castile Formation may flow up the borehole into the repository.

The brines in these three formations have considerably different compositions, and the solubilities of actinides are significantly different in each of the three end-member compositions. For example, the solubilities of actinides in each oxidation state in Salado and Castile brines provided by the Actinide Source Term Program (Siegel 1996) are shown in Table 2-1.

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Table 2-1. Solubilities (moles/liter) of the Actinide Oxidation States in Salado and Castile Brines Controlled by the MgO/MgCO₃ Buffer

Brine Source	Oxidation State			
	+III	+IV	+V	+VI
Salado	5.82×10^{-7}	4.4×10^{-6}	2.3×10^{-6}	8.7×10^{-6}
Castile	6.52×10^{-8}	6.0×10^{-9}	2.2×10^{-6}	8.8×10^{-6}

The composition of the more dilute brines of the Rustler and Dewey Lake Formations are expected to change rapidly upon entering the repository due to fast dissolution of host Salado Formation minerals (about 93.2 percent halite and about 1.7 percent each of polyhalite, gypsum, anhydrite, and magnesite, Brush 1990). EQ3/6 calculations (see Appendix A) titrating Salado rock into a dilute brine show that the brine becomes saturated with gypsum, anhydrite, and magnesite before it saturates with halite. When halite saturates, the brine composition is very similar to that of Castile brine. The brine saturates with polyhalite only when 100 times more Salado rock is added to the system than is needed to saturate the brine with halite. The resulting brine would then have a composition within the range observed for Salado brines. Thus, if dilute brines dissolve only the surfaces of the repository, they will attain Castile-like compositions. But, if they circulate through the Salado Formation after saturating with halite, they may attain compositions similar to Salado brine. Similarly, if Castile brine circulates through enough host rock, it may also approach Salado brine composition. In either case, the actual brine within the repository may be described as a mixture of the two concentrated brine "end members": Salado and Castile. The brine ratio in this mixture is, however, difficult to quantify because it is both temporally and spatially variable. Only in the undisturbed scenario is the mixture well defined as 100 percent Salado brine over the 10,000-year time period.

For a panel intersected by a borehole, the BRAGFLO calculations show that the ratio of brine inflow that enters via the borehole versus inflow from the surrounding DRZ is variable both in time and sampled realization. This ratio was the only measure of brine mixing available during the Source Term ALGEBRA calculations in the 1996 CCA PA. The ratio is somewhat crude because it (1) did not account for brine composition changes that occurred when water was consumed by corrosion reactions, (2) did not resolve the details of flow, diffusion, and brine interaction with internal pillars and the DRZ, and (3) was an average over the entire panel. It is expected that the fraction of Salado brine within the mixture will be high in areas of the repository distant from the borehole and much lower near the borehole. Because radioisotope transport up the borehole is required for significant release, it is the solubility of radioisotopes

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near the borehole that is most important. Given these uncertainties, and NUTS' requirement for time-independent solubilities, calculation of brine mixing was not attempted in the CCA calculations. Instead, actinide solubilities in Castile brine were used for scenarios where a borehole hit a pressurized brine pocket, and solubilities in Salado brine were used for scenarios where it did not. This simplification should bracket the range of behavior of the repository and should therefore suffice for CCDF calculations.

2.4 The Effects of Oxidation State on Actinide Solubility

The solubilities of actinides are dependent on actinide oxidation state distributions (Weiner 1996). The oxidation state distributions are expected to be determined by reactions of the actinides with the major components of the waste. Microbially mediated reactions with the organic waste and reactions with the $\text{Fe}(0)^2$ and resulting dissolved $\text{Fe}(+II)$, are expected to have the largest impact on the oxidation state distribution, but because the kinetics of these reactions are uncertain, it is impossible to define a single redox potential (Eh) for the repository. It is expected that the redox state of the repository may range from "reducing" to "extremely reducing," and experiments have shown that the more highly oxidized actinide oxidation states do not persist (Weiner 1996). The most likely persistent oxidation states for the six actinides are shown in Table 2-2 (Weiner 1996):

Table 2-2. Most Likely Persistent Oxidation States for Six Actinides

Actinide	Oxidation State
Am	+III
Cm	+III
Np	+IV, +V
Pu	+III, +IV
Th	+IV
U	+IV, +VI

For U, Np, and Pu, two oxidation states are likely to persist depending on the reducing power of the waste. It is expected that under likely repository conditions, one oxidation state will dominate the dissolved concentration of each actinide, with the more reduced state dominating the solubility if the repository is "extremely reducing" and the more oxidized state dominating if the repository is "reducing." The uncertainty in the repository reducing power and resultant

² The number in parenthesis is the oxidation state. $\text{Fe}(0)$ is iron metal.

oxidation state distribution is characterized in CCA modeling by the "OXSTAT" parameter. OXSTAT is sampled uniformly from 0 to 1. When the sampled OXSTAT is less than or equal to 0.5, the solubility of the lower oxidation state (U(+IV), Np(+IV), Pu(+III)) is used. When OXSTAT is greater than 0.5, the solubility of the higher oxidation state (U(+VI), Np(+V), Pu(+IV)) is used.

2.5 Choosing Source-Term Parameters for Sampling/Parameter Correlation

Up to 30 Source Term parameters were supplied with distributions, but many of them were expected to have limited impact on the final CCDF. The most important parameters were expected to be the oxidation state parameter (OXSTAT) and the solubilities of Pu(+III), Pu(+IV), and Am(+III) in the two brine end members.

A single distribution was used to model the uncertainty of the solubility of each oxidation state of all actinides in both brines (Bynum 1996). The cumulative distribution, as entered into the parameter database, is shown in Table 2-3 and plotted using SigmaPlot in Figure 2-1. However, the amount of correlation between the solubilities of the actinides was uncertain. Some factors that cause uncertainty in the solubility affect all oxidation states of all actinides similarly, and some factors affect only some actinides or some oxidation states. For example, uncertainties in the sulfate concentrations have more effect on the uncertainty of the solubility of the actinides in the IV oxidation state, while uncertainties in the ionic strength have a more generalized effect of increasing the uncertainty in the stability of any highly charged species. In nature, solubilities show correlation due to redox effects as well as major ion-concentration effects. It is therefore expected that solubilities within the WIPP should show some, but not complete, correlation. The use of end-member brines in the calculations results in a correlation of solubilities due to ionic-strength and major-ion effects, and the use of the oxidation state parameter results in a correlation due to redox effects. Because it was not possible to estimate the amount of correlation due to effects on solubility that were not modeled, for the first cut, no additional correlation was used. For detailed modeling of the relative movement of the actinides, a better estimate of this correlation would be necessary, but, for use in constructing CCDFs, this estimate was sufficient. With nine possible element/oxidation state combinations (Am(+III), Cm(+III), Np(+IV), Np(+V), Pu(+III), Pu(+IV), Th(+IV), U(+IV), and U(+VI)) and two brines, a zero-percent correlation implies 18 independent samples of the distribution.

With 18 samples of the solubility distribution, 11 sampled colloid parameters (Papenguth 1996 a, b, c, and d), and one oxidation state parameter, the calculation required 30 sampling slots to

Table 2-3. Distribution of Actinide Log Solubility about the Modeled Value

CDF	Difference Between Actual Log Solubility and Modeled Log Solubility
0.00	-2.00
0.04	-1.00
0.13	-0.50
0.27	-0.25
0.63	0.00
0.84	0.25
0.89	0.50
0.99	1.00
1.00	1.40

Distribution of Actinide Log Solubilities

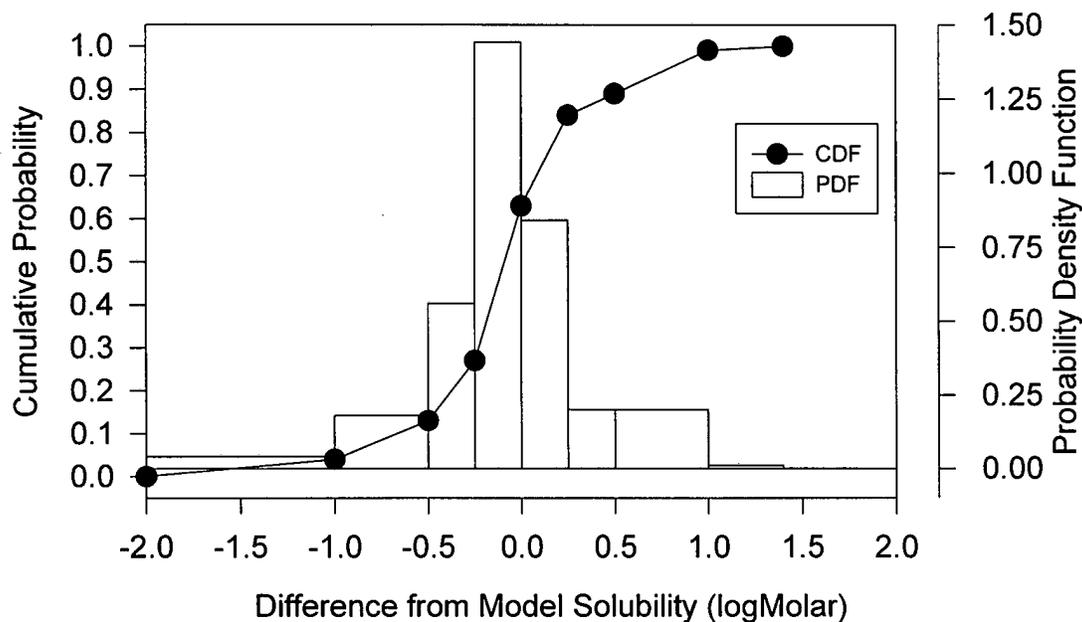


Figure 2-1. Solubility Distribution.

accommodate all parameters supplied with distributions. Many of the parameters supplied with distributions, however, were expected to have an insignificant effect on repository performance, so this list was reduced to 12 as follows:

- Cm is a minor contributor to the total EPA units, and it is expected to behave similarly to Am. A 100-percent correlation was made between Am and Cm. Only the parameters for Am were sampled, and these were copied for Cm.
- Np has a maximum of 0.48 EPA units during the 10,000-year regulatory period. Np solubilities were not sampled.
- The solubilities of U(+IV) and Th(+IV) in Castile brine were not sampled because (1) U and Th are only a little more important than Np, and (2) the solubility of the +IV oxidation state in Castile brine is low enough ($6 \times 10^{-9} \text{M}$) that it cannot adversely effect system performance. (Sampling around a number that is too low to effect performance will not change the result.)
- The actinide concentration on mineral fragment parameters was not sampled because the concentrations of actinides that may be mobilized on mineral fragments (2.6×10^{-10} to $2.6 \times 10^{-8} \text{M}$, Papenguth 1996a) were in most cases much lower than the possible concentrations of dissolved actinides.
- Of the humic acid proportionality constants, only the one for the +III oxidation state in Castile brine was sampled because it was high (0.065 to 1.6, Papenguth 1996b), and it applied to important elements (Pu and Am). The others were not sampled but were held fixed at their maximum values during the calculations.

The parameters that were sampled are listed below:

<u>Material Name</u>	<u>Property Name(s)³</u>
SOLAM3	SOLSIM, SOLCIM
SOLPU3	SOLSIM, SOLCIM
SOLPU4	SOLSIM, SOLCIM
SOLU4	SOLSIM
SOLU6	SOLSIM, SOLCIM
SOLTH4	SOLSIM
GLOBAL	OXSTAT
PHUMOX3	PHUMCIM

³ By convention, parameters are entered into the database using two identifiers: the material name and the parameter name. For hydrologic properties such as the permeability of Salado rock, it is clear that the material is the Salado Rock and the parameter is the permeability. For chemistry parameters, the naming convention does not have a literal meaning and the two identifies may not actually be material names and parameter names, but just two identifiers.

where

SOLAM3 = distribution parameter for solubility of AM(+III),

SOLSIM = solubility in Salado brine, inorganic only, Mg(OH)₂/MgCO₃ buffer⁴,

SOLCIM = solubility in Castile brine, inorganic only, Mg(OH)₂/MgCO₃ buffer,

OXSTAT = oxidation state parameter,

PHUMOX3 = the proportionality constant for humic colloids and actinides in the +3 oxidation state,

PHUMCIM = the proportionality constant for humic colloids in Castile brine, inorganic only, Mg(OH)₂/MgCO₃ buffer.

2.6 Constructing the Source Term Parameters

2.6.1 Effective Element Solubility

The parameters required for constructing the source term were (1) modeled solubilities for four oxidation states in each end-member brine, (2) a distribution to be applied about the model solubility values, (3) the scheme for assigning sampled dominant oxidation states, (4) colloidal concentrations or proportionality constants for the six actinides or the four oxidation states for each of four colloid types, and (5) caps on the actinide concentrations that may be carried on two colloid types. Use of these parameters in the performance assessment calculations required combining these into a single "effective solubility" or maximum concentration for each modeled actinide. This is performed with PANEL as shown below. Parameters that are sampled, and values derived from them, have been indicated by italics. Parameters read from the database during the Source Term ALGEBRA CDB calculations are in bold.

Dissolved Solubility = **Model Solubility** * 10 ^{*Sampled from Solubility Distribution*}

Humic Colloid Concentration = *Dissolved Solubility* * **Proportionality Constant**

if *Dissolved* * **Prop. Const.** < **Humic Cap**, otherwise

Humic Colloid Concentration = **Humic Cap**

Microbe Colloid Concentration = *Dissolved Solubility* * **Proportionality Constant**

if the *Total Mobile* < **Microbe Cap**, otherwise

Microbe Colloid Concentration = **Max (0, microbe cap - Dissolved - Humic - Mineral)**

Mineral Colloid Concentration = **Database Concentration**

⁴ When brine and MgO are added to a repository that already has MgCO₃, the brine and MgO will react to form brucite (Mg(OH)₂). If enough MgO is added, the pH and f(CO₂) of the resulting solution will be controlled by a brucite/magnesium carbonate buffer, represented here as the Mg(OH)₂/MgCO₃ buffer.

Intrinsic Colloid Concentration = Database Concentration

Total Mobile = Dissolved + Humic + Microbe + Mineral + Intrinsic

LOGSOLM = log₁₀(Total Mobile)

where LOGSOLM is the log of the "effective solubility" in moles/liter used by NUTS and PANEL. Table 2-3 shows LOGSOLM for each brine and oxidation state calculated using median values for all sampled parameters.

Table 2-3. Median "Effective Log Solubilities" for Each Brine and Oxidation State

Brine	Am(+III), Cm(+III)	Pu(+III)	Pu(+IV)	U(+IV)	U(+VI)	Th(IV)	Np(IV)	Np(V)
Salado	-5.64	-6.14	-4.80	-4.84	-5.10	-4.59	-4.17	-4.52
Castile	-6.47	-6.77	-7.19	-7.16	-4.96	-7.05	-6.85	-4.54

For actinides with more than one oxidation state, the above procedure is performed for each oxidation state, and the final total mobile concentration is set based on the oxidation state parameter:

Total Mobile = Total Mobile(lower oxidation state) if OXSTAT ≤ 0.5
 = Total Mobile(higher oxidation state) if OXSTAT > 0.5,

where OXSTAT is the oxidation-state parameter that is sampled uniformly from 0 to 1.

PANEL also calculates the fractions of each actinide that are mobilized by the five different mechanisms that are used by CCDFGF (see the Analysis Package for the CCDF Construction (Task 7) (WPO# 40524)) as follows:

Fraction dissolved = Dissolved/Total Mobile

Fraction on humics = Humic/Total Mobile

Fraction in/on microbes = Microbe/Total Mobile

Fraction on mineral fragments = Mineral/Total Mobile

Fraction as intrinsic colloid = Intrinsic/Total Mobile

2.6.2 "Lumped Effective Solubilities"

Because the Source Term calculation is used for both NUTS and PANEL, it performed the above calculation for each of the five actinides: Am, Np, Pu, Th, and U and copied the Am solubility to Cm for PANEL. NUTS, however, needs the "effective solubility" for the four "lumped" elements designated: AmL, PuL, ThL, and UL. For Am, there is only one important isotope (the amount of ^{241}Am is orders of magnitude larger than the other isotopes), so it is not necessary to adjust the Am solubility due to shared solubility effects with other non-modeled isotopes. Therefore, LOGSOLM of Am is just copied into LOGSOLM for AmL. Similarly, the NUTS modeled or "lumped" isotopes of Pu, (^{238}Pu ,⁵ ^{239}Pu , ^{240}Pu , ^{242}Pu) account for more than 99.8 percent of the moles of Pu and more than 99.999 percent of the EPA units of Pu in the repository, so the LOGSOLM for Pu is copied into PuL. For U and Th, however, there are long-lived isotopes, ^{238}U , ^{235}U , and ^{232}Th that are not modeled by NUTS, because they do not contribute significantly to the EPA normalized release, but that have large mole fractions within the repository. Because solubility is shared by isotopes on a mole-fraction basis, UL and ThL were assigned log solubilities equal to their log elemental solubilities plus their maximum log mole fraction during the 10,000-year regulatory period. (See Appendix C: for calculation of the maximum mole fractions.) Consequently, LOGSOLM of U234L was set to LOGSOLM of U minus 2.55, and LOGSOLM of Th234L was set to LOGSOLM of Th minus 2.9.

⁵ In newer versions of NUTS, a separate solubility for Pu238 is needed. Therefore, LOGSOLM of Pu238L was set to LOGSOLM of Pu minus 2.17 (the \log_{10} of the initial mole fraction of Pu238 to all Pu).

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APPENDIX A: EQ3/6 Calculation of Brine Compositions**Sandia National Laboratories**

Albuquerque, New Mexico 87185-1341

date: January 7, 1997

to: Christine T. Stockman (Org. 6849)

from: Yifeng Wang (Org. 6832)

subject: Compositions of Culebra Brines Modified by Reaction with Salado Formation

The compositions of dilute brines from Culebra formation are expected to change upon entering WIPP repository due to the dissolution of Salado evaporite minerals. This memorandum is to constrain, based on the chemical equilibrium calculations with computer code EQ3/6 (Wolery, 1992; Wolery and Daveler, 1992), the composition range that those brines can possibly attain after entering the repository.

Salado formation is composed of evaporite minerals: 93.2 wt% halite (NaCl), 1.7 wt% each of polyhalite ($K_2MgCa_2(SO_4)_4 \cdot 2H_2O$), gypsum ($CaSO_4 \cdot 2H_2O$), anhydrite ($CaSO_4$), and magnesite ($MgCO_3$) (Brush, 1990). The compositions of original Culebra brines are listed in Table 1. It is clear from Tables 1 and 3 that the original Culebra brines are much more dilute than Salado brines, which are directly derived from Salado formation and expected to be in equilibrium with most evaporite minerals. This implies that the dilute Culebra brines will inevitably dissolve the Salado evaporite minerals upon entering the WIPP repository. The composition changes of the Culebra brines due to the dissolution of Salado minerals have been calculated with computer code EQ3/6. In the calculations, the Salado minerals have been titrated into the brine in proportion to their molar fractions in the rock. The reaction path of Salado rock dissolution in Culebra brine AIS is shown in Figure 1. Figure 1 indicates that halite becomes saturated with the brine before polyhalite and the saturation of polyhalite is reached only when ~ 100 times more Salado rock is added to the brine than that needed for the halite saturation.

Table 1. Compositions of Original Culebra Brines (Siegel, 1996).

Brine type	AIS	H-17
Brine Source	Culebra facies "C" AIS seep	Culebra facies "A" well sample
Na ⁺ (M)	0.601	2.288
K ⁺ (M)	0.008	0.028
Ca ²⁺ (M)	0.023	0.042
Mg ²⁺ (M)	0.021	0.074
Cl (M)	0.560	2.522
HCO ₃ ⁻ (M)	0.001	0.001
SO ₄ ²⁻ (M)	0.079	0.077
pH	7.8	7.0
Density (g/cm ³)	1.04	1.1

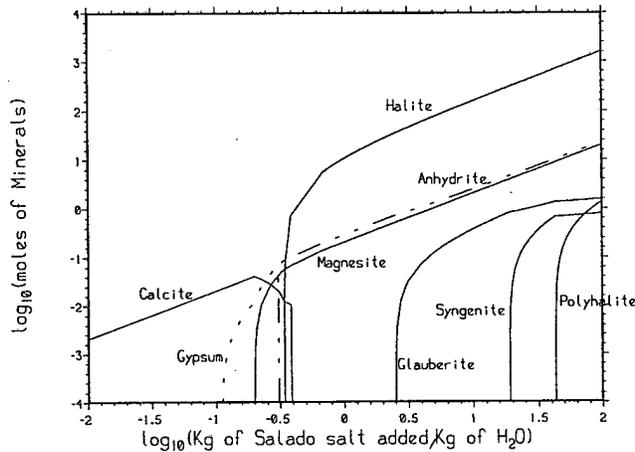


Figure 1. Moles of Secondary Minerals Precipitated as a Function of the Amount of Salado Rock Added to the Culebra Brine AIS. Note that the brine becomes saturated with polyhalite only when ~ 100 times more Salado rock is added than that needed for the brine to be saturated with halite.

The compositions of the Culebra brines after entering the repository will be determined by the extent of evaporite mineral dissolution. The extent of the mineral dissolution can be easily constrained for two extreme cases. *Case 1:* The bulk Salado rock will be dissolved until the Culebra brines become saturated with halite. Since halite accounts for 93.2 wt% of the bulk rock, the saturation of halite will prevent the other minerals such as polyhalite from further dissolution, and the Culebra brine in the repository will remain undersaturated with polyhalite. *Case 2:* The Culebra brines will circulate in Salado formation long enough to become saturated with a full assemblage of Salado evaporite minerals, especially polyhalite.

Because halite is the major component of the bulk rock and is highly soluble, any Culebra brine entering the repository will quickly become saturated with halite. Whether this brine will further react with other evaporite minerals depends on specific hydrologic conditions. At any rate, the compositions of the resulting brines in the two extreme cases certainly bracket the whole range of actual brine compositions. The compositions of Culebra brines AIS and H-17 reacted with Salado formation for the two extreme cases have been calculated with the computer code EQ3/6 and are given in Tables 2 and 3. The calculation results show that the compositions of the resulting brines in Case 1 are very similar those of Castile brines, both with high Na^+ and low Mg^{2+} concentrations, whereas the compositions of the resulting brines in Case 2 are very similar to those of Salado brines, both rich in Mg^{2+} . This implies that it is sufficient to use Salado and Castile brines as two end members to describe the WIPP brine composition, even for the cases where a significant amount of Culebra brines will be drawn into the repository. It is also interesting to note that the compositional difference of the two original Culebra brines AIS and H-17 has little effect on the final brine compositions (Tables 2 and 3).

Table 2. Compositions of Culebra Brines Which Just Become Saturated with Halite during the Dissolution of Salado Rock (Case 1). Note that the reacted Culebra brines and the Castile brines have similar chemical compositions.

Brine type	Culebra brines which just become saturated with halite during the dissolution of Salado rock ¹ (Molality)		Castile brines ² (Molality)	
	AIS	H-17	ERDA-6	WIPP-12
Na ⁺	6.087	5.923	5.472	6.726
K ⁺	0.027	0.039	0.109	0.083
Ca ²⁺	0.019	0.026	0.013	0.010
Mg ²⁺	0.042	0.074	0.021	0.074
Cl ⁻	6.048	6.135	5.393	5.628
HCO ₃ ⁻	0.001	0.0009	0.018	0.007
SO ₄ ²⁻	0.104	0.071	0.191	0.213
pH	6.8	6.5	6.17	7.06

1. Calculated with EQ3/6

2. From Brush (1990) and converted to molality

Table 3. Compositions of Culebra Brines Saturated with Full Assemblage of Salado Evaporite Minerals Including Polyhalite (Case 2). Note that the reacted Culebra brines and the Salado brines have similar chemical compositions.

Brine Type	Culebra brines saturated with a full assemblage of Salado minerals including polyhalite ¹ (Molality)		Salado brines ² (Molality)			
	AIS	H-17	Brine A	DH36	G Seep	SB-1
Na ⁺	4.178	4.180	2.047	4.200	4.697	4.671
K ⁺	0.921	0.921	0.863	0.540	0.400	0.599
Ca ²⁺	0.006	0.006	0.022	0.011	0.009	0.012
Mg ²⁺	1.040	1.018	1.611	0.935	0.720	1.198
Cl ⁻	6.404	6.446	5.984	6.144	5.829	7.234
HCO ₃ ⁻	0.0007	0.0007	0.011	0.000016	0.000014	0.00044
SO ₄ ²⁻	0.401	0.401	0.045	0.198	0.346	0.192
pH	5.55	5.55	6.5	6.0	6.1	6.0

1. Calculated with EQ3/6

2. From Brush (1990) and converted to molality

References:

- Brush L. H. (1990) *Test Plan for Laboratory and Modeling Studies of Repository and Radionuclide Chemistry for the Waste Isolation Pilot Plant*. SAND90-0266, Sandia National Lab., Albuquerque, NM.
- Siegel M. D. (1996) Calculation of pCO₂ and speciation of reference WIPP brines with EQ3NR. Memorandum to Y. Wang, May 8, 1996, SWCF-A:1.1.10.3.2.
- Wolery T. J. (1992) *EQ3NR, A Computer Program for Geochemical Aqueous Speciation-Solubility Calculations: Theoretical Manual, User's Guide, and Related Documentation (Version 7.0)*. Lawrence Livermore Lab., Livermore, CA.
- Wolery T. J. and Daveler S. A. (1992) *EQ6, A Computer Program for Reaction Path Modeling of Aqueous Geochemical Systems: Theoretical Manual, User's Guide, and Related Documentation (Version 7.0)*. Lawrence Livermore Lab., Livermore, CA.

Distribution:

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APPENDIX B: Source Term ALGEBRA Input File ALG_ST_CCA_S1.INP

This application of ALGEBRA is used to provide NUTS and PANEL with the parameters required to carry out dissolution-like calculations for the mobilization of radioisotopes by dissolution and colloidal transport, as described in the text. Note that an exclamation point in front of a line indicates that it is a comment and not executable.

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=====
!TITLE: SOURCE TERM CALCULATIONS, SALADO BRINE
!ANALYSTS: CHRISTINE STOCKMAN SNL Org 6749
!CREATED: MAY 29, 1996
!MODIFIED: OCT 25, 1996
!MODIFIED for: additional "lumping" of inventory
=====
!OX IS NEG AND 0 FOR LOW OX STATE AND POSITIVE FOR HIGH OX STATE
OX=OXSTAT[B:1]-0.5
!AM
!AM=32,SOLMOD3=45,SOLAM3=53,PHUMOX3=49
LIMIT BLOCKS 32
DIS=MAKEPROP(10**SOLSIM[B:53]*SOLSIM[B:45])
HUM=MAKEPROP(MIN(CAPHUM,10**SOLSIM[B:53]*SOLSIM[B:45]*PHUMSIM[B:49]))
MIC1=MAKEPROP(10**SOLSIM[B:53]*SOLSIM[B:45]*PROPMIC)
TOT=MAKEPROP(DIS+HUM+MIC1+CONCINT+CONCMIN)
TOTNM=MAKEPROP(DIS+HUM+CONCINT+CONCMIN)
TOTSOL = MAKEPROP(IFLT0(CAPMIC-TOT,MIN(TOTNM+CAPMIC,TOT),TOT))
MIC= MAKEPROP(IFLT0(CAPMIC-TOT,TOTSOL-TOTNM,MIC1))
LOGSOLM=MAKEPROP(LOG10(TOTSOL))
FRCDIS=MAKEPROP(DIS/TOTSOL)
FRCHUM=MAKEPROP(HUM/TOTSOL)
FRCMIC=MAKEPROP(MIC/TOTSOL)
FRCINT=MAKEPROP(CONCINT/TOTSOL)
FRCMIN=MAKEPROP(CONCMIN/TOTSOL)
!TH
!TH=43,SOLMOD4=46,PHUMOX4=50, SOLTH4=56
LIMIT BLOCKS 43
DIS=MAKEPROP(10**SOLSIM[B:56]*SOLSIM[B:46])
HUM=MAKEPROP(MIN(CAPHUM,10**SOLSIM[B:56]*SOLSIM[B:46]*PHUMSIM[B:50]))
MIC1=MAKEPROP(10**SOLSIM[B:56]*SOLSIM[B:46]*PROPMIC)
TOT=MAKEPROP(DIS+HUM+MIC1+CONCINT+CONCMIN)
TOTNM=MAKEPROP(DIS+HUM+CONCINT+CONCMIN)
TOTSOL = MAKEPROP(IFLT0(CAPMIC-TOT,MIN(TOTNM+CAPMIC,TOT),TOT))
MIC= MAKEPROP(IFLT0(CAPMIC-TOT,TOTSOL-TOTNM,MIC1))
LOGSOLM=MAKEPROP(LOG10(TOTSOL))
FRCDIS=MAKEPROP(DIS/TOTSOL)
FRCHUM=MAKEPROP(HUM/TOTSOL)
FRCMIC=MAKEPROP(MIC/TOTSOL)
FRCINT=MAKEPROP(CONCINT/TOTSOL)
FRCMIN=MAKEPROP(CONCMIN/TOTSOL)
!PU3
!PUT LOGSOLM ETC INTO SOLPU3 UNTIL CHECK OXIDATION STATE, THEN PUT INTO PU
!PU=40,SOLMOD3=45,SOLPU3=54,PHUMOX3=49
LIMIT BLOCKS 54
DIS=MAKEPROP(10**SOLSIM[B:54]*SOLSIM[B:45])
HUM=MAKEPROP(MIN(CAPHUM[B:40],10**SOLSIM[B:54]*SOLSIM[B:45]*PHUMSIM[B:49]))
MIC1=MAKEPROP(10**SOLSIM[B:54]*SOLSIM[B:45]*PROPMIC[B:40])

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TOTNM=MAKEPROP(DIS+HUM+CONCINT[B:40]+CONCMIN[B:40])
TOT=MAKEPROP(TOTNM+MIC1)
TOTSOL = MAKEPROP(IFLT0(CAPMIC[B:40]-TOT,MIN(TOTNM+CAPMIC[B:40],TOT),TOT))
MIC= MAKEPROP(IFLT0(CAPMIC[B:40]-TOT,TOTSOL-TOTNM,MIC1))
LOGSOLM=MAKEPROP(LOG10(TOTSOL))
FRCDIS=MAKEPROP(DIS/TOTSOL)
FRCHUM=MAKEPROP(HUM/TOTSOL)
FRCMIC=MAKEPROP(MIC/TOTSOL)
FRCINT=MAKEPROP(CONCINT[B:40]/TOTSOL)
FRCMIN=MAKEPROP(CONCMIN[B:40]/TOTSOL)
!PU4
!PUT LOGSOLM ETC INTO SOLPU4 UNTIL CHECK OXIDATION STATE, THEN PUT INTO PU
!PU=40,SOLMOD4=46,SOLPU4=55,PHUMOX4=50
LIMIT BLOCKS 55
DIS=MAKEPROP(10**SOLSIM[B:55]*SOLSIM[B:46])
HUM=MAKEPROP(MIN(CAPHUM[B:40],10**SOLSIM[B:55]*SOLSIM[B:46]*PHUMSIM[B:50]))
MIC1=MAKEPROP(10**SOLSIM[B:55]*SOLSIM[B:46]*PROPMIC[B:40])
TOTNM=MAKEPROP(DIS+HUM+CONCINT[B:40]+CONCMIN[B:40])
TOT=MAKEPROP(TOTNM+MIC1)
TOTSOL = MAKEPROP(IFLT0(CAPMIC[B:40]-TOT,MIN(TOTNM+CAPMIC[B:40],TOT),TOT))
MIC= MAKEPROP(IFLT0(CAPMIC[B:40]-TOT,TOTSOL-TOTNM,MIC1))
LOGSOLM=MAKEPROP(LOG10(TOTSOL))
FRCDIS=MAKEPROP(DIS/TOTSOL)
FRCHUM=MAKEPROP(HUM/TOTSOL)
FRCMIC=MAKEPROP(MIC/TOTSOL)
FRCINT=MAKEPROP(CONCINT[B:40]/TOTSOL)
FRCMIN=MAKEPROP(CONCMIN[B:40]/TOTSOL)
!NOW CHECK OX
LIMIT BLOCK 40
LOGSOLM=MAKEPROP(IFGT0(OX,LOGSOLM[B:55],LOGSOLM[B:54]))
FRCDIS =MAKEPROP(IFGT0(OX,FRCDIS[B:55],FRCDIS[B:54]))
FRCHUM =MAKEPROP(IFGT0(OX,FRCHUM[B:55],FRCHUM[B:54]))
FRCINT =MAKEPROP(IFGT0(OX,FRCINT[B:55],FRCINT[B:54]))
FRCMIN =MAKEPROP(IFGT0(OX,FRCMIN[B:55],FRCMIN[B:54]))
FRCMIC =MAKEPROP(IFGT0(OX,FRCMIC[B:55],FRCMIC[B:54]))
!U4
!PUT LOGSOLM ETC INTO SOLU4 UNTIL CHECK OXIDATION STATE, THEN PUT INTO U
!U=44,SOLMOD4=46,SOLU4=57,PHUMOX4=50
LIMIT BLOCKS 57
DIS=MAKEPROP(10**SOLSIM[B:57]*SOLSIM[B:46])
HUM=MAKEPROP(MIN(CAPHUM[B:44],10**SOLSIM[B:57]*SOLSIM[B:46]*PHUMSIM[B:50]))
MIC1=MAKEPROP(10**SOLSIM[B:57]*SOLSIM[B:46]*PROPMIC[B:44])
TOTNM=MAKEPROP(DIS+HUM+CONCINT[B:44]+CONCMIN[B:44])
TOT=MAKEPROP(TOTNM+MIC1)
TOTSOL = MAKEPROP(IFLT0(CAPMIC[B:44]-TOT,MIN(TOTNM+CAPMIC[B:44],TOT),TOT))
MIC= MAKEPROP(IFLT0(CAPMIC[B:44]-TOT,TOTSOL-TOTNM,MIC1))
LOGSOLM=MAKEPROP(LOG10(TOTSOL))
FRCDIS=MAKEPROP(DIS/TOTSOL)
FRCHUM=MAKEPROP(HUM/TOTSOL)
FRCMIC=MAKEPROP(MIC/TOTSOL)
FRCINT=MAKEPROP(CONCINT[B:44]/TOTSOL)
FRCMIN=MAKEPROP(CONCMIN[B:44]/TOTSOL)
!U6
!PUT LOGSOLM ETC INTO SOLU6 UNTIL CHECK OXIDATION STATE; THEN PUT INTO U
!U=44,SOLMOD6=48,SOLU6=58,PHUMOX6=52

```

LIMIT BLOCKS 58

DIS=MAKEPROP(10**SOLSIM[B:58]*SOLSIM[B:48])
HUM=MAKEPROP(MIN(CAPHUM[B:44],10**SOLSIM[B:58]*SOLSIM[B:48]*PHUMSIM[B:52]))
MIC1=MAKEPROP(10**SOLSIM[B:58]*SOLSIM[B:48]*PROPMIC[B:44])
TOTNM=MAKEPROP(DIS+HUM+CONCINT[B:44]+CONCMIN[B:44])
TOT=MAKEPROP(TOTNM + MIC1)
TOTSOL = MAKEPROP(IFLT0(CAPMIC[B:44]-TOT,MIN(TOTNM+CAPMIC[B:44],TOT),TOT))
MIC= MAKEPROP(IFLT0(CAPMIC[B:44]-TOT,TOTSOL-TOTNM,MIC1))
LOGSOLM=MAKEPROP(LOG10(TOTSOL))
FRCDIS=MAKEPROP(DIS/TOTSOL)
FRCHUM=MAKEPROP(HUM/TOTSOL)
FRCMIC=MAKEPROP(MIC/TOTSOL)
FRCINT=MAKEPROP(CONCINT[B:44]/TOTSOL)
FRCMIN=MAKEPROP(CONCMIN[B:44]/TOTSOL)
!NOW CHECK OX

LIMIT BLOCK 44

LOGSOLM=MAKEPROP(IFGT0(OX,LOGSOLM[B:58],LOGSOLM[B:57]))
FRCDIS =MAKEPROP(IFGT0(OX,FRCDIS[B:58],FRCDIS[B:57]))
FRCHUM =MAKEPROP(IFGT0(OX,FRCHUM[B:58],FRCHUM[B:57]))
FRCINT =MAKEPROP(IFGT0(OX,FRCINT[B:58],FRCINT[B:57]))
FRCMIN =MAKEPROP(IFGT0(OX,FRCMIN[B:58],FRCMIN[B:57]))
FRCMIC =MAKEPROP(IFGT0(OX,FRCMIC[B:58],FRCMIC[B:57]))

!

!NP

!PUT LOGSOLM ETC INTO SOLNP UNTIL CHECK OXIDATION STATE, THEN PUT INTO NP
!NP=36,SOLMOD4=46,PHUMOX4=50,SOLMOD5=47,PHIMOX5=51

LIMIT BLOCKS 36

DISNP4=MAKEPROP(SOLSIM[B:46])
HUMNP4=MAKEPROP(MIN(CAPHUM[B:36],SOLSIM[B:46]*PHUMSIM[B:50]))
MNP4=MAKEPROP(SOLSIM[B:46]*PROPMIC[B:36])
TNMNP4=MAKEPROP(DISNP4+HUMNP4+CONCINT[B:36]+CONCMIN[B:36])
TOT4=MAKEPROP(TNMNP4+MNP4)
TOTNP4 = MAKEPROP(IFLT0(CAPMIC-TOT4,MIN(TNMNP4+CAPMIC,TOT4),TOT4))
MICNP4=MAKEPROP(IFLT0(CAPMIC-TOT4,TOTNP4-TNMNP4,MNP4))

!

DISNP5=MAKEPROP(SOLSIM[B:47])
HUMNP5=MAKEPROP(MIN(CAPHUM[B:36],SOLSIM[B:47]*PHUMSIM[B:51]))
MNP5=MAKEPROP(SOLSIM[B:47]*PROPMIC[B:36])
TNMNP5=MAKEPROP(DISNP5+HUMNP5+CONCINT[B:36]+CONCMIN[B:36])
TOT5=MAKEPROP(TNMNP5+MNP5)
TOTNP5 = MAKEPROP(IFLT0(CAPMIC-TOT5,MIN(TNMNP5+CAPMIC,TOT5),TOT5))
MICNP5=MAKEPROP(IFLT0(CAPMIC-TOT5,TOTNP5-TNMNP5,MNP5))
LOGSOLM=MAKEPROP(IFGT0(OX,LOG10(TOTNP5),LOG10(TOTNP4)))
FRCDIS =MAKEPROP(IFGT0(OX,DISNP5/TOTNP5,DISNP4/TOTNP4))
FRCHUM =MAKEPROP(IFGT0(OX,HUMNP5/TOTNP5,HUMNP4/TOTNP4))
FRCMIC =MAKEPROP(IFGT0(OX,MICNP5/TOTNP5,MICNP4/TOTNP4))
FRCINT =MAKEPROP(IFGT0(OX,CONCINT[B:36]/TOTNP5,CONCINT[B:36]/TOTNP4))
FRCMIN =MAKEPROP(IFGT0(OX,CONCMIN[B:36]/TOTNP5,CONCMIN[B:36]/TOTNP4))

!

!PA

!PA=37, NP=36

LIMIT BLOCKS 37

LOGSOLM=MAKEPROP(LOGSOLM[B:36])

!

!CF,CM,PM SET TO AM=32

LIMIT BLOCKS 33, 34, 39
LOGSOLM=MAKEPROP(LOGSOLM[B:32])
!
!NOW TO LUMP FOR NUTS
!NOW INVENTORY ARE FOR SINGLE SPECIES, NEED TO ADD IN TH229, U233,
!Pu241, Pu240, Pu242
!
!use most conservative method: if added species is shorter-lived, add curies
!if added species is longer-lived, add curies scaled by halflives (add grams)
!
!U234L=63, U234=28, U233=27
LIMIT BLOCK 63
INVCHD=MAKEPROP(INVCHD[B:28]+INVCHD[B:27])
INVRHD=MAKEPROP(INVRHD[B:28]+INVRHD[B:27])
!
!TH230L=62, TH229=24, TH230=25
LIMIT BLOCK 62
INVCHD=MAKEPROP(INVCHD[B:25]+INVCHD[B:24])
INVRHD=MAKEPROP(INVRHD[B:25]+INVRHD[B:24])
!
!AM241L=59, AM241=3, PU241=18
!DECAY ALL PU241 TO AM241 AND ADD THIS IN TO AM241
!SO CONVERT CI PU241 TO KG PU241, CONVERT TO KG AM241, CONVERT BACK TO CI
M241
!THIS IS DONE USING RATIO OF HALFLIFES
LIMIT BLOCK 59
INVCHD=MAKEPROP(INVCHD[B:3]+INVCHD[B:18]*HALFLIFE[B:18]/HALFLIFE[B:3])
INVRHD=MAKEPROP(INVRHD[B:3]+INVRHD[B:18]*HALFLIFE[B:18]/HALFLIFE[B:3])
!
!PU239L=61, PU239=16, PU240=17, PU242=19
LIMIT BLOCK 61
LIFERATO = HALFLIFE[B:19]/HALFLIFE[B:16]
INVCHD=MAKEPROP(INVCHD[B:16]+INVCHD[B:17]+INVCHD[B:19]*LIFERATO)
INVRHD=MAKEPROP(INVRHD[B:16]+INVRHD[B:17]+INVCHD[B:19]*LIFERATO)
!
!REDUCE SOLUBILITIES BY RATIO'S WITH OTHER ISOTOPES
!AML=64,PUL=65,THL=66,UL=67: AM=32,PU=40,TH=43,U=44
!AML
LIMIT BLOCK 64
LOGSOLM=MAKEPROP(LOGSOLM[B:32])
FRCDIS=MAKEPROP(FRCDIS[B:32])
FRCHUM=MAKEPROP(FRCHUM[B:32])
FRCMIC=MAKEPROP(FRCMIC[B:32])
FRCINT=MAKEPROP(FRCINT[B:32])
FRCMIN=MAKEPROP(FRCMIN[B:32])
!PUL
LIMIT BLOCK 65
LOGSOLM=MAKEPROP(LOGSOLM[B:40])
FRCDIS=MAKEPROP(FRCDIS[B:40])
FRCHUM=MAKEPROP(FRCHUM[B:40])
FRCMIC=MAKEPROP(FRCMIC[B:40])
FRCINT=MAKEPROP(FRCINT[B:40])
FRCMIN=MAKEPROP(FRCMIN[B:40])
!THL
LIMIT BLOCK 66

```
LOGSOLM=MAKEPROP(LOGSOLM[B:43]-2.9)
FRCDIS=MAKEPROP(FRCDIS[B:43])
FRCHUM=MAKEPROP(FRCHUM[B:43])
FRCMIC=MAKEPROP(FRCMIC[B:43])
FRCINT=MAKEPROP(FRCINT[B:43])
FRCMIN=MAKEPROP(FRCMIN[B:43])
!UL
LIMIT BLOCK 67
LOGSOLM=MAKEPROP(LOGSOLM[B:44]-2.55)
FRCDIS=MAKEPROP(FRCDIS[B:44])
FRCHUM=MAKEPROP(FRCHUM[B:44])
FRCMIC=MAKEPROP(FRCMIC[B:44])
FRCINT=MAKEPROP(FRCINT[B:44])
FRCMIN=MAKEPROP(FRCMIN[B:44])
!
END
```

APPENDIX C: Maximum Mole Fractions for Th and U

The maximum mole fractions of "lumped ^{230}Th " and "lumped ^{234}U " were calculated in a spread sheet using Microsoft EXCEL versio 7.0a, based on the total Curies of each isotope calculated by an ORIGEN run as reported in Sanchez et. al. 1996. Sections of the spread sheet are reproduced below. Constants used in the calculations were:

$\text{Bq/Ci} = 3.7 \times 10^{10}$ *, $\text{days/year} = 365.25$, Avogadro's number. = 6.022137×10^{23} atoms/mole*. In Column B, molecular weights, MW, were approximated by the isotope name, i.e. MW of ^{229}Th was approximated as 229 gm/mole. Half-lives were obtained from Sanchez** and converted to seconds in Column E. Mole/Ci was calculated in Column F:

Column F = Column E * 3.7×10^{10} / (Avo. * $\ln(2)$)

Column G = 1 / (Column B * Column F)

A	B	C	D	E	F	G	
	MW	half-life**	half-life units**	half-life (seconds)	mole/Ci	Ci/g	
^{227}Th	227	1.87E+01	d	1.62E+06	1.43E-07	3.07E+04	
^{228}Th	228	1.91E+00	a	6.04E+07	5.35E-06	8.20E+02	
^{229}Th	229	7.30E+03	a	2.30E+11	2.04E-02	2.14E-01	
^{230}Th	230	7.54E+04	a	2.38E+12	2.11E-01	2.06E-02	
^{231}Th	231	1.06E+00	d	9.18E+04	8.14E-09	5.32E+05	
^{232}Th	232	1.40E+10	a	4.42E+17	3.92E+04	1.10E-07	
^{234}Th	234	2.41E+01	d	2.08E+06	1.85E-07	2.32E+04	
^{232}U	232	7.00E+01	a	2.21E+09	1.96E-04	2.20E+01	
^{233}U	233	1.59E+05	a	5.02E+12	4.45E-01	9.64E-03	
^{234}U	234	2.46E+05	a	7.76E+12	6.88E-01	6.21E-03	
^{235}U	235	7.04E+08	a	2.22E+16	1.97E+03	2.16E-06	
^{236}U	236	2.34E+07	a	7.39E+14	6.55E+01	6.46E-05	
^{237}U	237	6.75E+00	d	5.83E+05	5.17E-08	8.16E+04	d = days
^{238}U	238	4.47E+09	a	1.41E+17	1.25E+04	3.36E-07	a = years
^{240}U	240	1.41E+01	h	5.08E+04	4.50E-09	9.26E+05	h = hours

* CRC Handbook of Chemistry and Physics, 72nd edition, 1991 (constants rounded to 7 significant figures in spreadsheet)

** Half-lives were entered into spread sheet from an electronic copy of table 3 from the memo to M. Martell from L. C. Sanchez, 4/24/1996, "Justification for Choice of CCA Radionuclide Values". These half-lives were taken from the General Electric Chart of the Nuclides, 14th Edition, 1989. These values were compared to the half-lives in ORIGEN2 in the 3/28/1996 memo from L.C. Sanchez to M. Martell, "Radionuclide Half-lives and Specific Activities Obtained From ORIGEN2 Data" and found to be less than 3% different, and thus accurate enough for these calculations.

Section 2 of the spreadsheet has two parts. The top half of Section 2 of the spread sheet contains the total Curies within the repository at various times. This section was created by pointing to the appropriate cells in the spread sheet provided by Sanchez et. al^{***}. Note that all isotopes of Th and U contained in Sanchez et. al. are included in this section. The lower half of Section 2 contains the total moles of each isotope in the repository at the same times. The lower half was obtained by multiplying the Curies from the top half of the second section by the mole/Ci from column F of the first section. The total moles of Th and U at each time were summed in bold at the bottom of the columns for each time.

The third section calculates the ratio of the moles of "lumped isotopes" to the total moles of all isotopes for each element from Section 2. The "lumped isotope" for Th, designated "ThL," is the sum of ²²⁹Th and ²³⁰Th. The "lumped isotope" for U, designated "UL," is the sum of, and ²³³U and ²³⁴U. Finally, Section 4 takes the maximum over all times of the mole fractions calculated in Section 3. Notice that because of ingrowth and decay, the maximum mole fraction for ThL occurs at 10,038 years and the maximum mole fraction for UL occurs at 1,038 years.

^{***} Excel file used by Sanchez, L. C., and J. Liscum-Powell, J. S. Rath, and H. R. Trelue. (1996). WIPP PA Analysis Report for EPAUNI: Estimating Probability Distribution of EPA Unit Loading in the WIPP Repository for Performance Assessment Calculations, Version 1.01, WPO# 39529, Sandia National Laboratories, Albuquerque, NM.

Spreadsheet Section 2: Curies and Moles of isotopes at various times

total Curies ***:											
	t=0 (1995)	t=38	t=138	t=163	t=213	t=388	t=1038	t=3038	t=5038	t=7538	t=10038
²²⁷ Th	6.02E-01	4.99E-01	4.87E-01	4.95E-01	5.12E-01	5.74E-01	8.20E-01	1.56E+00	2.33E+00	3.33E+00	4.35E+00
²²⁸ Th	2.72E+01	1.94E+01	8.03E+00	6.53E+00	4.42E+00	1.64E+00	1.01E+00	1.01E+00	1.01E+00	1.01E+00	1.01E+00
²²⁹ Th	3.00E+00	9.97E+00	2.82E+01	3.27E+01	4.17E+01	7.30E+01	1.84E+02	4.85E+02	7.32E+02	9.78E+02	1.17E+03
²³⁰ Th	8.82E-02	3.06E-01	1.17E+00	1.44E+00	1.99E+00	4.11E+00	1.25E+01	3.79E+01	6.27E+01	9.30E+01	1.22E+02
²³¹ Th	1.74E+01	1.75E+01	1.76E+01	1.76E+01	1.76E+01	1.77E+01	1.82E+01	1.97E+01	2.11E+01	2.28E+01	2.43E+01
²³² Th	1.01E+00										
²³⁴ Th	5.01E+01										
²³² U	2.58E+01	1.79E+01	6.84E+00	5.37E+00	3.32E+00	6.16E-01	1.18E-03	5.13E-12	2.22E-20	0.00E+00	0.00E+00
²³³ U	1.95E+03	1.95E+03	1.95E+03	1.95E+03	1.95E+03	1.95E+03	1.94E+03	1.93E+03	1.91E+03	1.89E+03	1.87E+03
²³⁴ U	5.08E+02	7.51E+02	1.13E+03	1.19E+03	1.27E+03	1.40E+03	1.44E+03	1.43E+03	1.43E+03	1.42E+03	1.41E+03
²³⁵ U	1.74E+01	1.75E+01	1.76E+01	1.76E+01	1.76E+01	1.77E+01	1.82E+01	1.97E+01	2.11E+01	2.28E+01	2.43E+01
²³⁶ U	4.30E-01	6.72E-01	1.30E+00	1.46E+00	1.77E+00	2.85E+00	6.70E+00	1.70E+01	2.53E+01	3.35E+01	3.98E+01
²³⁷ U	6.01E+01	9.67E+00	8.12E-02	2.63E-02	4.90E-03	2.74E-03	2.60E-03	2.20E-03	1.87E-03	1.53E-03	1.25E-03
²³⁸ U	5.01E+01										
²⁴⁰ U	1.50E-06	1.51E-06	1.54E-06	1.55E-06	1.56E-06	1.61E-06	1.80E-06	2.36E-06	2.93E-06	3.64E-06	4.34E-06
total moles:											
	t=0 (1995)	t=38	t=138	t=163	t=213	t=388	t=1038	t=3038	t=5038	t=7538	t=10038
²²⁷ Th	8.63E-08	7.15E-08	6.98E-08	7.10E-08	7.34E-08	8.23E-08	1.18E-07	2.24E-07	3.34E-07	4.77E-07	6.24E-07
²²⁸ Th	1.45E-04	1.04E-04	4.30E-05	3.49E-05	2.36E-05	8.77E-06	5.39E-06	5.38E-06	5.38E-06	5.38E-06	5.38E-06
²²⁹ Th	6.12E-02	2.04E-01	5.76E-01	6.68E-01	8.52E-01	1.49E+00	3.76E+00	9.91E+00	1.49E+01	2.00E+01	2.39E+01
²³⁰ Th	1.86E-02	6.45E-02	2.48E-01	3.03E-01	4.19E-01	8.67E-01	2.63E+00	7.99E+00	1.32E+01	1.96E+01	2.58E+01
²³¹ Th	1.42E-07	1.42E-07	1.43E-07	1.43E-07	1.43E-07	1.44E-07	1.48E-07	1.61E-07	1.72E-07	1.85E-07	1.98E-07
²³² Th	3.94E+04										
²³⁴ Th	9.25E-06										
tot. Th	3.94E+04										
²³² U	5.05E-03	3.51E-03	1.34E-03	1.05E-03	6.50E-04	1.21E-04	2.31E-07	1.00E-15	4.35E-24	0.00E+00	0.00E+00
²³³ U	8.68E+02	8.68E+02	8.67E+02	8.67E+02	8.67E+02	8.67E+02	8.64E+02	8.57E+02	8.51E+02	8.42E+02	8.34E+02
²³⁴ U	3.50E+02	5.17E+02	7.78E+02	8.17E+02	8.75E+02	9.64E+02	9.92E+02	9.87E+02	9.81E+02	9.75E+02	9.68E+02
²³⁵ U	3.43E+04	3.44E+04	3.46E+04	3.46E+04	3.47E+04	3.49E+04	3.59E+04	3.88E+04	4.16E+04	4.48E+04	4.78E+04
²³⁶ U	2.82E+01	4.40E+01	8.54E+01	9.56E+01	1.16E+02	1.87E+02	4.39E+02	1.11E+03	1.66E+03	2.20E+03	2.61E+03
²³⁷ U	3.11E-06	5.00E-07	4.20E-09	1.36E-09	2.53E-10	1.41E-10	1.34E-10	1.14E-10	9.68E-11	7.89E-11	6.44E-11
²³⁸ U	6.27E+05										
²⁴⁰ U	6.75E-15	6.79E-15	6.92E-15	6.96E-15	7.02E-15	7.24E-15	8.08E-15	1.06E-14	1.32E-14	1.64E-14	1.95E-14
tot. U	6.62E+05	6.63E+05	6.63E+05	6.63E+05	6.63E+05	6.64E+05	6.65E+05	6.69E+05	6.72E+05	6.76E+05	6.79E+05

Spreadsheet Section 3: The ratio of the moles of "lumped isotopes" to the total moles of all isotopes

	t=0	t=38	t=138	t=163	t=213	t=388	t=1038	t=3038	t=5038	t=7538	t=10038
ThL	2.03E-06	6.80E-06	2.09E-05	2.46E-05	3.23E-05	5.98E-05	1.62E-04	4.54E-04	7.15E-04	1.00E-03	1.26E-03
UL	1.84E-03	2.09E-03	2.48E-03	2.54E-03	2.63E-03	2.76E-03	2.79E-03	2.76E-03	2.73E-03	2.69E-03	2.65E-03

Spreadsheet section 4:

	maximum mole fraction	log max. mole fraction
ThL	1.26E-03	-2.90
UL	2.79E-03	-2.55

APPENDIX D: Post-PANEL ALGEBRACDB Input Files

The application of ALGEBRACDB for the input-control file listed below post processes PANEL's results, converting units from kg to Curies and lumping PANEL's 21 radioisotope outputs to form the 5 equivalent lumped radioisotopes used by CCDFGF to scale SECOTP's outputs. The kg to Curie conversion factors were calculated in PANEL using PANEL's half-lives, and were copied from the PANEL debug file. The units of the five lumped isotopes are also converted to EPA units for display purposes. Note that an exclamation point at the start of a line indicates that the line is a comment and not executed. Some "commented out" sections of this file have been deleted for clarity.

```

!A00PB210=SD0PB210*7.6338E4
A00RA226=SD0RA226*9.8863E2
AL0RA226=SL0RA226*9.8863E2
AS0RA226=SS0RA226*9.8863E2
!A00RA228=SD0RA228*2.7268E5
A00TH229=SD0TH229*2.1268E2
AL0TH229=SL0TH229*2.1268E2
AS0TH229=SS0TH229*2.1268E2
A00TH230=SD0TH230*2.0186E1
AL0TH230=SL0TH230*2.0186E1
AS0TH230=SS0TH230*2.0186E1
!A00TH232=SD0TH232*1.0967E-4
!A00PA231=SD0PA231*4.7240E1
A00U233=SD0U233*9.6801E0
AL0U233=SL0U233*9.6801E0
AS0U233=SS0U233*9.6801E0
A00U234=SD0U234*6.2484E0
AL0U234=SL0U234*6.2484E0
AS0U234=SS0U234*6.2484E0
!A00U235=SD0U235*2.1615E-3
!A00U236=SD0U236*6.4679E-2
!A00U238=SD0U238*3.3618E-4
A00NP237=SD0NP237*7.0486E-1
AL0NP237=SL0NP237*7.0486E-1
AS0NP237=SS0NP237*7.0486E-1
A00PU238=SD0PU238*1.7119E4
AL0PU238=SL0PU238*1.7119E4
AS0PU238=SS0PU238*1.7119E4
A00PU239=SD0PU239*6.2143E1
AL0PU239=SL0PU239*6.2143E1
AS0PU239=SS0PU239*6.2143E1
A00PU240=SD0PU240*2.2786E2
AL0PU240=SL0PU240*2.2786E2
AS0PU240=SS0PU240*2.2786E2
A00PU242=SD0PU242*3.9257E0
A00AM241=SD0AM241*3.4321E3
AL0AM241=SL0AM241*3.4321E3
AS0AM241=SS0AM241*3.4321E3

```

```

!STATEMENTS BELOW ARE TO COMBINE CURIES FOR CCA96 CALCULATIONS
A09AM241=A00AM241
A09PU238=A00PU238
A09PU239=A00PU239+A00PU240+A00PU242

```

A09U234=A00U233+A00U234
A09TH230=A00TH229+A00TH230
epalwmbt=makehist(0.)

!SCALE=4.0736
SCALE=3.44

E09AM241=A09AM241/100./SCALE
E09PU238=A09PU238/100./SCALE
E09PU239=A09PU239/100./SCALE
E09U234=A09U234/100./SCALE
E09TH230=A09TH230/10./SCALE
EPATOT=E09AM241+E09PU238+E09PU239+E09U234+E09TH230
END

APPENDIX E: PANEL Concentration Algebra Input Files: ALG_PANEL_CCA.INP and ALG_PANEL_CCA_CON.INP

File ALG_PANEL_CCA.INP is the ALGEBRA input file that makes a BRAGFLO input file with volume equal to 4000 m³ and integrated flow of 10⁻⁵•time(years).

```
ALLTIMES
DELETE ALL
BRNVOL_W=MAKEGLOB(4000.)
BNBHUDRZ=MAKEGLOB(TIME*.00001/3.15570E+07)
```

File ALG_PANEL_CCA_CON.INP is the ALGEBRA input file that changes integrated releases in kg to concentrations in EPA units/m³.

```
SCALE=3.44
```

```
N00TH229=SD0TH229*2.1269E2/SCALE/100.
N00TH230=SD0TH230*2.0186E1/SCALE/10.
N00TH232=SD0TH232*1.0968E-4/SCALE/10.
N00U233=SD0U233*9.6803/SCALE/100.
```

```
N00U234=SD0U234*6.2485/SCALE/100.
N00U235=SD0U235*2.1615E-3/SCALE/100.
N00U236=SD0U236*6.468E-2/SCALE/100.
N00U238=SD0U238*3.3619E-4/SCALE/100.
N00NP237=SD0NP237*7.0487E-1/SCALE/100.
```

```
N00PU238=SD0PU238*1.712E4/SCALE/100.
N00PU239=SD0PU239*6.2144E1/SCALE/100.
N00PU240=SD0PU240*2.2787E2/SCALE/100.
N00PU242=SD0PU242*3.9257/SCALE/100.
```

```
N00PU244=SD0PU244*1.7738E-2/SCALE/100.
N00AM241=SD0AM241*3.4322E3/SCALE/100.
N00AM243=SD0AM243*1.9962E2/SCALE/100.
N00CM243=SD0CM243*5.0556E4/SCALE/100.
N00CM244=SD0CM244*8.0903E4/SCALE*0.
N00CM245=SD0CM245*1.7106E2/SCALE/100.
N00CM248=SD0CM248*4.2523/SCALE/100.
```

```
TOTTP=(N00TH229+N00TH230+N00TH232+N00U233+N00U234+N00U235+N00U236+N00U238+&
N00NP237+N00PU238+N00PU239+N00PU240+N00PU242+N00PU244+N00AM241+N00AM243+&
N00CM243+N00CM244+N00CM245+N00CM248)
```

```
DEN=SMFLOW00-SMFLOW00[T:-1]
DEN=IFGT0(TIME-TIME[T:-1],DEN,SMFLOW00)
NUM=TOTTP-TOTTP[T:-1]
NUM=IFGT0(TIME-TIME[T:-1],NUM,TOTTP)
EPACON=NUM/DEN
```

```
!back time up since in PANEL, concentration is constant over a time step
!at the value at the beginning of the time step. ie, A2-A1=C1*(V2-V1)
TIME=TIME-3.15570E+07*50.
```

```
! extend last concentration to 10,000 years
TIME=IFGT0(TIME-312.4E+9, 315.57E+9, TIME)
```

```
END
```

E-2
Information Only