Appendix E

NUCLEAR WASTE MANAGEMENT PROCEDURE Sandia National Laboratories	**Design Document Criteria**	**Form Number: NP 19-1-4** **Page 1 of 1**

1. **Software Name:** PANEL
2. **Software Version:** 5.02
3. **Document Version:** 5.02
4. **ERMS #:** 577751

Prior to sign-off of the DD, all items shall be appropriately addressed by the code sponsor so that "**Yes**" may be checked. Include this form as part of the DD.

Are the following appropriately defined and documented in the DD?

5.	Major Software Components	☒ Yes
6.	Technical description of the software with respect to: theoretical basis, embodied mathematical model, major control flow, control logic, and data structures	☒ Yes
7.	Functionalities and interfaces of object components, functions, and subroutines.	☒ Yes
8.	Allowable or prescribed ranges for inputs and outputs	☒ Yes
9.	Verifiability: Is the design verifiable through testing or other means?	☒ Yes
10.	Consistency and Traceability: Is the design consistent with and traceable to the software's requirements?	☒ Yes
11.	Technical Feasibility: Is the design technically feasible?	☒ Yes
12.	Implementation: Is the design presented in sufficient detail to allow for implementation as computer software?	☒ Yes

13.	Sungtae Kim **Code Team/Sponsor** (*print*)	*Signature on File* Signature	10/10/22 Date
14.	Seth King **Technical Reviewer** (*print*)	*Signature on File* Signature	10/10/22 Date
15.	Shelly R. Nielsen **QA Reviewer** (*print*)	Shelly R. Nielsen Signature	10-31-2022 Date
16.	Steve Wagner **Responsible Manager** (*print*)	Steve Wagner Signature	11/21/2022 Date
17.	Jennifer J. Long **SCM Coordinator** (*print*)	Jennifer Long Signature	11/2/22 Date

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Appendix G

NUCLEAR WASTE MANAGEMENT PROCEDURE Sandia National Laboratories	**User's Manual Criteria**	**Form Number: NP 19-1-6** **Page 1 of 1**

Does the User's Manual contain as appropriate:

1. **Software Name:** PANEL
2. **Software Version:** 5.02
3. **Document Version:** 5.02
4. **ERMS #:** 577751

Prior to sign-off of the User's Manual, all items shall be appropriately addressed by the code sponsor so that "**Yes**" or "**N/A**" may be checked. Include this form as part of the User's Manual.

5.	A statement(s) of functional requirements (consistent with those in the RD)?	☒ Yes	
6.	An explanation of the mathematical model and numerical models, where applicable as based on code functionality?	☒ Yes	☐ N/A
7.	Physical and mathematical assumptions, where applicable as based on code functionality?	☒ Yes	☐ N/A
8.	The capabilities and limitations inherent in the software?	☒ Yes	
9.	Instructions that describe the user's interaction with the software?	☒ Yes	
10.	The identification of input parameters, formats, and valid ranges?	☒ Yes	
11.	Messages initiated as a result of improper input and how the user can respond?	☒ Yes	
12.	The identification and description of output specifications and formats?	☒ Yes	
13.	A description of any required training necessary to use the software?	☒ Yes	
14.	The identification of components of the code that were not tested?	☒ Yes	☐ N/A

15.	Sungtae Kim **Code Team/Sponsor** (*print*)	Signature on File Signature	10/10/2022 Date
16.	Seth King **Technical Reviewer** (*print*)	Signature on File Signature	10/10/2022 Date
17.	Shelly R. Nielsen **QA Reviewer** (*print*)	Shelly R. Nielsen Signature	10-31-2022 Date
18.	Steve Wagner **Responsible Manager** (*print*)	Steve Wagner Signature	11/21/2022 Date
19.	Jennifer J. Long **SCM Coordinator** (*print*)	Jennifer Long Signature	11/2/22 Date

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WIPP PA

Design Document and User's Manual

for

PANEL Version 5.02

Document Version 5.02

ERMS # 577751

November 2022

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1.0 INTRODUCTION AND SCOPE

This Design Document and User's Manual for PANEL Version 5.02, describes the following major features of software design: software components, theoretical basis, mathematical model, control flow and logic, data structures, and functionality and the interfaces of subroutines. It also describes in detail the allowed or prescribed ranges for input data and user interface, in accordance with the Nuclear Waste Management Procedure NP 19-1 Software Requirements (Long, 2020). This code is used by the Sandia National Laboratories' Performance Assessment (PA) Department in support of the performance assessment calculations for the Waste Isolation Pilot Plant (WIPP). It is controlled under the software configuration management system CVS (Concurrent Versions System) on the Linux cluster.

1.1 Software Identification

Code Name:	PANEL
Version:	5.02
CVS Repository:	/data/cvs/CVSLIB/WIPP_CODES/PA_CODES/PANEL
Platform:	CentOS 7/Dell PowerEdge C6420
Host:	fwm.sandia.gov
Compiler:	Gfortran/GCC 8.2.0

1.2 Points of Contact

Code Sponsor:	Sungtae Kim	sunkim@sandia.gov	(575) 234-0001

1.3 Code Overview

PANEL serves three purposes in the WIPP PA calculations. First, PANEL calculates a "total mobile" (i.e. dissolved plus that associated with dispersed colloids) concentration limit for each element in the waste inventory. Second, PANEL uses these total mobile concentration limit values to calculate the mobile concentrations of various radionuclides in brine that is in contact with the solid waste inventory. Third, PANEL performs a mass balance over a single (or an interconnected group of) waste-filled repository *panel(s)*, accounting for time-varying brine volumes inside the panel and time-varying rates of brine exiting the panel, and calculates the cumulative amounts of radionuclides exiting the waste panel as a function of time.

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2.0 REQUIREMENTS

2.1 Functional Requirements

The functional requirements for PANEL, Version 5.02 are listed below.

R.1 Compute the total mobile concentration limits (i.e. the dissolved plus that associated-with-dispersed-colloids) for elements in accordance with the Source Term conceptual model including oxidation states of Pu, U and Np elements, microbial colloid model (biomass- or toxicity-based) and colloid enhancement factors.

R.2 Compute the instantaneous concentrations of each radionuclide by (1) portioning the respective elemental concentration limit according to the isotope-to-element mole fraction of the radionuclide and (2) saturating the brine (subject to the concentration limit) with the available radionuclide inventory.

R.3 Compute the total amount (stationary and mobile) of each radionuclide as a function of time, accounting for radioactive decay and ingrowth.

R.4 Compute the cumulative amount of each radionuclide that is removed from the simulated waste panel(s) by brine flow, as a function of time.

R.5 Translate (i.e. shift) the time values associated with the input brine volume and brine outflow data according to the (wellbore) intrusion time.

R.6 Scale the inventory and brine volume according to a user-defined number of waste panels.

R.7 Lump together sets of selected radionuclides to form "lumped" radionuclides for reporting output.

2.2 External Interface Requirements

The external interface requirements for PANEL, Version 5.02 are listed below:

R.8 Read input data from standard binary CAMDAT database (CDB) files.

R.9 Write output data to a binary CAMDAT database (CDB) file.

R.10 Rely on routines from CAMDAT_LIB, CAMCON_LIB, and CAMPSUPES_LIB to read and write to CDB files and to perform QA logging in those files.

PANEL links to the standard WIPP code libraries, namely CAMCON_LIB, CAMSUPES_LIB, and CAMDAT_LIB. User interactions consist of command line execution, batch files, and input files.

2.3 Other Requirements

There are no other requirements for PANEL.

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2.4 Functionality Not Tested

PANEL has a capability to calculate hydrogen gas generation rate by radiolysis but this capability has not been tested. Additionally, PANEL has capability of calculating historical instantaneous concentration changes that are affected by both decay and brine flow-out, when a BRAGFLO CDB file is used as input. These capabilitiies will not be tested. PANEL is not used to calculate the radiolysis-related effects and the brine flow-out related concentration changes in WIPP PA.

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3.0 MAJOR SOFTWARE COMPONENTS

PANEL consists of a set of core subroutines and functions that perform its calculations as related to the functional requirements. It is linked against the object libraries CAMDAT_LIB, CAMON_LIB, and CAMSUPES_LIB and calls upon subroutines and functions in those libraries to perform input/output operations on the CDB (CAMDAT Database) binary files, perform input/output operations related to QA records, and perform memory allocation.

3.1 Major Control Flow, Control Logic, and Subroutines

The major program units and subroutines are listed below. Their functionalities and major control flow and logic are included in the descriptions.

PROGRAM PANEL – Parses the command line arguments, prints QA records, opens the input and output CDB files, calls subroutine STERM to calculate the total mobile concentration limits, and calls subroutine CPANEL to perform the decay/mobilization/mass balance calculations.

SUBROUTINE STERM – Calculates the total mobile concentration limits for each element. Reads the necessary parameters from the input CDB file, performs parameter selection logic (e.g. by valency, brine type, and brine volume factor) and writes the results to the output CDB file. Subroutine MOBILE performs the actual total mobile concentration limit calculations for the five primary elements. Subroutine REPLICATE copies the values from the primary elements to the secondary elements.

SUBROUTINE CPANEL – Performs the decay/mobilization/mass balance calculations for the 10,000 year simulation. Calls subroutine GETFLX to read the inventory and other relevant parameters from the input CDB file. Calls subroutine WHICHE to index the elements. Calls subroutine GETFLX to read and set the brine volume and brine discharge values. Loops over timesteps. Calls subroutine BHFLO to interpolate the brine volume and brine discharge values to the current timestep. Calls subroutine LOAD to perform the decay and ingrowth calculations over the timestep period. Performs mobilization, mass balance, and cumulative discharge calculations. Performs lumping calculations. Outputs results to the output CDB file and updates remaining inventory for the next timestep iteration.

SUBROUTINE GETFLX – Reads the panel(s) brine volume and brine discharge time series data from the "flux" CDB file. Performs the time translation if necessary. Sets the brine volume and brine discharge to constant values if no "flux" CDB file is specified (i.e. DECAY and CONCENTRATION run modes).

SUBROUTINE LOAD – Dynamically assembles a decay chain (containing up to four generations) for each radionuclide based on parent/daughter relationships using subroutines WHICH and WHERE. Calculates the remaining inventory at the end of the timestep.

3.2 Data Structures

PANEL uses standard FORTRAN variables, arrays, and common blocks. Descriptions of the common blocks are given below.

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CHAIN – Arrays for the atomic weights and remaining inventory of each radionuclide

DATA – Arrays related to radionuclide atomic properties and release limits

DATAC – Arrays holding the radionuclide parent-daughter relationships

DBRDR – Variables for the CDB file FORTRAN file unit numbers

DECAY – Flags to determine PANEL's run mode

EB_P – Variables and arrays used to facilitate reading and writing to the CDB files

EB_PC – Variables and arrays used to facilitate reading and writing to the CDB files

FLUX – Variables and arrays related to the brine volume and brine discharge data

INPUT – Variables related to time integration and various unit conversion factors

PANLINFO – Variables related to inventory scaling

PANEL also uses fixed PARAMETERS defining the timestep size, number of radionuclides, and number of elements.

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4.0 MODELS AND METHODS

This section describes the technical basis and calculation methods of the four primary functionalities in PANEL (corresponding to Functional Requirements R.1 – R.4). The supplementary requirements (R.5 – R.7) are noted and discussed where relevant to the primary functionalities.

In general, an actinide isotope is notated as $^{actomic\ weight}actinide$ like ^{241}Am and ^{239}Pu. When notating an actinide isotope in equation and in the WIPP PA code input files, it is written in a convenient way as [*actinide*][*atomic weight*] like AM241 and PU239. For instance, concentration of ^{241}Am in equation can be notated like C^{Am}_{AM241} (concentration of ^{241}Am, isotope of Am actinide element) or C^{t}_{AM241} (instantaneous concentration of ^{241}Am).

4.1 Total Mobile Concentration Limit Calculations

PANEL computes the total mobile concentration limits (referred to as the "Total Mobilization Potential") for 14 elements in the tracked inventory. The total mobilization potential represents the "dissolved" (speciated or complexed with organic ligands) solubility limit plus a maximum concentration that could be associated with four types of dispersed colloids (mineral, intrinsic, humic, and microbial). The basis for this conceptual model is further described in Appendix-SOTERM (US DOE, 2014 and 2019), Sarathi (2019) and Kim (2022). It is important to note that, while dependent upon several parameters, the total mobilization potential values are constant for any given model realization and throughout the course of a simulation (these total mobilization potentials are distinct from instantaneous mobile concentrations discussed in Section 4.2, which vary with time based on the available inventory). In the context of WIPP PA calculations, the parameters vary across model realizations, thus different realizations and simulations will have different total mobilization potentials. The computed total mobilization potential values are used by PANEL internally and are output (as the logarithm to 10 base (hereinafter referred to as log10) of the value) for use by other PA codes (i.e. NUTS).

The set of 14 tracked elements includes five "primary" actinides, Am, Pu, Th, U, and Np, whose total mobilization potentials are computed according to the Solubility Model described in Appendix-SOTERM (US DOE, 2014 and 2019), three "secondary" actinides and one lanthanide, Cm, Cf, Pa, and Pm, whose total mobilization potentials are assumed to be the same as one of the five primary actinides, and five other elements, Cs, Sr, Ra, Sm, and Pb, whose total mobilization potentials are assumed fixed. Between the CCA-1996 and the CRA-2004, PANEL was changed to assign Cs and Sr total mobilization potentials of 1.0 mol/L (see Garner 1998a-b, and 2003a, also Garner 2003b page 8, reference to "PANEL computes the concentrations of 23 radionuclides") so that ^{137}Cs and ^{90}Sr would be included in the calculated DBR releases. This total mobilization potential is sufficiently large that it is unlikely to be reached. The molar inventories of Cs and Sr in WIPP PA calculations (PA PDB) are low enough that, if dissolved in 1× the minimum brine volume necessary for a DBR (PA PDB parameter REFCON:DBRMINBV), the concentrations would be several orders of magnitude smaller than 1.0 mol/L. PANEL assigns Pb, Ra, and Sm total mobilization potentials of 1.0×10^{-99} mol/L, which is effectively zero. This is to prevent their mobilization (Garner and Leigh 2005). This is because ^{210}Pb, ^{226}Ra, ^{228}Ra, and ^{147}Sm were historically deemed to represent small fractions of the total (solid) inventory on an EPA release-

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unit basis (CCA Appendix-WCA (US DOE, 1996a)). While this is not necessarily true if one considers their fractional representation in the *mobilized* inventory, they are still likely to contribute a small amount to DBR releases in absolute EPA units.

Figure 4-1 illustrates the steps involved in calculating the total mobilization potential values (S_TOT, and the log10 of this value, LOGSOLM) for each of the elements. While the calculations themselves are simple, the process is complicated by the need to select the appropriate model parameters according to the element, element valency (i.e. oxidation state), brine type, and brine (volume) factor. Figure 4-1 illustrates the logic involved in selecting the appropriate parameters. In general, database parameters are referred to with the convention MATERIAL:PROPERTY (i.e. material name colon property name). Terms in brackets refer to a portion of the name that is replaced with a value, e.g. SOLMOD[valency] could refer to SOLMOD3, SOLMOD4, etc.

The oxidation state condition is used to determine the valency of the actinide of interest (i.e. the oxidation state of the individual elements). If oxidation state index number (GLOBAL:OXSTAT) is lower than and equal to the oxidation state cutoff value (GLOBAL:OXSTAT $\leq$ [actinide]:OXCUTOFF), each actinide (of Pu, U, Np) is assigned its lower valency numbers (Pu^{3+}, U^{4+}, and Np^{4+}), whereas if GLOBAL:OXSTAT > [actinide]:OXCUTOFF, each actinide is assigned higher valency numbers (Pu^{4+}, U^{6+}, and Np^{5+}). The other two actinides are independent on GLOBAL:OXSTAT, and are assigned as Am^{3+} and Th^{4+}. The specific valency number (i.e. +3, +4, +5, or +6 oxidation state) determines the SOLMOD[valency] parameter name prefix (i.e. the database "material" name), e.g. SOLMOD3, SOLMOD4, SOLMOD5, or SOLMOD6. The name "SOLMOD" refers to the Solubility Model, i.e. the premise that each actinide in a specific oxidation state can be represented by an analog actinide (Appendix-SOTERM (US DOE 2014, and 2019)). The baseline solubilities (SOLMOD[valency]:SOL[S|C]OH[BV]), solubility uncertainty modifier (SOLMOD[valency]:SOLVAR), and the actinide-humic colloid proportionality constant (i.e. association factor) (PHUMOX[valency]:PHUM[S|C]IM) are all catalogued according to the valency number.

The simulation scenario (read as the command line argument -scenario) is used to determine the brine type, i.e. either Salado or Castile. The WIPP PA scenarios S1-BF, S4-BF, and S5-BF do not assume a borehole intrusion that encounters the Castile brine pocket, thus the Salado brine composition is selected. Scenarios S2-BF, S3-BF, and S6-BF assume a borehole intrusion that encounters the Castile brine pocket, thus the Castile brine composition is selected. The baseline solubilities (SOLMOD[valency]:SOL[S|C]OH[BV]) and the actinide-humic colloid proportionality constant (i.e. association factor) (PHUMOX[valency]:PHUM[S|C]IM) are all catalogued according to brine type (term S for Salado or C for Castile in the brackets).

The brine (volume) factor (GLOBAL:BRINEFAC[1]) is used to select the baseline solubility parameters. This is because the baseline solubilities employed in WIPP PA calculations are not truly intrinsic variables. The baseline solubilities depend on the concentration of organic ligands (acetate, citrate, EDTA, and oxalate) present in the waste-contaminated brine. Since the entire waste inventory of organic ligands is assumed to dissolve into the brine (which is consistent with the general assumption that all of the inventory is immediately available to mix with any brine that

[1] GLOBAL:BRINEFAC is not a PA parameter database value but typically set in an ALGEBRACDB pre-processing step before the PANEL calculations.

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may enter the repository), the baseline solubilities become implicitly dependent upon the volume of brine that is used to calculate the organic ligand concentrations. In WIPP PA, these baseline solubilities are calculated for several different brine volume bases, which correspond to multiples of the minimum volume of brine necessary for a direct brine release (DBR) event to occur. More details can be found in Brush and Domski (2013a-b). This multiple, or brine factor, is the numeric suffix (BV) on the baseline solubility parameter name SOLMOD[valency]:SOL[S|C]OH[BV] (however, a number is appended only if the factor is greater than 1).

The element name used to select the colloid solubility enhancement parameters ([actinide]:CONCMIN, [actinide]:CONCINT, [actinide]:CAPHUM, [actinide]:PROPMIC, [actinide]:CAPMIC), with the exception of the actinide-humic colloid proportionality constant (PHUMOX[valency]:PHUM[S|C]IM), which is catalogued according to the valency. Before PANEL calculation, the element with lower/higher oxidation state is used to select the colloid solubility enhancement parameters type in an ALGEBRACDB pre-processing step. When the oxidation state specific colloid solubility enhancement parameters are selected for PANEL calculations, the colloid solubility enhancement parameters are catalogued according to the actinide's oxidation state[2]:

$$\begin{aligned}
[actinide]\text{: CONCMIN} &= [actinide][valency]\text{: CONCMIN} \\
[actinide]\text{: CONCINT} &= [actinide][valency]\text{: CONCINT} \\
[actinide]\text{: CAPHUM} &= [actinide][valency]\text{: CAPHUM} \\
[actinide]\text{: PROPMIC} &= [actinide][valency]\text{: PROPMIC} \\
[actinide]\text{: CAPMIC} &= [actinide][valency]\text{: CAPMIC}
\end{aligned} \qquad \text{Eq. 4-1}$$

When the element specific colloid solubility enhancement parameters are selected for PANEL calculations, the colloid solubility enhancement parameters are catalogued according to the maximum of all parameter values of the valenced actinide. For Am and Th, Eq. 4-1 is used, because they have a single oxidation state.

For Pu, U and Np, which has lower and higher oxidation states, the colloid solubility enhancement parameters are defined (Eq. 4-2)[3]:

$$\begin{aligned}
[actinide]\text{: CONCMIN} &= max([actinide][lower\ valency]\text{: CONCMIN}, \\
&\quad [actinide][higher\ valency]\text{: CONCMIN})) \\
[actinide]\text{: CONCINT} &= max([actinide][lower\ valency]\text{: CONCINT}, \\
&\quad [actinide][higher\ valency]\text{: CONCINT}) \\
[actinide]\text{: CAPHUM} &= max([actinide][lower\ valency]\text{: CAPHUM}, \\
&\quad [actinide][higher\ valency]\text{: CAPHUM}) \\
[actinide]\text{: PROPMIC} &= max([actinide][lower\ valency]\text{: PROPMIC}, \\
&\quad [actinide][higher\ valency]\text{: PROPMIC}) \\
[actinide]\text{: CAPMIC} &= max([actinide][lower\ valency]\text{: CAPMIC}, \\
&\quad [actinide][higher\ valency]\text{: CAPMIC})
\end{aligned} \qquad \text{Eq. 4-2}$$

Once the proper model parameters have been selected, the total mobilization potentials can be calculated (Figure 4-1). The total mobilization potential is comprised of five terms: a dissolved concentration limit and four concentration limits that represent the actinide associated with

[2] This is done in an ALGEBRACDB pre-processing step.

[3] This is done in an ALGEBRACDB pre-processing step.

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dispersed "colloids" (mineral fragment, intrinsic, humic, and microbial). The dissolved concentration limit is calculated as the baseline solubility multiplied by 10 raised to the solubility uncertainty modifier (e.g. uncertainty multiplier of the log10 based baseline solubility). The mineral fragment-associated and intrinsic colloid-associated concentration limits are simply the input parameter values. The humic colloid-associated and microbial-colloid associated concentration limits are proportional to the previously calculated dissolved concentration limit and the respective proportionality constant. The humic colloid-associated concentration limit is subject to a maximum, or "cap", value that represents the actinide-specific sorption capacity of the theoretically maximum concentration of the dispersed colloid (it is assumed that the different actinides do not compete for sorption sites). This cap prevents the limits from becoming unrealistically large if the (e.g. stochastically determined) dissolved concentration limit is large. The microbial colloid model is selected with the GLOBAL:MICOL parameter value, which is input to the 2nd ALGEBRACDB pre-processing step input file (Section 5.0). The microbial colloid-associated concentration limit is subject to a cap value (CAPMIC; this cap value is biomass-based maximum value), when the biomass-based microbial colloid model is selected to use. When the toxicity-based microbial colloid model is selected to use, this concentration limit is subject to difference between CAPMIC (this cap value is toxicity-based maximum value) and the concentration limits of sub movables (dissolved + intrinsic colloids + mineral fragments + humic colloids). The final output parameter, LOGSOLM, is the log10 of the total mobilization potential value. PANEL also outputs each of the five terms as fractions of the total mobilization potential.

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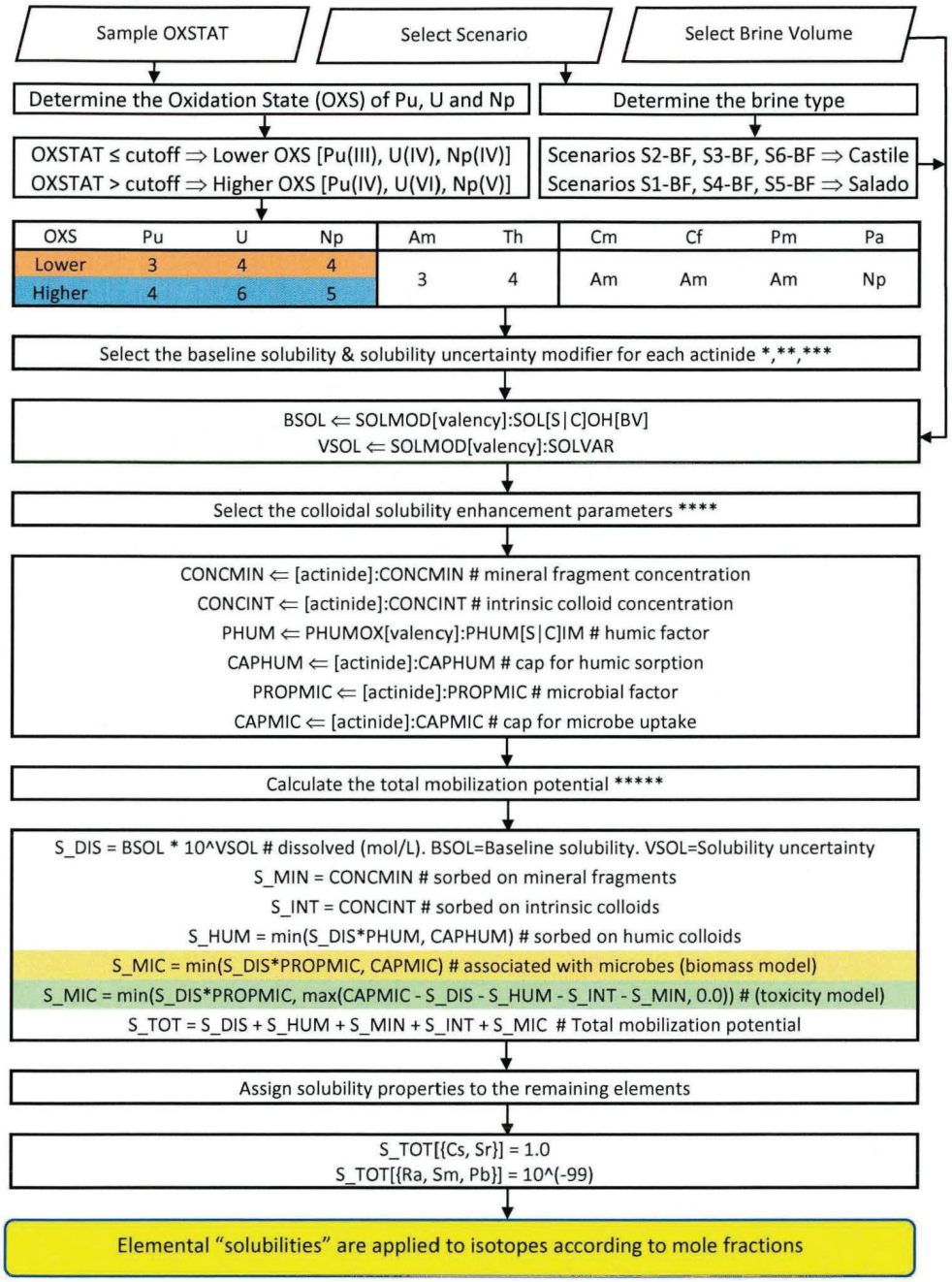

(*) Baseline solubilities are defined with respect to valency, not a particular element.
The premise is that each valency can be represented by an analog actinide [SOTERM-86].
(**) Cm, Cf, Pm, Pa are assumed the same solubilities as one of the 5 primary actinides.
(***) SOLMOD[5]:SOLVAR and SOLMOD[6]:SOLVAR are currently zero.
(****) The colloidal parameters are defined with respect to the element, except for PHUM.
(*****) CAPMIC *limits the amount of microbial colloids that can be mobilized in the presence of other mobilization processes* [Garner & Leigh 2005].

Figure 4-1. Flowchart for total mobilization potential (or mobile concentration limit) calculations using element solubility limit (or elemental solubility).l

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4.2 Instantaneous Mobilization Calculations

PANEL computes instantaneous (time-depenent) mobile concentrations as a function of time according to the available inventory and the resultant solubility limit of each radionuclide when the mole fraction of actinide isotope portioned the total mobilization potential of actinide. The instantaneous concentration (Eq. 4-3) is determined by a simple "saturation" type calculation – the lesser of the solubility limit and the resultant concentration if the entire available inventory of radionuclide were mobilized (i.e. the inventory-limited concentration) is selected:

$$C_j^t = min\left(C_j^k, \frac{I_{k,j}^t}{V_{br}}\right) = min\left(C_k X_j^k, \frac{I_{k,j}^t}{V_{br}}\right) = min\left(C_k \frac{I_{k,j}^t}{\sum_i I_{k,i}^t}, \frac{I_{k,j}^t}{V_{br}}\right) \quad \text{Eq. 4-3}$$

where the subscript j and i refer to the isotope of actinide element k, C_k refers to total mobilization potential of actinide k, C_j^k refers to the solubility limit of isotope j of actinide k, X_j^k refers to the instantaneous mole fraction of isotope j to actinide k, and $I_{k,i}^t$ and $I_{k,j}^t$ refer to the entire available inventory of i and j in waste area (*i.e.* 1 panel for CRA14, and 5 panels for CRA19). V_{br} refers to the brine volume of the waste area. Three sequential steps arise in computing this term.

The first step computes the inventory-limited mass (= entire available inventory). This inventory limit, $I_{k,j}^t$, is simply the available radionuclide inventory that is in the waste area.

Secondly, the total mobilization potentials are defined with respect to actinide elements (Section 4.1), but PANEL tracks a set of radionuclides wherein there are multiple isotopes of several of the elements. Thus an appropriate isotope specific solubility limit must be computed based on the element specific total mobilization potential (Eq. 4-3). PANEL does so by calculating the isotope-to-element mole fraction for each radionuclide in the inventory, and multiplying the elemental concentration limit by this mole fraction. PANEL employs a mid-point (in time) weighting scheme to evaluate radionuclide inventory for solubility calculations (Eq. 4-4 through Eq. 4-7):

$$I_{k,j}^{avg,t} = 0.5 \times \left(I_{k,j}^t + I_{k,j}^{t+\Delta t}\right) \quad \text{Eq. 4-4}$$

$$I_k^{avg,t} = \sum_{j \in k} I_{k,j}^{avg,t} \quad \text{Eq. 4-5}$$

$$X_j^{avg,k} = \frac{I_{k,j}^{avg,t}}{I_k^{avg,t}} \quad \text{Eq. 4-6}$$

$$C_j^t = min\left(C_k X_j^{avg,k}, \frac{I_{k,j}^{avg,t}}{V_{br}}\right) = min\left(C_k \frac{I_{k,j}^{avg,t}}{I_k^{avg,t}}, \frac{I_{k,j}^{avg,t}}{V_{br}}\right) \quad \text{Eq. 4-7}$$

where I refers to the instantaneous inventory mass (in moles), and X refers to the mole fraction. The superscript avg refers to a value averaged between the beginning and end of a time step (t and $t + \Delta t$). This portioning of the elemental total mobilization potential must be performed at each timestep because the isotope-element mole fractions vary over time since different radionuclides decay at different rates. Though in WIPP PA the total mobilization potential, C_k, of actinide k is time-independent, C_j^k, $I_{k,j}^{avg,t}$ and C_j^t varies over time.

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The third step computes the concentrations as a function of time, i.e. coupling the inventory decay calculations with the instantaneous mobilization calculations. The decay calculations are described in the next section (Section 4.3), but here we are concerned with the time interval used in calculating the concentrations. As indicated in Eq. 4-4 through Eq. 4-6, the instantaneous concentration represents an average concentration over the forward timestep. PANEL averages over a forward step of 50 years at all time steps, while at the final timestep the forward step of 10 years is used.

Eq. 4-3 through Eq. 4-6 show additionally that all of these steps are controlled by the instantaneous (average) inventory mass, $I_{k,j}^{avg,t}$ and the mole fraction, $X_j^{avg,k}$.

4.3 Decay Calculations

PANEL models the decay and ingrowth of 30 radionuclides that are subject to subject to the abridged decay chains (Figure 4-2). The last radionuclide in a chain decays to a stable isotope that is not tracked in PANEL.

The first four chains (Figure 4-2(a-d)) follow (or are collinear to) the Uranium Series, the Actinium Series, the Thorium Series, and the Neptunium Series (KAPL 2002). The abridged chains were originally formulated to include radionuclides called out in 40 CFR 191 (i.e. radionuclides with half-lives longer than 20 years) and deemed potentially significant to releases based on criteria set forth in the CCA Appendix-WCA (US DOE 1996a). Certain radionuclides with half-lives longer than 20 years were screened out based on small initial inventory and small potential for ingrowth during the 10,000 year regulatory period (CCA Appendix WCA (US DOE 1996a), Kicker and Zeitler (2013), and Kicker (2019)). Certain radionuclides with half-lives shorter than 20 years, but with significant inventories and which decay to radionuclides with half-lives longer than 20 years are included (e.g. ^{241}Pu).

In the abridged chains, intermediate radionuclides with short half-lives (i.e. less than 2 years) are excluded (PANEL assumes the parent decays directly to the next long-lived radionuclide), and stable isotopes are not tracked. Furthermore the Uranium Series chain omits ^{250}Cf, ^{246}Cm, and ^{250}Cm; the Actinium Series chain omits ^{251}Cf, ^{247}Cm, ^{247}Bk, and ^{227}Ac; the Thorium Series chain omits ^{236}Pu and ^{232}U (^{236}Np is not listed in the inventory); and the Neptunium Series chain omits ^{249}Cf.

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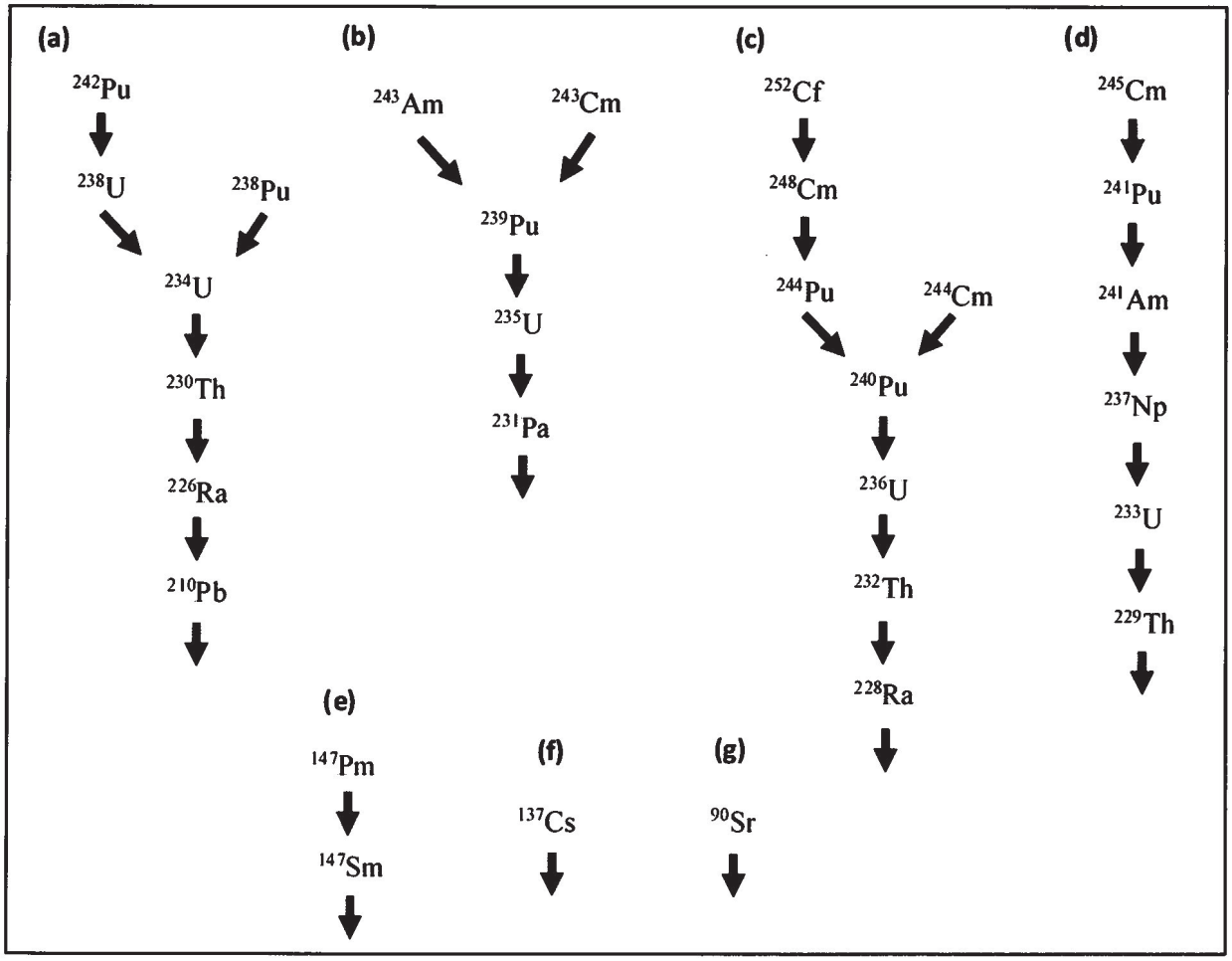

Figure 4-2. Abridged decay chains modeled in PANEL. The last isotope in a chain decays to the other isotope that is not tracked in PANEL.

PANEL performs the decay and ingrowth calculations by, for each of the 30 radionuclides, assembling a partial chain containing up to four generations (i.e. the originator and up to three generations of progeny), and calculating the (partial) updated amounts (in moles) of each member of the partial chain due to the decay of the originator. The partial updated amount of each radionuclide is summed across the 30 partial chains to give the total decay/ingrowth of each radionuclide. This is performed at each requested timestep – the inventory at the beginning of the timestep (i.e. time t) is used to calculate the updated inventory amounts at time $t + \Delta t$.

The Bateman equations (Bateman, 1910), which are a family of analytical solutions to the differential equations of radionuclide decay/ingrowth along a linear decay chain, are used to calculate the inventory updates at each timestep. The Bateman equations are commonly presented in the following form (adapted from Bateman (1910) and Vondy (1962)):

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$$N_{m,j,i}(t) = N_{m,m,1}(0)\left(\prod_{n=1}^{i-1}\lambda_n\right)\left[\sum_{n=1}^{i}\frac{\exp(-\lambda_n t)}{\prod_{l=1,l\neq n}^{i}(\lambda_l-\lambda_n)}\right] \quad \text{Eq. 4-8}$$

where $N_{m,m,1}(0)$ is initial amount of radionuclide m (decay parent) in moles (which, for our use case corresponds to the beginning of the timestep $t = 0$), $N_{m,j,i}(t)$ is the amount of radionuclide j ($(i-1)$th generation decay daughter) at time t, and λ_n is the decay constant of the $(n-1)$th generation decay daughter of radionuclide m (the decay constant is $ln(2)$ divided by the half-life).

PANEL uses the term inside the square brackets to calculate the decay/ingrowth along the partial chains. Because PANEL forms a partial chain for each of the 30 radionuclides, only the first term in the outer summation is included (i.e. only the "first" member of the partial chain is "initially present"). Thus, for ^{241}Am, the equations for the four members simplify to:

$$N_{AM241,AM241,1}(t) = N_{AM241,AM241,1}(0)\exp(-\lambda_1 t) \quad \text{Eq. 4-9}$$

$$N_{AM241,NP237,2}(\mathrm{t}) = N_{AM241,AM241,1}(0)\,\lambda_1\left(\frac{\exp(-\lambda_1 t)}{\lambda_2-\lambda_1}+\frac{\exp(-\lambda_2 t)}{\lambda_1-\lambda_2}\right) \quad \text{Eq. 4-10}$$

$$N_{AM241,U233,3}(t) = N_{AM241,AM241,1}(0)\,\lambda_1\lambda_2\left(\frac{exp(-\lambda_1 t)}{(\lambda_2-\lambda_1)(\lambda_3-\lambda_1)} + \frac{exp(-\lambda_2 t)}{(\lambda_1-\lambda_2)(\lambda_3-\lambda_2)} + \frac{exp(-\lambda_3 t)}{(\lambda_1-\lambda_3)(\lambda_2-\lambda_3)}\right) \quad \text{Eq. 4-11}$$

$$N_{AM241,TH229,4}(t) = N_{AM241,AM241,1}(0)\,\lambda_1\lambda_2\lambda_3\left(\frac{exp(-\lambda_1 t)}{(\lambda_2-\lambda_1)(\lambda_3-\lambda_1)(\lambda_4-\lambda_1)} + \frac{exp(-\lambda_2 t)}{(\lambda_1-\lambda_2)(\lambda_3-\lambda_2)(\lambda_4-\lambda_2)} + \frac{exp(-\lambda_3 t)}{(\lambda_1-\lambda_3)(\lambda_2-\lambda_3)(\lambda_4-\lambda_3)} + \frac{exp(-\lambda_4 t)}{(\lambda_1-\lambda_4)(\lambda_2-\lambda_4)(\lambda_3-\lambda_4)}\right) \quad \text{Eq. 4-12}$$

Figure 4-2(d) shows that the partial decay chain for ^{241}Am (n = 1) is ^{241}Am ➔ ^{237}Np ➔ ^{233}U ➔ ^{229}Th, giving that the first generation decay daughter (n = 2) is ^{237}Np, the 2nd generation (n = 3) is ^{233}U, and the 3rd generation (n = 4) is ^{229}Th.

PANEL accumulates the partial updated amount of each radionuclide over the 30 partial chains

$$I_{k,j}^{t} = \sum_{m} N_{m,j,i}(t) \quad \text{Eq. 4-13}$$

where the the isotope, j, of interest is only present in a subset of the partial decay chain of m.

Unfortunately, this particular form of the Bateman equations can suffer from round-off error, primarily because fractions that may be different orders of magnitude in size are being summed and differenced. The fourth generation and greater terms are susceptible, especially when the

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exponential terms are similar in magnitude. PANEL addresses the issue by setting the third generation and fourth generation terms equal to zero if they become less than zero. PANEL also includes logic to drop members of the partial chains if $t/t_{1/2} \geq \Delta t$, that is if the (current) time is very large compared to the half-life of the radionuclide.

4.4 Mass Balance Calculations

PANEL performs a mass balance to calculate the inventory changes over time and to combine the losses/gains due to both decay/ingrowth and (potentially) mobilization and discharge. The mass balance is performed in all of PANEL's run modes.

The mass balance equation for the waste area is

$$\{accumulation\} = \{mass\ flux\ in\} - \{mass\ flux\ out\} - \{decay\} + \{ingrowth\} \quad \text{Eq. 4-14}$$

PANEL always simulates in a 1×1×1 grid cell dimension, considering no $\{mass\ flux\ in\}$. In PANEL, brine that flows into the waste area is assumed to contain no radionuclides, thus brine-flow-rate is multiplied by a concentration of zero. The mass balance equation, in differential form, becomes:

$$\frac{dI_{k,j}^t}{dt} = -q_{out}^t C_j^t - \lambda_j I_{k,j}^t + \sum_m \lambda_p N_{m,p,i-1}(t)$$
$$\frac{dI_{k,j}^t}{dt} = -q_{out}^t C_j^t - \lambda_j \sum_m N_{m,j,i}(t) + \sum_m \lambda_p N_{m,p,i-1}(t) \quad \text{Eq. 4-15}$$

where j is the decay daughter of a decay parent p in the partial decay chain of a radionuclide m (e.g. $m \rightarrow \cdots \rightarrow p \rightarrow j \rightarrow \cdots$). At the same time, j is the $(i-1)$th generation decay daughter of m. q_{out}^t is brine flow out rate at time t. The first term in Eq. 4-15 represents the discharge rate of radionuclide j, the second term represents its decay rate, and the last term represents the ingrowth rate (the growth rate of j due to decay of its parent isotopes).

The mass balance is solved discretely in three stages within each timestep. First PANEL calculates decay/ingrowth of the entire inventory (i.e. regardless of whether it is stationary or mobile) to determine a tentative updated inventory amount at the end of the timestep, $I_{k,j}^{t+\Delta t}$ (as described in Section 4.3). PANEL then computes the time-averaged inventory within the timestep size (Eq. 4-4)

Next, PANEL uses this time-averaged inventory to compute the instantaneous mobile concentrations C_j^t (Eq. 4-7) (as described in Section 4.2). And lastly, PANEL uses the brine discharge rate q along with the mobile concentrations and the tentatively updated inventory to determine the updated inventory for the next timestep (Eq. 4-16):

$$I_{k,j}^{t+\Delta t} \Leftarrow max\left(I_{k,j}^{t+\Delta t} - q_{out}^t C_j^t \Delta t, 0\right) \quad \text{Eq. 4-16}$$

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The cumulative (in time) radionuclide discharge, $R_j(t)$, is calculated by integrating the mass flux out over time:

$$R_j(t) = \int_0^t q_{out}^t C_j^t dt \qquad \text{Eq. 4-17}$$

PANEL calculates this in discrete form as

$$R_j(t) = \sum_{l=1}^{n} C_j^{t_{l-1}} \left(q_{out}^{t_l} - q_{out}^{t_{l-1}}\right) \Delta t_l \qquad \text{Eq. 4-18}$$

where $\Delta t_l = t_l - t_{l-1}$ and n represents the total number of Δt_l time steps at a time step t. The same mass balance equation applies in all of PANEL's "run modes" – if there is no brine discharge, the q_{out} term is simply zero (the equation is still valid). However, the "bounding box" of the mass balance differs. In the DECAY run mode (in which PANEL outputs the inventory in the repository versus time), the mass balance is performed over the entire inventory (i.e. the inventory contained in the entire repository). In the CONCENTRATION run mode (in which PANEL outputs the mobile concentrations in the waste area versus time), the mass balance is performed over REFCON:NUMPANEL waste area. The inventory is scaled first by REFCON:INVSCALE (a factor which represents the volumetric ratio of waste contained in a single waste panel to that contained in the entire repository), then by REFCON:NUMPANEL, the number of waste panels (waste area) over which the mass balance should be performed. Because the static brine volume, REFCON:PANDFVOL, represents the volume of brine contained in a single waste panel, it too is scaled by REFCON:NUMPANEL. In the STANDARD run mode (in which PANEL outputs the cumulative discharge from the waste area versus time), PANEL scales the inventory in the same manner (multiplying it by both RECON:INVSCALE and REFCON:NUMPANEL). Both the brine volume and brine outflow rate (which are read in from a "flux" CDB file) are assumed to already represent the number of waste panels of interest, thus those values are not further scaled.

4.5 Lumping

PANEL contains functionality to lump together select radionuclides at each timestep for output reporting purposes (no internal mass balance calculations are performed on the lumped species). The lumping motivation and methodology is described further in Leigh and Trone (2005), also CCA Appendix-PANEL (US DOE, 1996b).

The lumping of select isotopes of actinide elements into a "lumped" species is notated with "L" following atomic weight number like ^{241L}Am, ^{238L}Pu, ^{239L}Pu, ^{234L}U and ^{230L}Th. The inventory of each select isotope (j) is added to the inventory of the lumped radionuclide ($lumped$) on a mole method, where $mole$ can be described with activity (Ci) and a conversion (mole per curie) factor (f_{mCi}):

$$mole = [Ci] \times [f_{mCi}] = [Ci] \times \left[\frac{(CITOBQ)(t_{1/2})}{(AVOGADRO)(ln2)}\right] \qquad \text{Eq. 4-19}$$

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$CITOBQ$ is a conversion factor from curie to Becquerel (= 3.7×10^{10}), $t_{1/2}$ is the half-life of j (in units of second), and $AVOGADRO$ is the Avogadro's constant (= 6.022137×10^{23}). $t_{1/2}$ of *lumped* is assigned to equal to the halflife of its namesake select (constituent) radionuclide such as $t_{1/2}^{PU239L} = t_{1/2}^{PU239}$, $t_{1/2}^{U234L} = t_{1/2}^{U234}$, and so on. Eq. 4-19 through Eq. 4-21 are utilized to transform the lumped radionuclide in terms of activity (Eq. 4-22 through Eq. 4-25).

$$mole^{lumped} = Ci^{lumped}\left[\frac{(CITOBQ)(t_{1/2}^{lumped})}{(AVOGADRO)(ln2)}\right] \quad \text{Eq. 4-20}$$

$$mole^{j} = Ci^{j}\left[\frac{(CITOBQ)(t_{1/2}^{j})}{(AVOGADRO)(ln2)}\right] \quad \text{Eq. 4-21}$$

Total moles of *lumped* are sum of constituent radionuclide moles (mole addition method in Leigh and Trone (2005)):

$$mole^{lumped} = \sum_j mole^{j} \quad \text{Eq. 4-22}$$

$$Ci^{lumped}\left[\frac{(CITOBQ)(t_{1/2}^{lumped})}{(AVOGADRO)(ln2)}\right] = \sum_j Ci^{j}\left[\frac{(CITOBQ)(t_{1/2}^{j})}{(AVOGADRO)(ln2)}\right] \quad \text{Eq. 4-23}$$

$$Ci^{lumped}t_{1/2}^{lumped} = \sum_j Ci^{j}t_{1/2}^{j} \quad \text{Eq. 4-24}$$

$$Ci^{lumped} = \sum_j Ci^{j}\frac{t_{1/2}^{j}}{t_{1/2}^{lumped}} \quad \text{Eq. 4-25}$$

The basis is to maximize the activity (curies) of the lumped radionuclide by setting $t_{1/2}^{j}/t_{1/2}^{lumped} = 1.0$ when a constituent radionuclide has shorter and equal half-life than the lumped radionuclide (activity addition method in Leigh and Trone (2005)). Therefore, when combining the Pu isotopes, ^{242}Pu, ^{240}Pu, and ^{239}Pu into ^{239L}Pu, the curies of ^{240}Pu and ^{239}Pu are added to the curies of ^{239L}Pu but the curies of ^{242}Pu multiplied by the relative half-life ratio, $t_{1/2}^{PU242}/t_{1/2}^{PU239L}$ (= $t_{1/2}^{PU242}/t_{1/2}^{PU239}$), are added to the curies of ^{239L}Pu (Eq. 4-26), where the half-lives of ^{242}Pu, ^{240}Pu, and ^{239}Pu are 1.221×10^{13}, 2.063×10^{11}, and 7.594×10^{11} seconds:

$$Ci^{PU239L} = Ci^{PU239} + Ci^{PU240} + Ci^{PU242}\frac{t_{1/2}^{PU242}}{t_{1/2}^{PU239}} \quad \text{Eq. 4-26}$$

^{241L}Am is treated uniquely. Because ^{241}Pu is a parent of ^{241}Am and it has a short half-life (~14 years), we assume that all of the ^{241}Pu "instantaneously" converts to ^{241}Am. Thus ^{241}Pu and ^{241}Am are simply combined based on Eq. 4-26.

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Table 4-1 lists the five lumped radionuclides that are tracked in PA calculations, the radionuclides that comprise each lumped radionuclide, and the unit basis used when combining quantities. As described in Leigh and Trone (2005), the inventory of each constituent radionuclide is added to the inventory of the lumped radionuclide on either a mole or activity addition method.

Table 4-1. Lumped radionuclides, where $t_{1/2}$ is the half-life of a constituent radionuclide and Ci represents a radionuclide in Curie unit.

Lumped Radionuclide	Constituent Radionuclides (in Curies)
^{241L}Am	$Ci^{AM241L} = Ci^{AM241} + Ci^{PU241}\left(t_{1/2}^{PU241}/t_{1/2}^{AM241}\right)$
^{239L}Pu	$Ci^{PU239L} = Ci^{PU239} + Ci^{PU240} + Ci^{PU242}\left(t_{1/2}^{PU242}/t_{1/2}^{PU239}\right)$
^{238L}Pu	$Ci^{PU238L} = Ci^{PU238}$
^{234L}U	$Ci^{U234L} = Ci^{U234} + Ci^{U233}$
^{230L}Th	$Ci^{TH230L} = Ci^{TH230} + Ci^{TH229}$

PANEL, during its total mobilization potential calculations, also calculates the log10 of the solubility limit values for the lumped radionuclides. It uses an input factor, LSOLDIF, which represents a maximum of negative log10 of the instantaneous mole fraction of the lumped radionuclide that is the sum of the isotope-to-element mole fractions for all isotopes included in the lumped species (due to its own decay/ingrowth rate the individual inventory of each radionuclde is changed with times, and resulting mole fraction is instantaneous). ^{234L}U, ^{238L}Pu, and ^{230L}Th are shown to have mole fractions much smaller than one, while maximum mole fractions of ^{241L}Am and ^{239L}Pu are close to one (for these lumped radionuclides, LSOLDIF ~ 0.0). PANEL subtracts the LSOLDIF value from the LOGSOLM value of the respective element to determine the solubility limit (LOGSOLM, used for both elements and radionuclides in PANEL) value for ^{234L}U, ^{238L}Pu, and ^{230L}Th (which is equivalent to multiplying the total mobilization potential by the mole fraction). Further details are given in Garner and Leigh (2005) and CCA Appendix-PANEL (US DOE, 1996b).

4.6 EPA Release Units

PANEL outputs radionuclide amounts with material units of kg, curies, and EPA release units. Because the EPA release unit is non-standard, the unit conversion procedure is described here. Appendix A of 40 CFR 191 (US EPA, 1993) defines release limits for containment requirements of the regulated radionuclides emplaced in WIPP. These release limits (EPAREL) have units Ci but are normalized with respect to a "waste unit factor" (WUF). The WUF is defined as "*an amount of transuranic wastes containing one million curies (10^6 Ci) of alpha-emitting transuranic radionuclides with half-lives greater than 20 years*" (all three clauses must be true for a radionuclide to be included in the WUF). The WUF acts as an normalization factor when scaling unit Ci to "EPA Units." For reference, the WUF is calculated as

$$WUF = \frac{\sum_j A_j}{10^6 Ci} \qquad \text{Eq. 4-27}$$

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where A_j is the inventory of a radionuclide j in Ci units, but it is calculated external to PANEL (see Kicker and Zeitler (2013), Kicker (2019) and Kicker (2022) for further details). Eq. 4-27 indicates that the larger initial radionuclide inventory results in the larger WUF value. The unit conversion factor from Ci to EPA Units is:

$$\frac{EPA\ unit}{Ci\ unit} = \frac{1}{EPAREL \cdot WUF} \qquad \text{Eq. 4-28}$$

This unit conversion factor is radionuclide-specific because the EPAREL parameter is dependent on radionuclide. Eq. 4-28 also indicates that a larger WUF embodies a larger number of Curies in an EPA unit. PANEL assigns radionuclides with zero EPA release limits (EPAREL) – ^{252}Cf, ^{244}Cm, ^{147}Pm, ^{241}Pu, and ^{228}Ra – a large value (1.0×10^{30}) so that the resulting amount is negligibly small.

4.7 Time Translation

PANEL includes unique functionality to translate the brine volume and brine discharge data (as supplied in the flux input file) in time. This was formulated to aid the WIPP PA code CCDFGF estimate releases as a function of repository intrusion time while reducing the need to perform additional BRAGLFO simulations.

The "intrusion time" information is supplied to PANEL via the command line option "-timeint". Unfortunately, the value required is not necessarily the true intrusion time and is also not a time offset. Rather, PANEL uses the input "intrusion time" TIMEINT to calculate a time offset DELTIME by which it translates the time values in brine volume and brine flux arrays. For historical reasons, the offset is defined with respect to 2000 years:

$$\text{DELTIME} = \text{TIMEINT} - 2000 \qquad \text{Eq. 4-29}$$

$$\text{TIMEINT} = \text{DELTIME} + 2000 \qquad \text{Eq. 4-30}$$

Thus, for a desired offset (e.g. time shift) of 6000 years, PANEL should be supplied TIMEINT = 6000 + 2000 = 8000. For a desired offset of -1000 years, PANEL should be supplied TIMEINT = -1000 + 2000 = 1000.

A negative time offset may require PANEL to extrapolate the time series brine volume and brine discharge data. In this case, PANEL performs a linear extrapolation based on the last two data points, and extrapolates to an additional 2100 years.

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5.0 INPUT AND OUTPUT FILES

PANEL relies upon two binary CDB files for its input data. The primary "input" CDB file contains static parameters related to mass balance volumes, unit conversions, atomic properties, radionuclide inventory, and concentration limits. This file is typically created by the WIPP PA code MATSET and may be further modified by POSTLHS and ALGEBRACDB. The secondary "flux" CDB file is only used in the "STANDARD" (i.e. intrusion) run mode and contains brine volume and brine outflow data as a function of time. That file is typically created by ALBEGRACDB based on BRAGFLO output data.

PANEL version 5.02 has been modified to utilize separate (decoupled) oxidation state cutoff values for Pu, U and Np. The cutoff values are typically read from the WIPP PA database through MATSET. The MATSET input file for PANEL is shown in Section 11.1. The used MATERIAL blocks are: block number 67 for AM+3, 68 for PU+3, 69 for PU+4, 70 for TH+4, 71 for U+4, 72 for U+6, 73 for NP+4, and 74 for NP+5 (yellow highlighted in Section 11.1). Oxidation state cutoff parameters (OXCUTOFF) are set to read from MATERIAL blocks PU (block # 40), U (block # 44) and NP (block # 36). In this file, oxidation state specific colloid enhancement parameters (CONCMIN, CONCINT, CAPHUM, CAPMIC, PROPMIC) are set to read from these MATERIAL blocks (block # 67 – 74) as well. The oxidation state specific values are translated into the colloid parameters used by PANEL in the 3rd ALEGEBRACDB step.

Given a set of mutually exclusive options of colloid enhancement parameters, which has to be oxidation state specific or element specific, and microbial colloid model, which has to be biomass-based or toxicity-based, PANEL calculates total mobilization potentials. Two ALGEBRACDB input parameters MICOL and ELEOXSTA determine colloid enhancement parameters type and microbial colloid model type, shown in Table 5-1. These two input parameters values are input to the ALGEBRACDB input files, *alg2_panel_bm.inp* (where *m* represents the brine volume multiplier (= 1, 2, 3, 4, 5)). *alg2_panel_b1.inp* is shown in Section 11.2.

Table 5-1. Types of the colloid enhancement parameters and microbial colloid model that are selected by the ALGEBRACDB input parameters MICOL (= 0 or 1) and ELEOXSTA (= 0 or 1).

MICOL	ELEOXSTA	Type of Parameter and Model
0	0	Biomass based microbial colloid model Oxidation state specific colloid enhancement parameters
0	1	Biomass based microbial colloid model Element specific colloid enhancement parameters
1	0	Toxicity based microbial colloid model Oxidation state specific colloid enhancement parameters
1	1	Toxicity based microbial colloid model Element specific colloid enhancement parameters

Both microbial colloid models (biomass- and toxicity-based) are embedded to PANEL code, and MICOL input parameter picks microbial colloid model type for total mobilization potential calculations. However, the PANEL code needs to be given a minimal modification and be more flexible in choosing colloid enhancement parameters types, which has to depend on ELEOXSTA

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parameter but MICOL = 1 forces to use toxicity-related microbial colloid enhancement parameter (PROPMIC and CAPMIC) values. These needs design to select colloid enhancement parameter type during the 3rd ALGEBRACDB step. Section 11.3 describes use of ELEOXSTA and shows the ALGEBRACDB input file, *alg3_panel_bm.inp*, used for this step when $m = 1$.

PANEL is designed to use colloid enhancement parameter values in MATERIAL blocks of AM, PU, TH, U and NP, so the 3rd ALGEBRACDB step has to assign select colloid enhancement parameters to these MATERIAL blocks. Table 5-2 lists the PU MATERIAL block that is assigned in Section 11.3. Firstly comparison of OXSTAT and PU:OXCUTOFF parameter values determines the oxidation state of Pu, which indicates the MATERIAL block for colloid enhancement parameters: PU+3 block for +III oxidation state and PU+4 block for +IV oxidation state. Currently the existing IF-statements in the ALGEBRACDB code are IFEQ0 (*argument = 0*), IFLT0 (*argument < 0*) and IFGT0 (*argument > 0*), and no IF-statement corresponding to (*argument ≤ 0* exist. To approximate OXSTAT ≤ PU:OXCUTOFF condition, OXCUTDIF parameter (of very small value, here *1.0E-10* is used) is introduced and used as OXSTAT < (PULOXCUTOFF + OXCUTDIF).

Table 5-2. PU MATERIAL block in the 3rd ALGEBRACDB input file in Section 11.3.

```
!
! PU(III), or PU(IV)
LIMIT BLOCK 40
OXCUT=OXSTAT[B:1]-OXCUTOFF
OXCUTDIF=1.0E-10
CONCINT=IFEQ0(ELEOXSTA[B:1],IFLT0(OXCUT-OXCUTDIF,CONCINT[B:68], &
        CONCINT[B:69]), MAX(CONCINT[B:68],CONCINT[B:69]))
CONCMIN=IFEQ0(ELEOXSTA[B:1],IFLT0(OXCUT-OXCUTDIF,CONCMIN[B:68], &
        CONCMIN[B:69]), MAX(CONCMIN[B:68],CONCMIN[B:69]))
CAPMIC=IFEQ0( ELEOXSTA[B:1],IFLT0(OXCUT-OXCUTDIF,CAPMIC[B:68] , &
        CAPMIC[B:69] ), MAX(CAPMIC[B:68] ,CAPMIC[B:69] ))
PROPMIC=IFEQ0(ELEOXSTA[B:1],IFLT0(OXCUT-OXCUTDIF,PROPMIC[B:68], &
        PROPMIC[B:69]), MAX(PROPMIC[B:68],PROPMIC[B:69]))
CAPHUM=IFEQ0( ELEOXSTA[B:1],IFLT0(OXCUT-OXCUTDIF,CAPHUM[B:68] , &
        CAPHUM[B:69] ), MAX(CAPHUM[B:68] ,CAPHUM[B:69] ))
```

5.1 "Input" CDB Files

Table 5-3 through Table 5-9 list the parameters that PANEL reads from the "input" CDB file along with the default values used if the parameter is not present. The parameters are organized according to the CDB file "Element Block" which typically corresponds to a "Material" in the WIPP PA Parameter Database. In general, PANEL does not check the validity of the parameter values since most come from the WIPP PA Parameter Database.

Table 5-4 lists the radionuclide specific parameters (whole-repository initial inventory amounts and atomic properties) for the 30 radionuclides of interest. Table 5-5 lists the default values used for the radionuclide atomic properties and EPA release limits. These values are consistent with

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those found in the WIPP PA Parameter Database, with the exception of the EPAREL values for those radionuclides with no release limits. PANEL assigns any radionuclide with a release limit of zero (i.e. no release limit) a very large number (1.0×10^{30}) instead. Thus, when that radionuclide's amount is expressed in EPA release units, that number will be negligibly small.

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Table 5-3. Problem specification, mass balance, and unit conversion parameters.

Block	Property	Units	Default	Description
GLOBAL	OXSTAT	N/A	0.0	Continuous variable used to establish the oxidation condition of the brine. When OXSTAT≤OXCUTOFF, the brine is reducing, when OXSTAT>OXCUTOFF, the brine is oxidizing.
GLOBAL	MICOL	N/A	0	Flag used to define microbial colloid model type: biomass-based microbial colloid model (MICOL=0) or toxicity-based microbial colloid model (MICOL=1).
GLOBAL	BRINEFAC	N/A	1.0	Brine (volume) factor (1, 2, 3, 4, or 5) used to select the baseline solubility parameters SOLMOD[n]:SOL[S|C]OH[BRINEFAC]. The brine factor corresponds to the multiple of the brine volume basis used to calculate the baseline solubilities. If BRINEFAC =1, no numeric suffix is added to the baseline solubility parameter name.
REFCON	NUMPANEL	N/A	1.0	Number of waste panels to include in the mass balance. Not used in DECAY mode. Used to scale the inventory in both CONCENTRATION and STANDARD modes. Scales the brine volume (PANDFVOL) in CONCENTRATION mode, but not in STANDARD mode (because the brine volume in that case comes from time-varying BRAGFLO data).
REFCON	INVSCALE	N/A	1.0	Inventory scaling factor used to scale the inventory in the entire repository (INVCHD and INVRHD) to that contained in a single, representative waste panel.
REFCON	PANDFVOL	m^3	1000.0	Static brine volume contained in a single waste panel. Only used in CONCENTRATION mode. If not included in the CDB file, PANEL attempts to read DBRMINBV.
GLOBAL	DBRMINBV	m^3	1000.0	Minimum brine volume, contained in the entire repository, necessary for a DBR. PANEL attempts to read this value if PANDFVOL is not included in the CDB file, but it is otherwise not directly used by PANEL.
REFCON	YRSEC	s/yr	0.0	Number of seconds in a year (annum). The WIPP convention is to use mean solar tropical years.
REFCON	CITOBQ	Bq/Ci	3.7×10^{10}	Number of becquerels in a curie.
REFCON	AVOGADRO	1/mol	6.022045×10^{23}	Avogadro constant (number per mole). This historical default value was used in previous versions of PANEL.
BOREHOLE	WUF	$Ci / 10^6 Ci$	3.44	WIPP inventory Waste Unit Factor. Number of millions of curies of radionuclides that (1) are transuranic, (2) are α-emitting, and (3) have half-lives greater than 20 years contained in the inventory.
WAS_AREA	PROBDEG	N/A	1.0	Probability of plastics/rubber biodegradation in the event of microbial gas generation. In PANEL it is used to determine if microbial colloids are to be modeled. True if PROBDEG>0.

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Table 5-4. Radionuclide specific property parameters

Property	Units	Default	Description
INVCHD	*Ci*	0.0	Activity of radionuclide inventory contained in waste that is classified as "contact handled".
INVRHD	*Ci*	0.0	Activity of radionuclide inventory contained in waste that is classified as "remote handled".
ATWEIGHT	kg/mol		Atomic mass
HALFLIFE	s		Isotope half life
EPAREL	*Ci* / WUF		EPA release limit. Used, along with the WUF, to convert radionuclide activity to EPA release units.

Table 5-5. Default values for radionuclide parameters (MATERIAL:PROPERTY)

Radionuclide	MATERIAL parameter	PROPERTY parameter		
		ATWEIGHT (kg/mol)	HALFLIFE (s)	EPAREL (*Ci*/WUF)
^{241}Am	AM241	2.41057×10^{-1}	1.36400×10^{10}	100
^{243}Am	AM243	2.43061×10^{-1}	2.32900×10^{11}	100
^{252}Cf	CF252	2.52082×10^{-1}	8.32500×10^{7}	1.0×10^{30}
^{243}Cm	CM243	2.43061×10^{-1}	8.99400×10^{8}	100
^{244}Cm	CM244	2.44063×10^{-1}	5.71500×10^{8}	1.0×10^{30}
^{245}Cm	CM245	2.45065×10^{-1}	2.68200×10^{11}	100
^{248}Cm	CM248	2.48072×10^{-1}	1.07000×10^{13}	100
^{137}Cs	CS137	1.36907×10^{-1}	9.46700×10^{8}	1000
^{237}Np	NP237	2.37048×10^{-1}	6.75300×10^{13}	100
^{231}Pa	PA231	2.31036×10^{-1}	1.03400×10^{12}	100
^{210}Pb	PB210	2.09984×10^{-1}	7.03700×10^{8}	100
^{147}Pm	PM147	1.46915×10^{-1}	8.27900×10^{7}	1.0×10^{30}
^{238}Pu	PU238	2.38050×10^{-1}	2.76900×10^{9}	100
^{239}Pu	PU239	2.39052×10^{-1}	7.59400×10^{11}	100
^{240}Pu	PU240	2.40054×10^{-1}	2.06300×10^{11}	100
^{241}Pu	PU241	2.41057×10^{-1}	4.54400×10^{8}	1.0×10^{30}
^{242}Pu	PU242	2.42059×10^{-1}	1.22100×10^{13}	100
^{244}Pu	PU244	2.44064×10^{-1}	2.60700×10^{15}	100
^{226}Ra	RA226	2.26025×10^{-1}	5.04900×10^{10}	100
^{228}Ra	RA228	2.28031×10^{-1}	2.11430×10^{8}	1.0×10^{30}
^{147}Sm	SM147	1.46915×10^{-1}	3.37700×10^{18}	100
^{90}Sr	SR90	8.99080×10^{-2}	9.19000×10^{8}	1000
^{229}Th	TH229	2.29032×10^{-1}	2.31600×10^{11}	100
^{230}Th	TH230	2.30033×10^{-1}	2.43000×10^{12}	10
^{232}Th	TH232	2.32038×10^{-1}	4.43400×10^{17}	10
^{233}U	U233	2.33040×10^{-1}	5.00200×10^{12}	100
^{234}U	U234	2.34041×10^{-1}	7.71600×10^{12}	100
^{235}U	U235	2.35044×10^{-1}	2.22100×10^{16}	100
^{236}U	U236	2.36046×10^{-1}	7.38900×10^{14}	100
^{238}U	U238	2.38051×10^{-1}	1.41000×10^{17}	100

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Table 5-6 lists the lumped-radionuclide associated parameters. The Block (Material) name corresponds to one of: AM241L, PU238L, PU239L, TH230L, U234L. Table 5-7 lists the element-associated parameters (parameters used in the mobile concentration limit calculations that are catalogued by element). The Block (Material) name corresponds to one of: AM, NP, PU, TH, U.

Table 5-8 lists the Solubility Model associated parameters. Here the Block (Material) name corresponds to one of: SOLMOD3, SOLMOD4, SOLMOD5, SOLMOD6. The numeric suffix corresponds to the oxidation state of the element being modeled. The input CDB file should contain baseline solubility parameters (SOL[S|C]OH) for both the Salado brine (SOLSOH) and the Castile brine (SOLCOH). It should also contain baseline solubility parameters for each of the brine factors used in calculating the organic ligand concentrations, i.e. SOLSOH (1× brine factor) and SOLSOH2, SOLSOH3, SOLSOH4, and SOLSOH5 for 2×, 3×, 4×, and 5× brine factors. PANEL will use the no dilution factor baseline solubility parameter (SOLSOH or SOLCOH) if no parameter is supplied with a suffix corresponding to the GLOBAL:BRINEFAC value.

The solubility uncertainty parameter SOLVAR is also associated with SOLMOD[n], but unlike the baseline solubility parameters, it does not depend on the brine type or the dilution factor.

To maintain backwards compatibility with input files used in previous versions of PANEL, PANEL will first try to read the parameters SOLMOD[x]:SOLS and SOLMOD[x]:SOLC before invoking logic to select the appropriate SOLMOD[x]:SOLSOH[n] and SOLMOD[x]:SOLCOH[n] parameters based on the brine factor GLOBAL:BRINEFAC. Additionally, PANEL will attempt to read parameters SOL[AM3|TH4|NP5|U6]:SOL[S|C]IM if the parameter SOLMOD[x]:SOLVAR is not present (and defaults to zero if neither is found).

Table 5-6. Lumped radionuclide specific property parameter

Property	Units	Default	Description
LSOLDIF	N/A	0.0	Negative log10 of the mole fraction of the sum of the isotopes included in the lumped isotope to the sum of all of the isotopes of the element. The value is intended to represent a static, e.g. maximum, isotope:element mole fraction over the regulatory period. It is used to scale the respective elemental concentration limit to a value appropriate for the lumped radionuclide (i.e. LOGSOLM + LSOLDIF). See Garner and Leigh (2005).

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Table 5-7. Element associated property parameters. Values of these parameters except OXCUTOFF are assigned at an ALGEBRACDB pre-processing step.

Property	Units	Default	Description
CONCMIN	mol/L	0.0	Concentration limit of actinide associated with mobile mineral fragment colloids.
CONCINT	mol/L	0.0	Concentration limit of actinide associated with mobile intrinsic actinide colloids.
CAPHUM	mol/L	0.0	Maximum (cap) concentration limit of actinide associated with mobile humic colloids.
CAPMIC	mol/L	0.0	Maximum (cap) concentration limit of actinide associated with mobile microbes.
PROPMIC	N/A	0.0	Proportionality constant for concentration limit of actinides associated with mobile microbes.
OXCUTOFF	N/A	0.5	For Pu, U, and Np elements, threshold values are used to decide the oxidation condition of the brine. The value splits the OXSTAT distribution into two states, higher or lower.

Table 5-8. Solubility model associated property parameters

Property	Units	Default	Description
SOLSOH	mol/L	0.0	*Baseline* solubility in Salado brine (GWB) (includes complexation with organic ligands and equilibration with hydromagnesite).
SOLCOH	mol/L	0.0	*Baseline* solubility in Castile brine (ERDA-6) (includes complexation with organic ligands and equilibration with hydromagnesite).
SOLSOH[n]	mol/L	0.0	*Baseline* solubility in Salado brine (GWB) (includes complexation with organic ligands and equilibration with hydromagnesite). Organic ligand concentration was diluted *n* times (where *n* is 2, 3, 4, or 5) in the calculation of the baseline solubility.
SOLCOH[n]	mol/L	0.0	*Baseline* solubility in Castile brine (ERDA-6) (includes complexation with organic ligands and equilibration with hydromagnesite). Organic ligand concentration was diluted *n* times (where *n* is 2, 3, 4, or 5) in the calculation of the baseline solubility.
SOLVAR	N/A	0.0	(Baseline) solubility uncertainty modifier. The baseline solubility value gets multiplied by 10^SOLVAR.

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Table 5-9. Humic colloid property parameters

Property	Units	Default	Description
PHUMSIM	N/A	0.0	Proportionality constant for the concentration limit of actinides associated with humic colloids in Salado brine (GWB).
PHUMCIM	N/A	0.0	Proportionality constant for the concentration limit of actinides associated with humic colloids in Castile brine (ERDA-6).

In the STANDARD run mode, the brine volume and brine flow data are provided as time series data in a "flux" CDB input file. This CDB file is typically BRAGFLO output CDB file that is further post-processed by ALGEBRACDB. It contains the global time step variables BRNVOL_P (brine volume summed over the group of interconnected panels) and BNBHUDRZ (cumulative brine discharge, i.e. the time-integrated gross brine outflow rate, through the borehole) (Table 5-10). As a fallback, PANEL will read BRNVOL_W (brine volume in the BRAGFLO waste panel) if BRNVOL_P is not provided, but internally it treats the data in the same manner.

Table 5-10. Time series data read by PANEL from the "flux" CDB file

Variables	Units	Description
BRNVOL_W	m^3	Brine volume in the waste panel (as a function of time).
BRNVOL_P	m^3	Brine volume summed over the group of interconnected waste panels that hydraulically communicate with the borehole (as a function of time).
BNBHUDRZ	m^3	Cumulative (over time) brine flow exiting the waste panels through the borehole to upper MB138.

5.2 "Output" CDB File

PANEL produces an output CDB file that includes the same information (i.e. static parameters) contained in the input CDB file along with PANEL's calculation results. PANEL adds the total mobile concentration limit results as static parameters to the CDB "Element Blocks" section. It also creates CDB "History Variables" that are output every 50 years.

Table 5-11 lists the added output element-associated parameters. The Block (Material) name corresponds to one of: AM, NP, PU, TH, U (the five primary elements in the solubility model), and also CF, CM, PA, PM (the secondary elements that are assigned the same values as one of the primary elements). PANEL also outputs the parameters for the five lumped radionuclides: AM241L, PU238l, PU239l, TH230L, and U234L.

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Table 5-11. Element associated parameters

Block	Property	Description
*	LOGSOLM	log10 of the actinide total mobile concentration limit (log10(mol/L))
*	FRCDIS	Fraction of the actinide total mobile concentration limit that is dissolved.
*	FRCHUM	Fraction of the actinide total mobile concentration limit that is associated with dispersed humic colloids.
*	FRCMIC	Fraction of the actinide total mobile concentration limit that is associated with dispersed microbial colloids.
*	FRCINT	Fraction of the actinide total mobile concentration limit that is associated with dispersed intrinsic actinide colloids.
*	FRCMIN	Fraction of the actinide total mobile concentration limit that is associated with dispersed mineral fragment colloids.

PANEL outputs LOGSOLM only for CS and SR, and no parameters for PB, RA, or SM. PANEL outputs different history variables according to the run mode. In DECAY mode, PANEL outputs the remaining radionuclide inventory versus time (Table 5-12). In CONCENTRATION mode, PANEL outputs the mobile radionuclide concentrations versus time (Table 5-13). And in STANDARD mode, PANEL outputs the cumulative radionuclide discharge versus time (Table 5-14). PANEL outputs each in material units of mass (kg), activity (*Ci*), and EPA release units. It also outputs the same information for the five lumped radionuclides: AM241L, PU238l, PU239l, TH230L, and U234L. However, the suffix "L" is not included in the history variable name.

PANEL also writes an ASCII "debug" file that may aid the user in diagnosing its activities, but all WIPP PA relevant results are written to the output CDB file.

Table 5-12. History variables outputs by PANEL in DECAY run mode

History Variable	Units	Description
BRNVOL00	m^3	Brine volume in the waste panel(s)
SMFLOW00	m^3	Cumulative (over time) brine discharge from waste panel(s)
SDETOTAL	EPA units	Total (sum of all radionuclides) remaining inventory in EPA units
SDM[radionuclide]	kg	Remaining inventory in mass units
SDC[radionuclide]	*Ci*	Remaining inventory in activity units
SDE[radionuclide]	EPA units	Remaining inventory in EPA release units
LDETOTAL	EPA units	Total (sum of all lumped radionuclides) remaining inventory in EPA units
LDM[radionuclide]	Kg	Remaining inventory of the lumped radionuclide in mass units
LDC[radionuclide]	*Ci*	Remaining inventory of the lumped radionuclide in activity units
LDE[radionuclide]	EPA units	Remaining inventory of the lumped radionuclide in EPA release units

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Table 5-13. History variables outputs by PANEL in CONCENTRATION run mode

History Variable	Units	Description
BRNVOL00	m^3	Brine volume in the waste panel(s)
SMFLOW00	m^3	Cumulative (over time) brine discharge from waste panel(s)
CNETOTAL	EPA units/m^3	Total (sum of all radionuclides) concentration in EPA units/m^3
CNM[radionuclide]	kg/m^3	Concentration in mass/m^3 units
CNC[radionuclide]	*Ci*/m^3	Concentration in activity/m^3 units
CNE[radionuclide]	EPA units/m^3	Concentration in EPA unit release/m^3 units
CLETOTAL	EPA units/m^3	Total (sum of all lumped radionuclides) concentration in EPA units/m^3
CLM[radionuclide]	kg/m^3	Concentration of the lumped radionuclide in mass/m^3 units
CLC[radionuclide]	*Ci*/m^3	Concentration of the lumped radionuclide in activity/m^3 units
CLE[radionuclide]	EPA units/m^3	Concentration of the lumped radionuclide in EPA unit release/m^3

Table 5-14. History variables outputs by PANEL in STANDARD run mode

History Variable	Units	Description
BRNVOL00	m^3	Brine volume in the waste panel(s)
SMFLOW00	m^3	Cumulative (over time) brine discharge from waste panel(s)
SDETOTAL	EPA units	Total (sum of all radionuclides) discharge in EPA units
SDM[radionuclide]	kg	Discharge in mass units
SDC[radionuclide]	*Ci*	Discharge in activity units
SDE[radionuclide]	EPA units	Discharge in EPA release units
LDETOTAL	EPA units	Total (sum of all lumped radionuclides) discharge in EPA units
LDM[radionuclide]	Kg	Discharge of the lumped radionuclide in mass units
LDC[radionuclide]	*Ci*	Discharge of the lumped radionuclide in activity units
LDE[radionuclide]	EPA units	Discharge of the lumped radionuclide in EPA release units

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6.0 REQUIRED USER TRAINING AND/OR BACKGROUND

To exercise the code PANEL, users should have a working knowledge of Linux operating systems, including how to execute commands via a system shell (such as BASH), and of Sandia's CAMDAT database (CDB) file format. The input/output CDB files can be manipulated with PA codes ALGEBRACDB, GROPECDB, and SUMMARIZE, thus having a working knowledge of these codes is helpful when preparing inputs and analyzing outputs from PANEL. To understand PANEL's technical basis and calculations methods, users should have a basic knowledge of calculus, linear algebra, numerical methods for ordinary differential equations, chemistry, nuclear decay transformations, fluid flow, and mass transport.

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7.0 CAPABILITIES AND LIMITATIONS

PANEL's embodied model contains several assumptions.

- Because PANEL scales the repository-wide inventory to the inventory contained in a single (or group of) waste panels, its mobile concentration and discharge calculations reflect the "repository-average" inventory, not a panel-specific inventory. This does not necessarily require that the waste inventory composition be homogenous between waste panels, however. Because a borehole intrusion could occur into any of the waste panels, the mobile concentration and discharge values aggregated across all possible panel intrusions would result in "expected" values that are similar to the repository-average values (as long as isotopes of the same element are present in similar ratios in different panels).
- Brine and the waste inventory are well mixed and are continuously in equilibrium (i.e. the chemical system equilibration time is fast compared to the brine residence time, decay half-lives, and PANEL timestep size).
- Diffusion, dispersion, adsorption, filtration, and chromatographic separation are ignored in the radionuclide discharge calculations. The discharged brine contains radionuclides at the same concentration as found in the waste panel.
- Mobile radionuclide concentrations are determined using a "saturation" type calculation – the concentration is the smaller of the radionuclide concentration limit or the value resulting from mobilizing the currently remaining inventory of that radionuclide. The radionuclides mobilize according to their isotope-to-element mole fraction and their elemental concentration limit.
- The elemental concentration limits are fixed during the course of a simulation – e.g. they do not change over time due to possible changes in the brine composition, reequilibration with the current radionuclide inventory, changes in organic ligand concentrations, or changes in colloid concentrations. These possible changes are addressed by running multiple PANEL simulations with stochastically sampled input parameters.
- A more detailed discussion of the assumptions behind the Solubility Model and the Colloid Model that form the basis of the total mobile concentration limit calculations is available in Appendix-SOTERM (US DOE, 2014 and 2019).

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8.0 USER INTERACTIONS WITH THE SOFTWARE

PANEL expects a number of command line arguments. The program arguments may either be positional (provided in order) or flagged (preceded by the appropriate flag). Flags always start with "-"; they may be abbreviated. All positional arguments must be listed before any flagged arguments. The only difference between using positional and flagged arguments is that optional arguments may be omitted for flagged arguments.

PANEL is executed from the system shell. The user must reference the executable by its absolute path if its location is not already included in the user's shell PATH variable. PANEL requires seven arguments (the arguments are specified with argument flags) so that it can set the run mode, scenario, time translation option, and file input/output locations. These are listed in Table 8-1.

Table 8-2 through Table 8-5 list examples of executing PANEL for different run modes. Each table shows two command line arguments but are executing the same runs. The first command line uses the positional arguments. The second command line uses the flagged arguments. Table 8-5 lists an example to execute PANEL where the time series data in the "flux" input CDB file is translated by 4000 years. This would correspond to the second intrusion in the E1E2 case being shifted from year 2000 to year 6000

Table 8-1. PANEL command line arguments

Argument flag	Value	Description
-run	DECAY | CONCENTRAION | STANDARD. Optionally, only the first letter may be specified.	Run mode. The mode determines the type of mass balance calculation and the output history variables. In DECAY mode, PANEL outputs the remaining inventory vs. time. In CONCENTRATION mode, PANEL outputs the mobile concentrations vs. time. In STANDARD mode, PANEL outputs the cumulative radionuclide discharge vs. time.
-input		File name for the "input" CDB file containing static parameters.
-output		File name for the output CDB file.
-scenario	1 | 2 | 3 | 4 | 5 | 6	PA scenario number (corresponds to a BRAGFLO scenario). PANEL only uses this value to select the brine type in the concentration limit calculations. Thus any scenario can be combined with in run mode. Note that the scenario is only supplied via the command line argument; it is not listed in the input CDB file.
-timeint	100 – 9000	Time offset (years) plus 2000 by which to translate the time series data contained in the "flux" CDB file. For an offset of zero, specify 2000. While this only applies to STANDARD mode, a value is required for all modes (it is recommended to specify 2000 for modes DECAY and CONCENTRATION).
-flux		File name for the "flux" CDB file that contains the time-varying panel brine volume and cumulative brine discharge data.
-debug		File name for the ASCII debug output file.

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Table 8-2. Example to execute PANEL in DECAY mode

```
panel DECAY my_panel_input.cdb my_panel_output.cdb 1 2000 CANCEL my_panel_output.dbg

panel -run DECAY -input my_panel_input.cdb -output my_panel_output.cdb -scenario 1 -timeint 2000 -
flux CANCEL -debug my_panel_output.dbg
```

Table 8-3. Example to execute PANEL in CONCENTRATION mode

```
panel CONCENTRATION my_panel_input.cdb my_panel_output.cdb 1 2000 CANCEL my_panel_output.dbg

panel -run CONCENTRATION -input my_panel_input.cdb -output my_panel_output.cdb -scenario 1 -timeint
2000 -flux CANCEL -debug my_panel_output.dbg
```

Table 8-4. Example to execute PANEL in STANDARD mode

```
panel STANDARD my_panel_input.cdb my_panel_output.cdb 6 2000 my_flux_input.cdb
my_panel_output.dbg

panel -run STANDARD -input my_panel_input.cdb -output my_panel_output.cdb -scenario 6 -timeint 2000
-flux my_flux_input.cdb -debug my_panel_output.dbg
```

Table 8-5. Example to execute PANEL in STANDARD mode with time intursion at 6,000 years

```
panel STANDARD my_panel_input.cdb my_panel_output.cdb 6 6000 my_flux_input.cdb
my_panel_output.dbg

panel -run STANDARD -input my_panel_input.cdb -output my_panel_output.cdb -scenario 6 -timeint 6000
-flux my_flux_input.cdb -debug my_panel_output.dbg
```

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9.0 ERROR MESSAGES

Table 9-1 contains a list of potential error messages generated by PANEL.

Table 9-1. Listing of potential error messages

Error message	Description
INCORRECT FILE ASSIGNMENTS	The list of command line arguments supplied to PANEL were not sufficient or not valid.
PROBLEM WITH INPUT CDB	The input CDB file could not be opened (e.g. was not found or the file is invalid).
PROBLEM WITH OUTPUT CDB	The output CDB file could not be created.
INVALID SCENARIO NUMBER	The scenario number could not be parsed from the command line arguments.
INVALID TIME OF INTRUSION	The intrusion time could not be parsed from the command line arguments.
PROBLEM WITH FLUX CDB FILE	The flux CDB file could not be opened (e.g. was not found or the file is invalid).
PROBLEM WITH DBOQAREC	Could not add QA information to the output CDB file.
PROBLEM WITH DBOHEAD	Could not add QA information to the output CDB file.
PROBLEM WITH DBOCLOSE	Could not close the output CDB file.
DT PROBLEM	The flux CDB file contains excessively large brine flux rates compared to the brine volume and timestep size.
DBOVAR ERROR 0-6	Could not write a History Variable to the output CDB file.
PROBLEM 1-3 WITH FLUXIN CDB	Could not read brine volume or brine flux data from the flux CDB file.
BRINEV=0,TFLXOUT>0	The flux CDB file contains invalid data – brine discharge occurs when there is no brine in the panel.
IN BHFLO,TIME PROBLEM	Could not interpolate brine volume/brine flux time series data, likely due to the data not encompassing the simulation period.
IN DBIELBK	Problem reading block/property data from the input CDB file.
OVER 200 EL BLKS IN DBVALUE	Insufficient memory allocation to read from the input CDB file.
OVER 50 PROPERTIES IN DBVALUE	Insufficient memory allocation to read from the input CDB file.
ELBNAM NOT FOUND IN LIST	PANEL is trying to write a property to an element block (in the output CDB file) that does not exist in the input CDB file.
OVER 50 PROPERTIESIN OUTDBVAL	Insufficient memory allocation to write to the input CDB file.
ERROR WRITEING PROPERTIES TO OUTPUT CDB	Could not write element property to the output CDB file, possibly because the property already exists in the input CDB file.

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10.0 REFERENCES

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11.0 APPENDICES

Changes for version 5.02 are highlighted in yellow.

11.1 MATSET Input File

```
!
*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, 66, 67, 68, 69, 70, 71, 72, 73, 74
*RETRIEVE*NAME
 COORDINATE, DIM=3, NAMES=X, Y, Z
 MATERIAL,    1=GLOBAL, 2=REFCON, &
    3=AM241,  4=AM243,  5=CF252,  6=CM243,  7=CM244,  8=CM245, &
    9=CM248, 10=CS137, 11=NP237, 12=PA231, 13=PB210, 14=PM147, &
   15=PU238, 16=PU239, 17=PU240, 18=PU241, 19=PU242, 20=PU244, &
   21=RA226, 22=RA228, 23=SR90,  24=TH229, 25=TH230, 26=TH232, &
   27=U233,  28=U234,  29=U235,  30=U236,  31=U238,  &
   32=AM, 33=CF, 34=CM, 35=CS, 36=NP, 37=PA, 38=PB, 39=PM, 40=PU, &
   41=RA, 42=SR, 43=TH, 44=U,  &
   45=SOLMOD3, 46=SOLMOD4, 47=SOLMOD5, 48=SOLMOD6, &
   49=PHUMOX3, 50=PHUMOX4, 51=PHUMOX5, 52=PHUMOX6, &
   53=SOLAM3,  54=SOLPU3,  55=SOLPU4,  56=SOLTH4,  57=SOLU4,  58=SOLU6, &
   59=AM241L, 60=PU238L, 61=PU239L, 62=TH230L, 63=U234L,  64=BOREHOLE, &
   65=WAS_AREA, 66=SM147, 67=AM+3, 68=PU+3, 69=PU+4, 70=TH+4, 71=U+4, &
   72=U+6, 73=NP+4, 74=NP+5
!MATERIALS 59-63 ARE LUMPED PARAMETERS FOR NUTS
!
 PROPERTY   MATERIAL=WAS_AREA,  NAMES =PROBDEG
 PROPERTY   MATERIAL=Global,    NAMES =OXSTAT,DBRMINBV
 PROPERTY   MATERIAL=REFCON,    NAMES =YRSEC,VPANLEX,VREPOS,CITOBQ,AVOGADRO
!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
```

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```
 PROPERTY   MATERIAL=Ra228,      NAMES =InvCHD,InvRHD,ATWEIGHT,HALFLIFE,EPAREL
 PROPERTY   MATERIAL=Sm147,      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=NP,         NAMES =OXCUTOFF
 PROPERTY   MATERIAL=PU,         NAMES =OXCUTOFF
 PROPERTY   MATERIAL=U,          NAMES =OXCUTOFF
!OXSTAT-ELEMENTS
 PROPERTY   MATERIAL=AM+3,       NAMES =CONCMIN,CONCINT,CAPHUM,CAPMIC,PROPMIC
 PROPERTY   MATERIAL=PU+3,       NAMES =CONCMIN,CONCINT,CAPHUM,CAPMIC,PROPMIC
 PROPERTY   MATERIAL=PU+4,       NAMES =CONCMIN,CONCINT,CAPHUM,CAPMIC,PROPMIC
 PROPERTY   MATERIAL=TH+4,       NAMES =CONCMIN,CONCINT,CAPHUM,CAPMIC,PROPMIC
 PROPERTY   MATERIAL=U+4,        NAMES =CONCMIN,CONCINT,CAPHUM,CAPMIC,PROPMIC
 PROPERTY   MATERIAL=U+6,        NAMES =CONCMIN,CONCINT,CAPHUM,CAPMIC,PROPMIC
 PROPERTY   MATERIAL=NP+4,       NAMES =CONCMIN,CONCINT,CAPHUM,CAPMIC,PROPMIC
 PROPERTY   MATERIAL=NP+5,       NAMES =CONCMIN,CONCINT,CAPHUM,CAPMIC,PROPMIC
!OXIDATION STATES
 PROPERTY   MATERIAL=SOLMOD3,    NAMES
=SOLSOH,SOLCOH,SOLSOH2,SOLCOH2,SOLSOH3,SOLCOH3,SOLSOH4,SOLCOH4,SOLSOH5,SOLCOH5,SOLVAR
 PROPERTY   MATERIAL=SOLMOD4,    NAMES
=SOLSOH,SOLCOH,SOLSOH2,SOLCOH2,SOLSOH3,SOLCOH3,SOLSOH4,SOLCOH4,SOLSOH5,SOLCOH5,SOLVAR
 PROPERTY   MATERIAL=SOLMOD5,    NAMES
=SOLSOH,SOLCOH,SOLSOH2,SOLCOH2,SOLSOH3,SOLCOH3,SOLSOH4,SOLCOH4,SOLSOH5,SOLCOH5
 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
!-----------------------------------------------------------------------------
```

11.2 ALGEBRACDB Input File, *alg2_panel_bm.inp (m=1)*

```
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
STEP 201

DELETE HISTORY

! PU238L
LIMIT BLOCK 60
LSOLDIFF = MAKEPROP(LSD_PU[T:1])

! TH230L
LIMIT BLOCK 62
LSOLDIFF = MAKEPROP(LSD_TH[T:1])
```

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```
! U234L
LIMIT BLOCK 63
LSOLDIFF = MAKEPROP(LSD_U[T:1])

! LSOLDIFF for AM241L and PU239L are assumed zero (i.e. the mol frac is one)


! SET UP SCALING FOR INVENTORY AND MIN DBR BRINE VOLUME.
!
!    BRINEFAC=FACTOR TO SCALE MINIMUM DBR BRINE VOLUME
!             SET AT 1,2,3,4,5X
!    NUMPANEL=NUMBER OF PANELS WITH DIRECT ACCESS TO THE
!             BOREHOLE
!    INVSCALE=SCALING FACTOR FROM FULL REPOSITORY TO A SINGLE
!             PANEL
!    PANDFVOL=MINIMUM DBR BRINE VOLUME SCALED TO A SINGLE
!             PANEL, AS ADJUSTED BY THE 1,2,3,4,5X SCALING

LIMIT BLOCK 1
BRINEFAC=MAKEPROP(1.0)
DBRMINBV=DBRMINBV*BRINEFAC
!
! Microbial Colloid Model Criteria Parameter
! MICOL = 0.0 (default) Use Biomass based Microbial Colloid Model
!       = 1.0           Use Toxicity based Microbial Colloid Model
MICOL=MAKEPROP(0.0)
!
! Colloid Enhancement Parameters
! ELEOXSTA = 0.0 (default) Oxidation state-specific
!          = 1.0           Element-specific
ELEOXSTA=MAKEPROP(1.0)

LIMIT BLOCK 2
NUMPANEL=MAKEPROP(5.0)
INVSCALE=MAKEPROP(VPANLEX/VREPOS)
PANDFVOL=MAKEPROP(DBRMINBV[B:1]*INVSCALE)

EXIT
```

11.3 ALGEBRACDB Input File, *alg3_panel_bm.inp (m=1)*

The ELEOXSTA and MICOL parameters values are input into the 2nd step ALGEBRACDB input file that determine the colloid enhancement parameter type and the microbial colloid model type. The MICOL parameter is used within the PANEL code but the ELEOXSTA parameter is used the 3rd ALGEBRACDB pre-processing step.

When ELEOXSTA = 0 (oxidation state specific colloid enhancement parameters) and OXSTAT ≤ *actinide*:OXCUTOFF (*actinide* = PU, U, and NP), property parameters (CONCINT, CONCMIN, CAPMIC, PROPMIC, and CAPHUM) of the lower oxidation state *actinide* MATERIAL block (PU+3, U+4, and NP+4) are assigned to the *actinide* MATERIAL block. When ELEOXSTA = 0 (oxidation state specific colloid enhancement parameters) and OXSTAT > *actinide*:OXCUTOFF, property parameters of the higher oxidation state *actinide* MATERIAL block (PU+4, U+6, and NP+5) are assigned to the *actinide* MATERIAL block. When ELEOXSTA = 1 (element specific colloid enhancement parameters), maximum property parameters between the lower and higher oxidation state *actinide* MATERIAL blocks are assigned to the *actinide* MATERIAL block.

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```
!
! 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])
!
```

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```
! SET HALFLIFE AND ATWEIGHT FOR U234L SAME AS FOR U234
!
LIMIT BLOCK 63 ! (U234L)
ATWEIGHT=MAKEPROP(ATWEIGHT[B:28])
HALFLIFE=MAKEPROP(HALFLIFE[B:28])
!
! Colloid Enhancement Parameters
!
! AM and TH : No difference between element-specific and ox-state-specific
! PU, U and NP : Difference between element-specific and ox-state-specific
!
LIMIT BLOCK 1
ELEOXSTA=IFLT0(ABS(1.0-ELEOXSTA)-1.0d-3,1.0,0.0)
MICOL=IFLT0(ABS(1.0-MICOL)-1.0d-3,1.0,0.0)
! for toxicity, refere CCA data for PROPMIC and CAPMIC
!
! AM(III)
LIMIT BLOCK 32
CONCINT=CONCINT[B:67]
CONCMIN=CONCMIN[B:67]
CAPMIC=CAPMIC[B:67]
PROPMIC=PROPMIC[B:67]
CAPHUM=CAPHUM[B:67]
!
! PU(III), or PU(IV)
LIMIT BLOCK 40
OXCUT=OXSTAT[B:1]-OXCUTOFF
OXCUTDIF=1.0E-10
CONCINT=IFEQ0(ELEOXSTA[B:1],IFLT0(OXCUT-OXCUTDIF,CONCINT[B:68], &
        CONCINT[B:69]), MAX(CONCINT[B:68],CONCINT[B:69]))
CONCMIN=IFEQ0(ELEOXSTA[B:1],IFLT0(OXCUT-OXCUTDIF,CONCMIN[B:68], &
        CONCMIN[B:69]), MAX(CONCMIN[B:68],CONCMIN[B:69]))
CAPMIC=IFEQ0( ELEOXSTA[B:1],IFLT0(OXCUT-OXCUTDIF,CAPMIC[B:68] , &
        CAPMIC[B:69] ), MAX(CAPMIC[B:68] ,CAPMIC[B:69] ))
PROPMIC=IFEQ0(ELEOXSTA[B:1],IFLT0(OXCUT-OXCUTDIF,PROPMIC[B:68], &
        PROPMIC[B:69]), MAX(PROPMIC[B:68],PROPMIC[B:69]))
CAPHUM=IFEQ0( ELEOXSTA[B:1],IFLT0(OXCUT-OXCUTDIF,CAPHUM[B:68] , &
        CAPHUM[B:69] ), MAX(CAPHUM[B:68] ,CAPHUM[B:69] ))
!
! TH(IV)
LIMIT BLOCK 43
CONCINT=CONCINT[B:70]
CONCMIN=CONCMIN[B:70]
CAPMIC=CAPMIC[B:70]
PROPMIC=PROPMIC[B:70]
CAPHUM=CAPHUM[B:70]

! U, U(IV), or U(VI)
LIMIT BLOCK 44
OXCUT=OXSTAT[B:1]-OXCUTOFF
OXCUTDIF=1.0E-10
CONCINT=IFEQ0(ELEOXSTA[B:1],IFLT0(OXCUT-OXCUTDIF,CONCINT[B:71], &
        CONCINT[B:72]), MAX(CONCINT[B:71],CONCINT[B:72]))
CONCMIN=IFEQ0(ELEOXSTA[B:1],IFLT0(OXCUT-OXCUTDIF,CONCMIN[B:71], &
        CONCMIN[B:72]), MAX(CONCMIN[B:71],CONCMIN[B:72]))
CAPMIC=IFEQ0( ELEOXSTA[B:1],IFLT0(OXCUT-OXCUTDIF,CAPMIC[B:71] , &
        CAPMIC[B:72] ), MAX(CAPMIC[B:71] ,CAPMIC[B:72] ))
PROPMIC=IFEQ0(ELEOXSTA[B:1],IFLT0(OXCUT-OXCUTDIF,PROPMIC[B:71], &
        PROPMIC[B:72]), MAX(PROPMIC[B:71],PROPMIC[B:72]))
CAPHUM=IFEQ0( ELEOXSTA[B:1],IFLT0(OXCUT-OXCUTDIF,CAPHUM[B:71] , &
        CAPHUM[B:72] ), MAX(CAPHUM[B:71] ,CAPHUM[B:72] ))

! NP, NP(IV), or NP(V)
LIMIT BLOCK 36
OXCUT=OXSTAT[B:1]-OXCUTOFF
OXCUTDIF=1.0E-10
CONCINT=IFEQ0(ELEOXSTA[B:1],IFLT0(OXCUT-OXCUTDIF,CONCINT[B:73], &
        CONCINT[B:74]), MAX(CONCINT[B:73],CONCINT[B:74]))
CONCMIN=IFEQ0(ELEOXSTA[B:1],IFLT0(OXCUT-OXCUTDIF,CONCMIN[B:73], &
```

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        CONCMIN[B:74]), MAX(CONCMIN[B:73],CONCMIN[B:74]))
CAPMIC=IFEQ0( ELEOXSTA[B:1],IFLT0(OXCUT-OXCUTDIF,CAPMIC[B:73] , &
        CAPMIC[B:74] ), MAX(CAPMIC[B:73] ,CAPMIC[B:74] ))
PROPMIC=IFEQ0(ELEOXSTA[B:1],IFLT0(OXCUT-OXCUTDIF,PROPMIC[B:73], &
        PROPMIC[B:74]), MAX(PROPMIC[B:73],PROPMIC[B:74]))
CAPHUM=IFEQ0( ELEOXSTA[B:1],IFLT0(OXCUT-OXCUTDIF,CAPHUM[B:73] , &
        CAPHUM[B:74] ), MAX(CAPHUM[B:73] ,CAPHUM[B:74] ))
END
```

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