

Appendix E

<p style="text-align: center;">NUCLEAR WASTE MANAGEMENT PROCEDURE</p> <p><small>Sandia National Laboratories</small></p>	<h2 style="margin: 0;">Design Document Criteria</h2>	<p>Form Number: NP 19-1-4</p> <p>Page 1 of 1</p>	
<p>1. Software Name: <u>PANEL</u></p> <p>2. Software Version: <u>5.00</u></p> <p>3. Document Version: <u>5.00</u></p> <p>4. ERMS #: <u>570821</u></p> <p style="font-size: small;">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.</p>			
<p>Are the following appropriately defined and documented in the DD?</p> <p>5. Major Software Components <input checked="" type="checkbox"/> Yes</p> <p>6. Technical description of the software with respect to: theoretical basis, embodied mathematical model, major control flow, control logic, and data structures <input checked="" type="checkbox"/> Yes</p> <p>7. Functionalities and interfaces of object components, functions, and subroutines. <input checked="" type="checkbox"/> Yes</p> <p>8. Allowable or prescribed ranges for inputs and outputs <input checked="" type="checkbox"/> Yes</p> <p>9. Verifiability: Is the design verifiable through testing or other means? <input checked="" type="checkbox"/> Yes</p> <p>10. Consistency and Traceability: Is the design consistent with and traceable to the software's requirements? <input checked="" type="checkbox"/> Yes</p> <p>11. Technical Feasibility: Is the design technically feasible? <input checked="" type="checkbox"/> Yes</p> <p>12. Implementation: Is the design presented in sufficient detail to allow for implementation as computer software? <input checked="" type="checkbox"/> Yes</p>			
13.	<p><u>Ramesh Sarathi</u> Code Team/Sponsor <i>(print)</i></p>	<p><u><i>Ramesh Sarathi</i></u> Signature</p>	<p><u>3/19/2019</u> Date</p>
14.	<p><u>Paul Mariner</u> Technical Reviewer <i>(print)</i></p>	<p><u><i>Paul Mariner</i></u> Signature</p>	<p><u>3/26/19</u> Date</p>
15.	<p><u>Shelly Nielsen</u> QA Reviewer <i>(print)</i></p>	<p><u><i>Shelly R. Nelson</i></u> Signature</p>	<p><u>4-2-19</u> Date</p>
16.	<p><u>Chris Camphouse</u> Responsible Manager <i>(print)</i></p>	<p><u><i>Chris Camphouse</i></u> Signature</p>	<p><u>3/15/19</u> Date</p>
17.	<p><u>Jennifer Long</u> SCM Coordinator <i>(print)</i></p>	<p><u><i>Jennifer Long</i></u> Signature</p>	<p><u>4/2/19</u> Date</p>

Appendix G



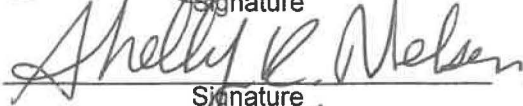

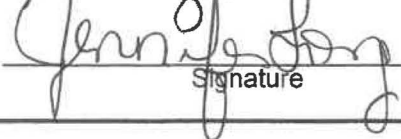
<p style="text-align: center;">NUCLEAR WASTE MANAGEMENT PROCEDURE</p> <p><small>Sandia National Laboratories</small></p>	<h2 style="margin: 0;">User's Manual Criteria</h2>	<p>Form Number: NP 19-1-6</p> <p>Page 1 of 1</p>
---	--	--

Does the User's Manual contain as appropriate:

- 1. **Software Name:** PANEL
- 2. **Software Version:** 5.00
- 3. **Document Version:** 5.00
- 4. **ERMS #:** 570821

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) and system limitations? 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. <u>Ramesh Sarathi</u> Code Team/Sponsor <i>(print)</i>	 Signature	<u>3/19/2019</u> Date
16. <u>Paul Mariner</u> Technical Reviewer <i>(print)</i>	 Signature	<u>3/20/19</u> Date
17. <u>Shelly Nielsen</u> QA Reviewer <i>(print)</i>	 Signature	<u>4-2-19</u> Date
18. <u>Chris Camphouse</u> Responsible Manager <i>(print)</i>	 Signature	<u>3/15/19</u> Date
19. <u>Jennifer Long</u> SCM Coordinator <i>(print)</i>	 Signature	<u>4/2/19</u> Date

WIPP PA

**Design Document and User's Manual
for
PANEL Version 5.00**

Document Version 5.00

ERMS #570821

February 2019

Information Only

Table of Contents

1.0	Introduction.....	4
1.1	Software Identifier	4
1.2	Points of Contact.....	4
1.3	Description.....	4
2.0	Functional Requirements	5
2.1	Functional Requirements	5
2.2	External Interfaces	5
2.3	Functionality Not Tested.....	5
3.0	Required User Training and/or Background.....	6
4.0	Description of the Models and Methods	6
4.1	Total Mobile Concentration Limit Calculations	6
4.2	Instantaneous Mobilization Calculations.....	11
4.3	Decay Calculations	12
4.4	Mass Balance Calculations	14
4.5	Lumping.....	16
4.6	EPA Release Units.....	17
4.7	Time Translation.....	18
5.0	Major Software Components.....	19
5.1	Major Control Flow, Control Logic, and Subroutines.....	19
5.2	Data Structures.....	20
6.0	Capabilities and Limitations of the Software for the WIPP PA Application.....	20
7.0	User Interactions with the Software.....	21
8.0	Description of Input Files.....	22
8.1	“Input” CDB File.....	22
8.2	“Flux” CDB File	27
9.0	Description of Output Files	27
10.0	Error Messages.....	29
11.0	Example MATSET File.....	30
12.0	References.....	33
Appendix-A.0	Expanded Decay Chain Figures	35

List of Figures

Figure 4-1 - Flowchart for total mobile concentration limit calculations (part 1).....	8
Figure 4-2 – Flowchart for total mobile concentration limit calculations (part 2)	9
Figure A-1 – Uranium Series; includes branches starting from radionuclides with half-lives greater than 1 year.....	36
Figure A-2 – Actinium Series; includes branches starting from radionuclides with half-lives greater than 1 year.....	37
Figure A-3 Thorium Series; includes branches starting from radionuclides with half-lives greater than 1 year.....	38
Figure A-4 Neptunium Series; includes branches starting from radionuclides with half-lives greater than 1 year.....	39
Figure A-5 – Decay chain for ^{147}Pm	40
Figure A-6 – Decay chain for ^{90}Sr	40
Figure A-7 – Decay chain for ^{137}Cs	40

List of Tables

Table 4-1 – Abridged decay chains modeled in PANEL.....	12
Table 4-2 – Lumped radionuclides and their constituents.....	16
Table 7-1 – PANEL command line arguments.....	21
Table 7-2 – Example to execute PANEL in DECAY mode.....	22
Table 7-3 – Example to execute PANEL in CONCENTRATION mode.....	22
Table 7-4 – Example to execute PANEL in STANDARD mode.....	22
Table 7-5 – Example to execute PANEL in STANDARD mode with time translation of 4000 years.....	22
Table 8-1 – Problem specification, mass balance, and unit conversion parameters.....	23
Table 8-2 – Radionuclide specific parameters.....	24
Table 8-3 – Default values for radionuclide parameters.....	24
Table 8-4 – Lumped-radionuclide specific parameters	25
Table 8-5 – Element-associated parameters	25
Table 8-6 – Solubility Model-associated (i.e. oxidation state specific) parameters	26
Table 8-7 – Oxidation state specific humic colloid parameters.....	27
Table 8-8 – Time series data read by PANEL from the “flux” CDB file.....	27
Table 9-1 – Element-associated parameters	28
Table 9-2 – CDB History Variables output by PANEL in DECAY run mode.	28
Table 9-3 – CDB History Variables output by PANEL in CONCENTRATION run mode.	28
Table 9-4 – CDB History Variables output by PANEL in STANDARD run mode.	29
Table 10-1 – Listing of potential error messages.....	29
Table 11-1 – Example to execute PANEL in DECAY mode.....	30

1.0 Introduction

The purpose of this document is to provide a technical description of PANEL's functionalities and calculation methods, major software components, and user interface. The documentation is developed in accordance with the Nuclear Waste Management Procedure NP 19-1 (Long 2017).

1.1 Software Identifier

Code Name: PANEL
WIPP Prefix: PANEL
Version: 5.00

1.2 Points of Contact

Code Sponsor:	Ramesh Sarathi	rsarath@sandia.gov	575-234-0004
Build/Run Consultant:	Jennifer Long	jlong@sandia.gov	575-234-0106

1.3 Description

The code PANEL serves three purposes in the context of WIPP Performance Assessment (PA) calculations. First, PANEL calculates a dissolved solubility limit and a "total mobile" (i.e. dissolved plus associated with dispersed colloids) concentration limit for each element in the waste inventory. These total mobile concentration limits are used by PANEL itself and by other PA codes such as NUTS. 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 (these concentration values vary with time due to the radioactive decay of the inventory). The PA code CCDFGF combines these concentration values with Direct Brine Release (DBR) volumes to determine DBR radionuclide releases. 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 (over time) amounts of radionuclides exiting the waste panel as a function of time. These "transport" calculation releases are used by the PA code CCDFGF when estimating long-term releases for the PA scenario in which a waste panel is intruded by human-drilled boreholes multiple times over a 10,000 year future (CRA-2014 Appendix-PA).

2.0 Functional Requirements

2.1 Functional Requirements

PANEL must:

1. Compute the total mobile concentration limits (i.e. the dissolved plus associated-with-dispersed-colloids "solubility" limits) for chemical elements in accordance with the Source Term conceptual model (CRA-2014 Appendix SOTERM).
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.
3. Compute the total amount (stationary and mobile) of each radionuclide as a function of time, accounting for radioactive decay and ingrowth.
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.
5. Translate (i.e. shift) the time values associated with the input brine volume and brine outflow data according to the (wellbore) intrusion time.
6. Scale the inventory and brine volume according to a user-defined number of waste panels.
7. Lump together sets of selected radionuclides to form "lumped" radionuclides for reporting output.

2.2 External Interfaces

In addition to the function requirements, PANEL shall:

1. Read input data from binary CAMDAT database files (CDB files).
2. Write output data to a binary CAMDAT database file (CDB files).
3. 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.

2.3 Functionality Not Tested

The radiolysis capability in PANEL will not be tested. PANEL is not used to calculate radiolysis-related effects in WIPP PA.

3.0 Required User Training and/or Background

To exercise the code PANEL, users should have a working knowledge of Unix-like 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.

4.0 Description of the Models and Methods

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

4.1 Total Mobile Concentration Limit Calculations

PANEL computes the total mobile concentration limits (sometimes referred to as the "Source Term" in other WIPP literature) for 14 elements in the tracked inventory. The total mobile concentration limit 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 CRA-2014 Appendix-SOTERM (2014) and Sarathi (2019). It is important to note that, while dependent upon several parameters, the total mobile concentration limit values are constant for any given model realization and throughout the course of a simulation (these concentration limits 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 mobile concentration limits. The computed total mobile concentration limit values are used by PANEL internally and are output (as the \log_{10} 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 limits are computed according to the Solubility Model described in CRA-2014 Appendix-SOTERM (2014), three "secondary" actinides and one lanthanide, Cm, Cf, Pa, and Pm, whose limits are assumed to be the same as one of the five primary actinides, and five other elements, Cs, Sr, Ra, Sm, and Pb, whose limits are assumed fixed. Sometime between the 1996 CCA and the 2004 CRA, PANEL was changed to assign Cs and Sr solubility limits of 1.0 mol/L (see Garner 1998, also Garner 2003 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 limit 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 1x 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 solubility limits of 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-unit basis (CCA Appendix-WCA). 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 and Figure 4-2 illustrate the steps involved in calculating the total mobile concentration limit values (S_TOT, and the \log_{10} 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 dilution 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[n] could refer to SOLMOD3, SOLMOD4, etc.

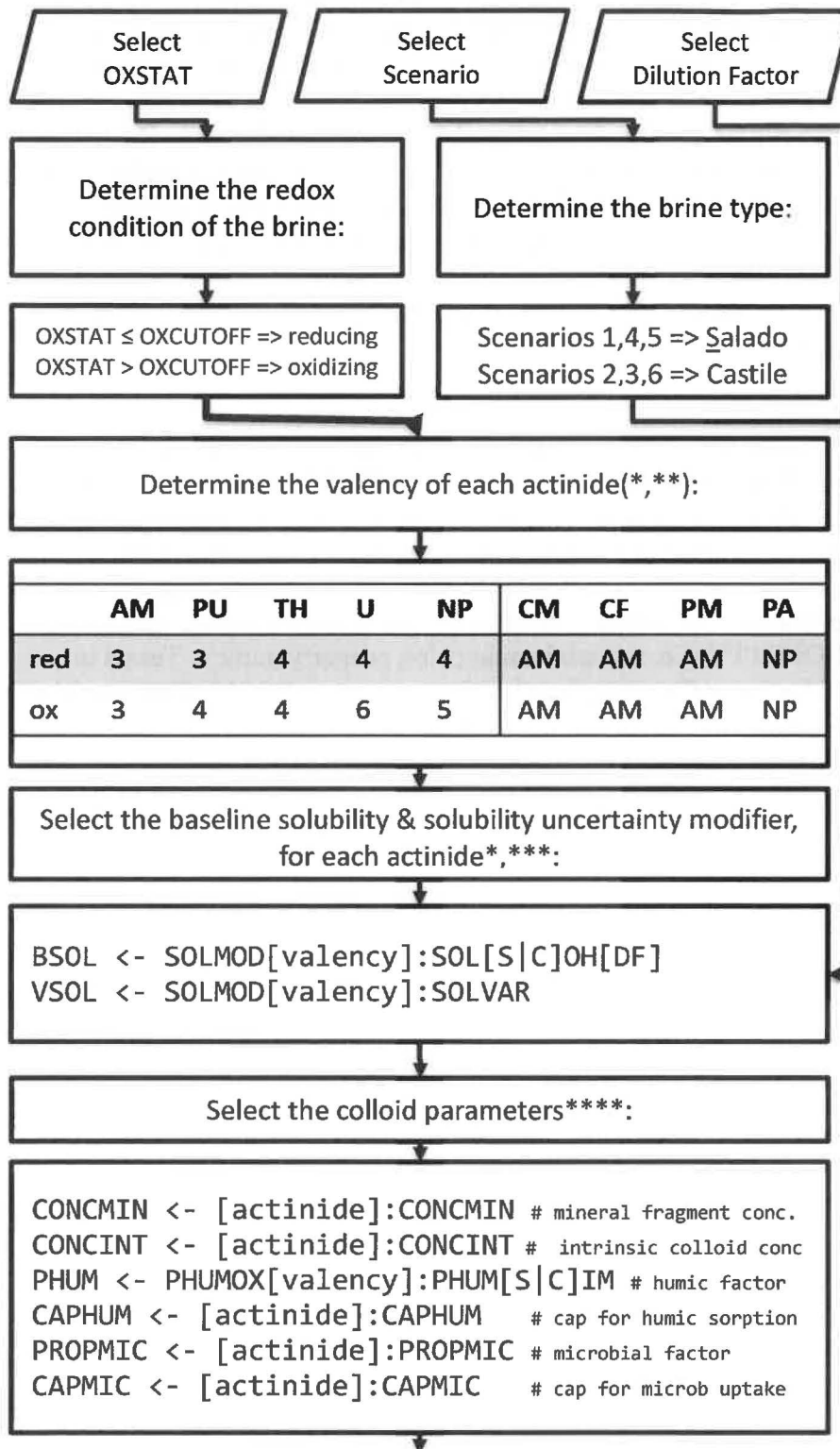


Figure 4-1 - Flowchart for total mobile concentration limit calculations (part 1)

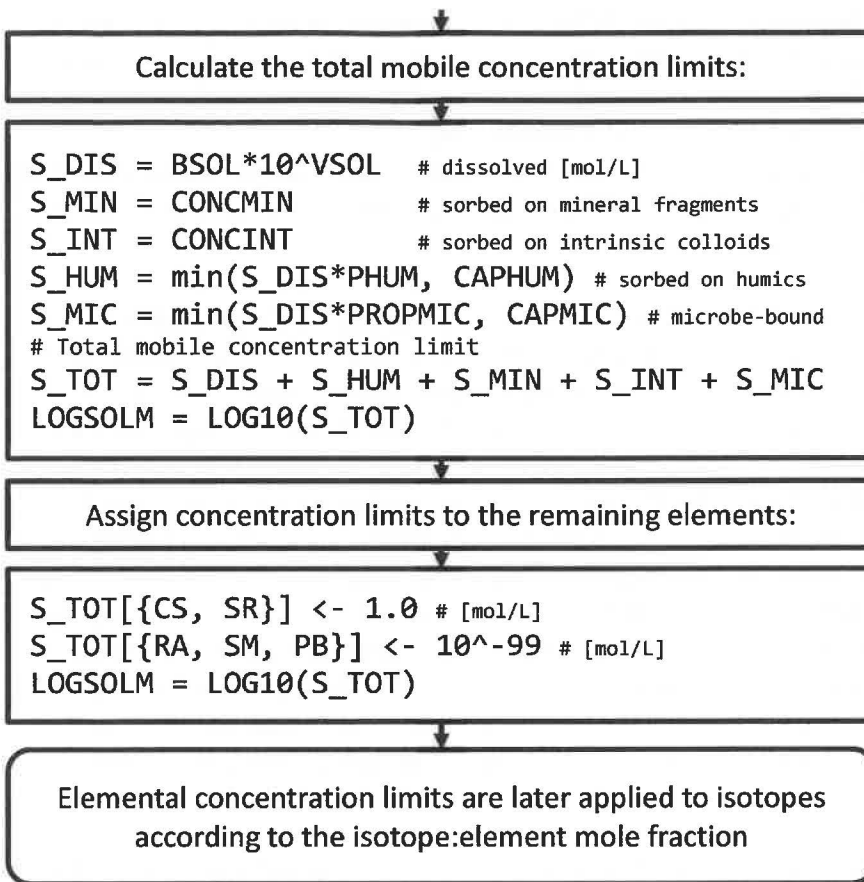


Figure 4-2 – Flowchart for total mobile concentration limit calculations (part 2)

The brine redox condition (i.e. whether the solution is reducing or oxidizing) is used to determine the valency of the actinide of interest (i.e. its oxidation state; however we use the term valency to more clearly distinguish between the oxidizing condition of the brine and the oxidation state of the individual elements). If the brine exhibits reducing conditions ($GLOBAL:OXSTAT \leq GLOBAL:OXCUTOFF$), the five actinides are assigned one set of valencies, whereas if the brine exhibits oxidizing conditions ($GLOBAL:OXSTAT > GLOBAL:OXCUTOFF$), the five actinides are assigned a different set of valencies. The specific valency number (i.e. oxidation state 3, 4, 5, or 6) 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 whose solubilities are redox insensitive (CRA-2014 Appendix-SOTERM, page 86). The baseline solubilities (SOLMOD[valency]:SOL[S|C]OH[DF]), 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 composition, i.e. either Salado or Castile. WIPP PA scenarios 1, 4, and 5 do not assume a borehole intrusion that intersects the Castile brine pocket, thus the Salado brine composition is selected. Scenarios 2, 3, and 6 do assume a borehole intrusion that interests the Castile, thus the Castile brine composition is selected. The baseline solubilities (SOLMOD[valency]:SOL[S|C]OH[DF]) and the actinide-humic colloid proportionality constant (i.e. association factor) (PHUMOX[valency]:PHUM[S|C]IM) are all catalogued according to brine composition (term S or C in the brackets).

The brine dilution factor (GLOBAL:BRINEFAC) 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 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 dilution factor, is the numeric suffix (DF) on the baseline solubility parameter name SOLMOD[valency]:SOL[S|C]OH[DF] (however, a number is appended only if the factor is greater than 1).

Lastly, the element name is used to select the colloid solubility enhancement parameters. The colloid solubility enhancement parameters are catalogued according to the actinide name, with the exception of the actinide-humic colloid proportionality constant (PHUMOX[valency]:PHUM[S|C]IM), which is catalogued according to the valency.

Once the proper model parameters have been selected, the total mobile concentration limits can be calculated. The total mobile concentration limit is comprised of five terms: a dissolved concentration limit and four concentration limits that represent the actinide associated with 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. the solubility modifier is input as the \log_{10} of the multiplier). 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. Each of these concentration limits is also 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 final output parameter, LOGSOLM, is the \log_{10} of the total mobile concentration limit value. PANEL also outputs each of the five terms as fractions of the total mobile concentration limit.

4.2 Instantaneous Mobilization Calculations

PANEL computes instantaneous mobile concentrations as a function of time according to the available inventory and the total mobile concentration limit of each radionuclide. The instantaneous concentration is determined by a simple “saturation” type calculation – the lesser of the total mobile concentration limit and the resultant concentration if the entire available inventory were mobilized (i.e. the inventory-limited concentration) is selected:

$$C_{iso}(t) = \min(C_{max,mob,iso}, C_{max,inv,iso}(t))$$

where the subscript *iso* refers to the isotope, *mob* refers to the total mobile concentration limit, and *inv* refers to the inventory-limited concentration. Three complications arise in computing this term.

First, the total mobile concentration limits are defined with respect to chemical 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 concentration limit must be computed based on the element-specific concentration limit. 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:

$$M_{ele}^{avg} = \sum_{isotope \in element} M_{iso}^{avg}$$

$$X_{iso}^{avg} = M_{iso}^{avg} / M_{ele}^{avg}$$

$$C_{max,mob,iso} = X_{iso}^{avg} \cdot C_{max,mob,ele}$$

where *M* refers to the available inventory (in moles) and *X* refers to the mole fraction. The superscript *avg* refers to a value averaged over the time step, the subscript *iso* refers to the isotope, and the subscript *ele* refers to the element. This portioning of the elemental total mobile concentration limit must be performed at each timestep because the isotope-element mole fractions vary over time since different radionuclides decay at different rates.

The second complication occurs in computing 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. PANEL employs a forward midpoint-in-time weighing scheme and averages the inventory that is computed at time *t* and at time *t + dt* when computing the inventory-limited concentrations. Thus the concentrations represent an average concentration over the forward timestep. At the final timestep, PANEL averages over a forward step of 10 years.

The third complication arises in computing the inventory-limited concentration. This concentration is simply the available radionuclide inventory divided by the volume of brine that is in the waste panel:

$$C_{max,inv,iso}(t) = \frac{M_{iso}^{avg}}{V}$$

However, PANEL scales both the inventory and the brine volume V to a representative number of waste panels. This is further discussed in Section 4.4.

4.3 Decay Calculations

PANEL models the decay and ingrowth of 30 radionuclides

²⁴¹ Am	²³⁷ Np	²⁴² Pu	²³² Th
²⁴³ Am	²³¹ Pa	²⁴⁴ Pu	²³³ U
²⁵² Cf	²¹⁰ Pb	²²⁶ Ra	²³⁴ U
²⁴³ Cm	¹⁴⁷ Pm	²²⁸ Ra	²³⁵ U
²⁴⁴ Cm	²³⁸ Pu	¹⁴⁷ Sm	²³⁶ U
²⁴⁵ Cm	²³⁹ Pu	⁹⁰ Sr	²³⁸ U
²⁴⁸ Cm	²⁴⁰ Pu	²²⁹ Th	
¹³⁷ Cs	²⁴¹ Pu	²³⁰ Th	

subject to the abridged decay chains:

Table 4-1 – Abridged decay chains modeled in PANEL

		²³⁸ Pu											
		↓											
²⁴² Pu	→	²³⁸ U	→	²³⁴ U	→	²³⁰ Th	→	²²⁶ Ra	→	²¹⁰ Pb	→		
		²⁴³ Cm											
		↓											
²⁴³ Am	→	²³⁹ Pu	→	²³⁵ U	→	²³¹ Pa	→						
						²⁴⁴ Cm							
						↓							
²⁵² Cf	→	²⁴⁸ Cm	→	²⁴⁴ Pu	→	²⁴⁰ Pu	→	²³⁶ U	→	²³² Th	→	²²⁸ Ra	→
²⁴⁵ Cm	→	²⁴¹ Pu	→	²⁴¹ Am	→	²³⁷ Np	→	²³³ U	→	²²⁹ Th	→		
¹⁴⁷ Pm	→	¹⁴⁷ Sm	→										
¹³⁷ Cs	→												
⁹⁰ Sr	→												

*The last radioisotope in a chain decays to a stable isotope that is not tracked in PANEL.

The first four chains follow (or are collinear to) the Uranium Series, the Actinium Series, the Thorium Series, and the Neptunium Series (KAPL 2002). An expanded version of the chains containing branches beginning from radionuclides with half-lives greater than 1 year is presented in the Appendix-A.0 so that the abridged chains can be verified, and for illustration purposes. The expanded chains were derived from data in ICRP Publication 107 (2008) using network (graph) analysis.

The abridged chains were originally formulated to include radionuclides called out in 10 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 (1996, especially page 23). 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 1996 and Kicker and Zeitler 2013). 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 .

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 $t + dt$.

The Bateman equations, 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):

$$M_i(t) = \sum_{k=1}^i \left[M_k \cdot \prod_{n=k}^{i-1} (\lambda_n) \cdot \sum_{j=k}^i \left(\frac{\exp(-\lambda_j \cdot t)}{\prod_{n=k \neq j}^{i-1} (\lambda_n - \lambda_j)} \right) \right]$$

where M_i is initial amount of radionuclide i in moles (which, for our use case corresponds to the beginning of the timestep), $M_i(t)$ is the amount of radionuclide i at time t (which for our use case corresponds to the end of the timestep, $t+dt$), and λ_i is the decay constant of radionuclide i (the decay constant is $\ln(2)$ divided by the half-life).

PANEL uses the term inside the square brackets (i.e. inside the outer summation) 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 the equations for the four members simplify to:

$$M_{1,i}^*(t) = M_1 \cdot \exp(-\lambda_1 \cdot t)$$

$$M_{2,l}^*(t) = M_1 \cdot \lambda_1 \cdot \left(\frac{\exp(-\lambda_1 \cdot t)}{\lambda_2 - \lambda_1} + \frac{\exp(-\lambda_2 \cdot t)}{\lambda_1 - \lambda_2} \right)$$

$$M_{3,l}^*(t) = M_1 \cdot \lambda_1 \cdot \lambda_2 \cdot \left(\frac{\exp(-\lambda_1 \cdot t)}{(\lambda_2 - \lambda_1) \cdot (\lambda_3 - \lambda_1)} + \frac{\exp(-\lambda_2 \cdot t)}{(\lambda_1 - \lambda_2) \cdot (\lambda_3 - \lambda_2)} + \frac{\exp(-\lambda_3 \cdot t)}{(\lambda_1 - \lambda_3) \cdot (\lambda_2 - \lambda_3)} \right)$$

$$M_{4,l}^*(t) = M_1 \cdot \lambda_1 \cdot \lambda_2 \cdot \lambda_3 \cdot \left(\frac{\exp(-\lambda_1 \cdot t)}{(\lambda_2 - \lambda_1) \cdot (\lambda_3 - \lambda_1) \cdot (\lambda_4 - \lambda_1)} + \frac{\exp(-\lambda_2 \cdot t)}{(\lambda_1 - \lambda_2) \cdot (\lambda_3 - \lambda_2) \cdot (\lambda_4 - \lambda_2)} + \frac{\exp(-\lambda_3 \cdot t)}{(\lambda_1 - \lambda_3) \cdot (\lambda_2 - \lambda_3) \cdot (\lambda_4 - \lambda_3)} + \frac{\exp(-\lambda_4 \cdot t)}{(\lambda_1 - \lambda_4) \cdot (\lambda_2 - \lambda_4) \cdot (\lambda_3 - \lambda_4)} \right)$$

where the numeric subscripts (1, 2, 3, 4) represent the i^{th} radionuclide in the partial chain, subscript l signifies the partial chain, and the superscript asterisk is added to signify that the updated inventory amounts are tentative (in that they only include decay/ingrowth effects and not discharge).

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

$$M_{iso}^* = \sum_l M_{iso \in l, l}^*$$

where the subscript $iso \in l, l$ signifies that the isotope of interest is only present in a subset of the partial chains.

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 exponential terms are similar in magnitude. Vondy (1962) presents a form that is much less susceptible to roundoff error – this is used and discussed further in the PANEL Validation and Verification Document. 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 $t / t_{1/2,(i,l)} \geq dt$, 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 is

$\{accumulation\} = \{mass\ flux\ in\} - \{mass\ flux\ out\} - \{decay\} + \{ingrowth\}$
 which, in differential form, becomes

$$\frac{dM_{iso}}{dt} = q_{in} \cdot 0 - q_{out} \cdot C_{iso} + -\lambda_{iso} \cdot M_{iso} + \sum_{p \in parents(iso)} \lambda_p \cdot M_p$$

where M is the amount of radionuclide in the waste panel, q is the brine flow rate, C is the mobile concentration of the radionuclide in the waste panel, and λ is the decay constant. The second term represents the discharge rate, the third term represents the decay rate, and the last term represents ingrowth rate (i.e. the growth rate of the isotope due to decay of its parent isotopes). In PANEL, brine that flows into the waste panel is assumed to contain no radionuclides, thus q_{in} is multiplied by a concentration of zero.

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, M_{iso}^* (as described in Section 4.3). PANEL then computes the time-averaged inventory within the timestep:

$$M_{iso}^{avg} = \frac{M_{iso}^{(n)} + M_{iso}^*}{2}$$

where the superscript (n) refers to the timestep level.

Next, PANEL uses this time-averaged inventory to compute the mobile concentrations C_{iso} (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:

$$M_{iso}^{(n+1)} = M_{iso}^* - C_{iso}^{avg} \cdot q_{out}^{(n)} \cdot \Delta t$$

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

$$R_{iso}(t) = \int_{t_i}^t q_{out} \cdot C_{iso} \cdot dt$$

PANEL calculates this in discrete form as

$$R_{iso}^{(n+1)} = R_{iso}^{(n)} + C_{iso}^{avg} \cdot q_{out}^{(n)} \cdot \Delta t$$

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 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 versus time), the mass balance is performed over REFCON:NUMPANEL waste panels. 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 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 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 (1996, page 38).

Table 4-2 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 (remaining) inventory of each auxiliary radionuclide is added to the (remaining) inventory of the namesake radionuclide on either a mole or activity (i.e. curie) basis. If the radionuclides to be combined belong to different chains (as for the constituents of PU239L, U234L, and TH230L), the basis is selected in order to maximize the activity of the lumped radionuclide. When the auxiliary radionuclide has a shorter half-life than the namesake radionuclide, the auxiliary radionuclide is added on an activity basis (because shorter half-lives indicate higher activity-per-mole). When the auxiliary radionuclide has a longer half-life than the namesake radionuclide, the auxiliary radionuclide is added on a mole basis (because the namesake radionuclide has a larger activity-per-mole). AM241L is treated uniquely. Because ²⁴¹Pu is a parent of ²⁴¹Am, and because it has a short half-life (14 years), we assume that all of the ²⁴¹Pu “instantaneously” converts to ²⁴¹Am. Thus ²⁴¹Pu and ²⁴¹Am are simply combined on a mole basis.

Table 4-2 – Lumped radionuclides and their constituents

“Lumped” Radionuclides	Constituent Radionuclides, addition basis
AM241L	²⁴¹ Am + ²⁴¹ Pu (molar)
PU239L	²³⁹ Pu + ²⁴⁰ Pu (activity) + ²⁴² Pu (molar)
PU238L	²³⁸ Pu
U234L	²³⁴ U + ²³³ U (activity)
TH230L	²³⁰ Th + ²²⁹ Th (activity)

If the inventory of each radionuclide is represented in moles, then combining isotopes on a mole basis requires only addition. In order to combine radionuclides on an activity basis, the auxiliary radionuclide inventory must be scaled by the ratio of mole-per-Curie conversion factor for the namesake radionuclide to that of the auxiliary radionuclide; this ratio simplifies to the ratio of half-lives:

$$\frac{\text{mol}_{Ci, \text{namesake}}}{\text{mol}_{Ci, \text{auxiliary}}} = \frac{t_{1/2, \text{namesake}}}{t_{1/2, \text{auxiliary}}}$$

The equations to perform the lumping are:

$$M_{Am241L} = M_{Am241} + M_{Pu241}$$

$$M_{Pu239L} = M_{Pu239} + M_{Pu240} \cdot \frac{t_{1/2,Pu239}}{t_{1/2,Pu240}} + M_{Pu242}$$

$$M_{Pu238L} = M_{Pu238}$$

$$M_{U234L} = M_{U234} + M_{U233} \cdot \frac{t_{1/2,U234}}{t_{1/2,U233}}$$

$$M_{Th230L} = M_{Th230} + M_{Th229} \cdot \frac{t_{1/2,Th230}}{t_{1/2,Th229}}$$

where M is the inventory in moles, and $t_{1/2}$ is the half-life. When the inventory is represented in curies, the equations become (this is the form given by Leigh and Trone 2005):

$$A_{Am241L} = A_{Am241} + A_{Pu241} \cdot \frac{t_{1/2,Pu241}}{t_{1/2,Am241}}$$

$$A_{Pu239L} = A_{Pu239} + A_{Pu240} + A_{Pu242} \cdot \frac{t_{1/2,Pu242}}{t_{1/2,Pu239}}$$

$$A_{Pu238L} = A_{Pu238}$$

$$A_{U234L} = A_{U234} + A_{U233}$$

$$A_{Th230L} = A_{Th230} + A_{Th229}$$

where A is the inventory in Ci.

PANEL, during its total mobile concentration limit calculations, also calculates the (\log_{10}) total mobile concentration limit values (LOGSOLM) for the lumped radionuclides. It uses an input factor, LSOLDIF, which represents the (negative \log_{10}) mole fraction of the isotopes *included* in the lumped species to all of the (modeled) isotopes of the element (i.e. it is the sum of the isotope-to-element mole fractions for all isotopes included in the lumped species). PANEL subtracts this value from the LOGSOLM value of the respective element to determine the LOGSOLM value for the lumped radionuclide (which is equivalent to multiplying the concentration limit by the mole fraction). Further details are given in Garner and Leigh (2005) and CCA Appendix-PANEL (1996, page 38).

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 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 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). For reference, the WUF is calculated as

$$WUF = \frac{\sum_{iso \in \{TRU \cap \alpha\text{-emitter} \cap t_{1/2} > 20yr\}} A_{iso}}{10^6 Ci}$$

where A is the inventory in Ci, but it is calculated external to PANEL (see Kicker and Zeitler 2013 for further details).

The unit conversion factor from Ci to EPA release units then is:

$$\frac{EPA \text{ unit}}{Ci} = \frac{1}{EPAREL \cdot WUF}$$

note that this unit conversion factor is isotope-specific because the EPAREL value is isotope-specific. PANEL assigns radionuclides with no EPA release limits (EPAREL), ^{252}Cf , ^{244}Cm , ^{147}Pm , ^{241}Pu , and ^{228}Ra , a large value (1.0E+30) so that the resulting amount is negligibly small.

For completeness, the unit conversion factor from Ci to moles is:

$$mol_{Ci} = \frac{Bq_{Ci}}{N_a} \cdot \frac{1}{\lambda}$$

where Bq_{Ci} is the Becquerel per Ci conversion constant (3.7E+10), N_a is Avogadro's constant, and λ is the radionuclide's decay constant ($\lambda = \ln(2) / t_{1/2}$, where $t_{1/2}$ is the half-life in seconds).

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:

$$DELTIME = TIMEINT - 2000$$

$$TIMEINT = DELTIME + 2000$$

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.

5.0 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.

5.1 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 STERM to calculate the total mobile concentration limits, and calls 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 dilution factor) and writes the results to the output CDB file. The helper MOBILE performs the actual total mobile concentration limit calculations for the five primary elements. The helper 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 GETFLX to read the inventory and other relevant parameters from the input CDB file. Calls WHICHE to index the elements. Calls GETFLX to read and set the brine volume and brine discharge values. Loops over timesteps. Calls BHFLO to interpolate the brine volume and brine discharge values to the current timestep. Calls 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.

5.2 Data Structures

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

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.

6.0 Capabilities and Limitations of the Software for the WIPP PA Application

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, re-equilibration 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 CRA-2014 Appendix-SOTERM (2014).

7.0 User Interactions with the Software

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 7-1.

Table 7-1 – PANEL command line arguments

Argument flag	Value	Description
-run	DECAY CONCENTRATION 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). In PA runs, “timeint” corresponds to the (shifted) time of the second intrusion (E1) in the E2E1 case (scenario 6).
-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.

Table 7-2 through Table 7-4 list examples of executing PANEL for different run modes.

Table 7-2 – Example to execute PANEL in DECAY mode

```
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 7-3 – Example to execute PANEL in CONCENTRATION mode

```
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 7-4 – Example to execute PANEL in STANDARD mode

```
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 7-5 list 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 E2E1 case being shifted from year 2000 to year 6000.

Table 7-5 – Example to execute PANEL in STANDARD mode with time translation of 4000 years

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

8.0 Description of Input 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.

8.1 “Input” CDB File

Table 8-1 through Table 8-7 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 8-1 – 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 $OXSTAT \leq OXCUTOFF$, the brine is reducing, when $OXSTAT > OXCUTOFF$, the brine is oxidizing.
GLOBAL	OXCUTOFF	N/A	0.5	Threshold value used to decide the oxidation condition of the brine. The value splits the OXSTAT distribution into two states, reducing or oxidizing.
GLOBAL	BRINEFAC	N/A	1.0	Brine dilution factor (1, 2, 3, 4, or 5) used to select the baseline solubility parameters $SOLMOD[n]:SOL[S]C]OH[BRINEFAC]$. The brine dilution 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/a	0.0	Number of seconds in a year (annum). The WIPP convention is to use mean solar tropical years.
REFCON	CITOBQ	Bq/Ci	3.7E+10	Number of becquerels in a curie.
REFCON	AVOGADRO	1/mol	6.022045 E+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 $PROBDEG > 0$.

Table 8-2 lists the radionuclide specific parameters (whole-repository initial inventory amounts and atomic properties) for the 30 radionuclides of interest. The Block (Material) name corresponds to one of:

AM241	CS137	PU240	SR90	U236
AM243	NP237	PU241	TH229	U238
CF252	PA231	PU242	TH230	
CM243	PB210	PU244	TH232	
CM244	PM147	RA226	U233	
CM245	PU238	RA228	U234	
CM248	PU239	SM147	U235	

Table 8-2 – Radionuclide specific parameters

Block	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 8-3 lists the default values used for the radionuclide atomic properties and EPA release limits. These values are consistent with 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 (1E+30) instead. Thus, when that radionuclide’s amount is expressed in EPA release units, that number will be negligibly small.

Table 8-3 – Default values for radionuclide parameters

Isotope	ATWEIGHT	HALFLIFE	EPAREL
	kg/mol	s	Ci/WUF
AM241	2.41057E-01	1.36400E+10	100
AM243	2.43061E-01	2.32900E+11	100
CF252	2.52082E-01	8.32500E+07	1E+30
CM243	2.43061E-01	8.99400E+08	100
CM244	2.44063E-01	5.71500E+08	1E+30
CM245	2.45065E-01	2.68200E+11	100
CM248	2.48072E-01	1.07000E+13	100
CS137	1.36907E-01	9.46700E+08	1000
NP237	2.37048E-01	6.75300E+13	100
PA231	2.31036E-01	1.03400E+12	100
PB210	2.09984E-01	7.03700E+08	100
PM147	1.46915E-01	8.27900E+07	1E+30
PU238	ratories. G	2.76900E+09	100
PU239	2.39052E-01	7.59400E+11	100
PU240	2.40054E-01	2.06300E+11	100
PU241	2.41057E-01	4.54400E+08	1E+30

PU242	2.42059E-01	1.22100E+13	100
PU244	2.44064E-01	2.60700E+15	100
RA226	2.26025E-01	5.04900E+10	100
RA228	2.28031E-01	2.11430E+08	1E+30
SM147	1.46915E-01	3.37700E+18	100
SR90	8.99080E-02	9.19000E+08	1000
TH229	2.29032E-01	2.31600E+11	100
TH230	2.30033E-01	2.43000E+12	10
TH232	2.32038E-01	4.43400E+17	10
U233	2.33040E-01	5.00200E+12	100
U234	2.34041E-01	7.71600E+12	100
U235	2.35044E-01	2.22100E+16	100
U236	2.36046E-01	7.38900E+14	100
U238	2.38051E-01	1.41000E+17	100

Table 8-4 lists the lumped-radionuclide associated parameters. The Block (Material) name corresponds to one of: AM241L, PU238L, PU239L, TH230L, U234L.

Table 8-4 – Lumped-radionuclide specific parameters

Block	Property	Units	Default	Description
	LSOLDIF	log ₁₀ (mol/mol)	0.0	Negative log ₁₀ 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).

Table 8-5 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 8-5 – Element-associated parameters

Block	Property	Units	Default	Description
*	CONCMIN	mol mineral-bound-actinide/L	0.0	Concentration limit of actinide associated with mobile mineral fragment colloids.
*	CONCINT	mol intrinsic-bound-actinide/L	0.0	Concentration limit of actinide associated with mobile intrinsic actinide colloids.
*	CAPHUM	mol humic-bound-actinide/L	0.0	Maximum (cap) concentration limit of actinide associated with mobile humic colloids.
*	CAPMIC	mol microbe-bound-actinide/L	0.0	Maximum (cap) concentration limit of actinide associated with mobile microbes.

*	PROPMIC	mol microbe- bound- actinide/mol dissolved actinide	0.0	Proportionality constant for concentration limit of actinides associated with mobile microbes.
---	---------	--	-----	--

Table 8-6 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 dilution factors used in calculating the organic ligand concentrations, i.e. SOLSOH (no dilution) and SOLSOH2, SOLSOH3, SOLSOH4, and SOLSOH5 for 2x, 3x, 4x, and 5x dilution 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.

Table 8-6 – Solubility Model-associated (i.e. oxidation state specific) parameters

Block	Property	Units	Default	Description
*	SOLSOH	mol/L	0.0	Oxidation state specific <i>baseline</i> solubility in Salado brine (GWB) (includes complexation with organic ligands and equilibration with hydromagnesite).
*	SOLCOH	mol/L	0.0	Oxidation state specific <i>baseline</i> solubility in Castile brine (ERDA-6) (includes complexation with organic ligands and equilibration with hydromagnesite).
*	SOLSOH[x]	mol/L	0.0	Oxidation state specific <i>baseline</i> solubility in Salado brine (GWB) (includes complexation with organic ligands and equilibration with hydromagnesite). Organic ligand concentration was diluted <i>n</i> times (where x is 2, 3, 4, or 5) in the calculation of the baseline solubility.
*	SOLCOH[x]	mol/L	0.0	Oxidation state specific <i>baseline</i> solubility in Castile brine (ERDA-6) (includes complexation with organic ligands and equilibration with hydromagnesite). Organic ligand concentration was diluted <i>n</i> times (where x 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} .

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

Table 8-7 lists the oxidation state-specific humic colloid parameters. Here the Block (Material) name corresponds to one of: PHUMOX3, PHUMOX4, PHUMOX5, PHUMOX6.

Table 8-7 – Oxidation state specific humic colloid parameters

Block	Property	Units	Default	Description
*	PHUMSIM	mol humic-bound-actinide/mol dissolved actinide	0.0	Oxidation state specific proportionality constant for the concentration limit of actinides associated with humic colloids in <u>S</u> alado brine (GWB).
*	PHUMCIM	mol humic-bound-actinide/mol dissolved actinide	0.0	Oxidation state specific proportionality constant for the concentration limit of actinides associated with humic colloids in <u>C</u> astile brine (ERDA-6).

8.2 “Flux” CDB File

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 8-8). 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 8-8 – Time series data read by PANEL from the “flux” CDB file

Global Variable	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 /s	Cumulative (over time) brine flow exiting the waste panels through the borehole.

9.0 Description of Output Files

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 9-1 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.

Table 9-1 – Element-associated parameters

Block	Property	Description
*	LOGSOLM	\log_{10} of the actinide total mobile concentration limit ($\log_{10}(\text{mol/L})$)
*	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 DECA Y mode, PANEL outputs the remaining radionuclide inventory versus time (Table 9-2). In CONCENTRATION mode, PANEL outputs the mobile radionuclide concentrations versus time (Table 9-3). And in STANDARD mode, PANEL outputs the cumulative radionuclide discharge versus time (Table 9-4). 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.

Table 9-2 – CDB History Variables output by PANEL in DECA Y 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

Table 9-3 – CDB History Variables output 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
CNM[radionuclide]	kg/m ³	Concentration in mass units
CNC[radionuclide]	Ci/m ³	Concentration in activity units
CNE[radionuclide]	EPA units/m ³	Concentration in EPA release units
CNETOTAL	EPA units/m ³	Total (sum of all lumped radionuclides) concentration in EPA units
CNM[radionuclide]	kg/m ³	Concentration of the lumped radionuclide in mass units
CNC[radionuclide]	Ci/m ³	Concentration of the lumped radionuclide in activity units
CNE[radionuclide]	EPA units/m ³	Concentration of the lumped radionuclide in EPA release units

Table 9-4 – CDB History Variables output 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

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.

10.0 Error Messages

Table 10-1 contains a list of potential error messages generated by PANEL.

Table 10-1 – 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.

11.0 Example MATSET File

Below is an example MATSET file used to generate the input CDB file for PANEL.

Table 11-1 – Example to execute PANEL in DECAY mode

```

=====
! PURPOSE:      MATSET input file for PANEL
! ANALYSIS:    Example
! ANALYSIS PLAN:
! ANALYST:     Brad Day
! DATE:       05/01/18
!=====
! DESCRIPTION:
! This input file is to prepare input CDB files for PANEL.
!=====
*HEADING
  RUN=0
  SCALE=SOURCE
  SCENARIO=00
  TITLE=SOURCE TERM
!
*PRINT_ASSIGNED_VALUES
!
*UNITS=SI
!
*CREATE_BLOCK
  BLOCKID=      2,  3,  4,  5,  6,  7,  8,  9, 10, 11, 12, 13, 14, 15, &
                16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, &
                31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, &
    
```



```
46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60, &
61, 62, 63, 64, 65, 66
*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
!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
!ISOTOPES
PROPERTY MATERIAL=Am241, NAMES =InvCHD,InvRHD,ATWEIGHT,HALFLIFE,EPAREL
PROPERTY MATERIAL=Am243, NAMES =InvCHD,InvRHD,ATWEIGHT,HALFLIFE,EPAREL
PROPERTY MATERIAL=Cf252, NAMES =InvCHD,InvRHD,ATWEIGHT,HALFLIFE,EPAREL
PROPERTY MATERIAL=Cm243, NAMES =InvCHD,InvRHD,ATWEIGHT,HALFLIFE,EPAREL
PROPERTY MATERIAL=Cm244, NAMES =InvCHD,InvRHD,ATWEIGHT,HALFLIFE,EPAREL
PROPERTY MATERIAL=Cm245, NAMES =InvCHD,InvRHD,ATWEIGHT,HALFLIFE,EPAREL
PROPERTY MATERIAL=Cm248, NAMES =InvCHD,InvRHD,ATWEIGHT,HALFLIFE,EPAREL
PROPERTY MATERIAL=Cs137, NAMES =InvCHD,InvRHD,ATWEIGHT,HALFLIFE,EPAREL
PROPERTY MATERIAL=Np237, NAMES =InvCHD,InvRHD,ATWEIGHT,HALFLIFE,EPAREL
PROPERTY MATERIAL=Pa231, NAMES =InvCHD,InvRHD,ATWEIGHT,HALFLIFE,EPAREL
PROPERTY MATERIAL=Pb210, NAMES =InvCHD,InvRHD,ATWEIGHT,HALFLIFE,EPAREL
PROPERTY MATERIAL=Pm147, NAMES =InvCHD,InvRHD,ATWEIGHT,HALFLIFE,EPAREL
PROPERTY MATERIAL=Pu238, NAMES =InvCHD,InvRHD,ATWEIGHT,HALFLIFE,EPAREL
PROPERTY MATERIAL=Pu239, NAMES =InvCHD,InvRHD,ATWEIGHT,HALFLIFE,EPAREL
PROPERTY MATERIAL=Pu240, NAMES =InvCHD,InvRHD,ATWEIGHT,HALFLIFE,EPAREL
PROPERTY MATERIAL=Pu241, NAMES =InvCHD,InvRHD,ATWEIGHT,HALFLIFE,EPAREL
PROPERTY MATERIAL=Pu242, NAMES =InvCHD,InvRHD,ATWEIGHT,HALFLIFE,EPAREL
PROPERTY MATERIAL=Pu244, NAMES =InvCHD,InvRHD,ATWEIGHT,HALFLIFE,EPAREL
PROPERTY MATERIAL=Ra226, NAMES =InvCHD,InvRHD,ATWEIGHT,HALFLIFE,EPAREL
PROPERTY MATERIAL=Ra228, NAMES =InvCHD,InvRHD,ATWEIGHT,HALFLIFE,EPAREL
PROPERTY MATERIAL=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=AM, NAMES =CONCMIN,CONCINT,CAPHUM,CAPMIC,PROPMIC
PROPERTY MATERIAL=NP, NAMES =CONCMIN,CONCINT,CAPHUM,CAPMIC,PROPMIC
PROPERTY MATERIAL=PU, NAMES =CONCMIN,CONCINT,CAPHUM,CAPMIC,PROPMIC
```

```
PROPERTY MATERIAL=TH, NAMES =CONCMIN, CONCINT, CAPHUM, CAPMIC, PROPMIC
PROPERTY MATERIAL=U, NAMES =CONCMIN, CONCINT, CAPHUM, CAPMIC, PROPMIC
!OXIDATION STATES
PROPERTY MATERIAL=SOLMOD3, NAMES
=SOLSOH, SOLCOH, 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
!-----
```

12.0 References

Bateman H. 1910. *The solution of a system of differential equations occurring in the theory of radioactive transformations*. Proceedings of the Cambridge Philosophical Society, Vol. 15.

Brush, L.H. and P. Domski. 2013a. *Calculation of Organic-Ligand Concentrations for the WIPP CRA-2014 PA*. Sandia National Laboratories. Carlsbad, NM. ERMS 559005.

Brush, L.H. and P. Domski. 2013b. *Prediction of Baseline Actinide Solubilities for the WIPP CRA-2014 PA*. Sandia National Laboratories. Carlsbad, NM. ERMS 559138.

Garner, J.W. 1998. *Change Control Form for PANEL Version 4.00*. ERMS 526499. Carlsbad, NM: Sandia National Laboratories.

Garner, J.W. 1998a. *Design Document for PANEL (Version 4.00)*. ERMS 252169. Carlsbad, NM: Sandia National Laboratories.

Garner, J.W. 1998b. *User's Manual for PANEL Version 4.00*. ERMS 248790. Carlsbad, NM: Sandia National Laboratories.

Garner, J.W. 2003. *Analysis Package for PANEL: Compliance Recertification Application*. ERMS 530165. Carlsbad, NM: Sandia National Laboratories.

Garner, J.W. 2003a. *User's Manual for PANEL Version 4.02*. ERMS 526652. Carlsbad, NM: Sandia National Laboratories.

Garner, J.W., and C. Leigh. 2005. *Analysis Package for PANEL: CRA-2004 Performance Assessment Baseline Calculation (Revision 0)*. ERMS 540572. Carlsbad, NM: Sandia National Laboratories.

ICRP 2008. ICRP Publication 107. *Nuclear Decay Data for Dosimetric Calculations*. Annals of the ICRP. Volume 38 No. 3.

Kicker, D.C. and T. Zeitler 2013. *Radionuclide Inventory Screening Analysis for the 2014 Compliance Recertification Application Performance Assessment (CRA-2014 PA)*. ERMS 559257. Sandia National Laboratories, Carlsbad, NM.

Knolls Atomic Power Laboratory. 2002. *Nuclides and Isotopes. Chart of the Nuclides*. Sixteenth Edition.

Leigh, C. and Trone, J. 2005. *Calculation of Radionuclide Inventories for Use in NUTS in the Performance Assessment Baseline Calculation Revision 0*. ERMS 539644. Sandia National Laboratories. Carlsbad, NM.

Sarathi. 2019. *Memo: Explanation of CAPMIC definition and usage in PA calculations*. ERMS 570685. Sandia National Laboratories. Carlsbad, NM.

U.S. Department of Energy (DOE). 1996. *Title 40 CFR Part 191 Compliance Certification Application for the Waste Isolation Pilot Plant (October). Appendix PANEL*. DOE/CAO-1996-2184. Carlsbad, NM: Carlsbad Field Office.

U.S. Department of Energy (DOE). 1996. *Title 40 CFR Part 191 Compliance Certification Application for the Waste Isolation Pilot Plant (October). Appendix WCA*. DOE/CAO-1996-2184. Carlsbad, NM: Carlsbad Field Office.

U.S. Department of Energy (DOE). 2014. *Title 40 CFR Part 191 Subparts B and C Compliance Recertification Application 2014, Appendix SOTERM-2014*. DOE/WIPP 14-3503. Carlsbad, NM: Carlsbad Field Office.

U.S. Environmental Protection Agency (EPA). 1993. *40 CFR 191: Environmental Radiation Protection Standards for the Management and Disposal of Spent Nuclear Fuel, High-Level and Transuranic Radioactive Wastes; Final Rule*. Federal Register, vol. 58 (December 20, 1993): 66398-416.

Vondy, D.R. 1962. *Development of a General Method of Explicit Solution to the Nuclide Chain Equations for Digital Machine Calculations*. ORNL-TM-361. Oak Ridge National Laboratory, Oak Ridge, TN.

WIPP PA Parameter Database. <http://bto.sandia.gov>.

Appendix-A.0 Expanded Decay Chain Figures

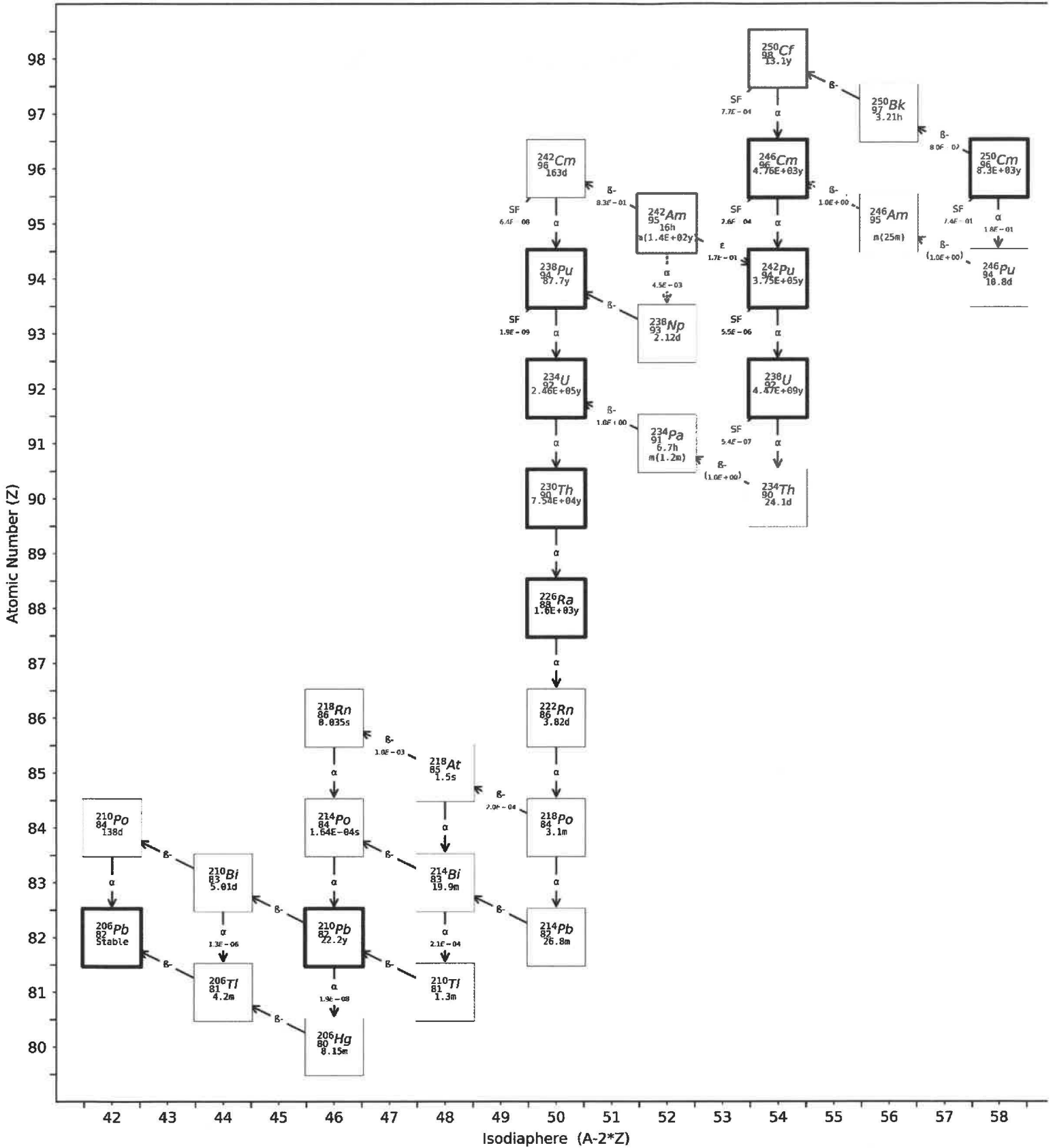


Figure A-1 – Uranium Series; includes branches starting from radionuclides with half-lives greater than 1 year

Information Only

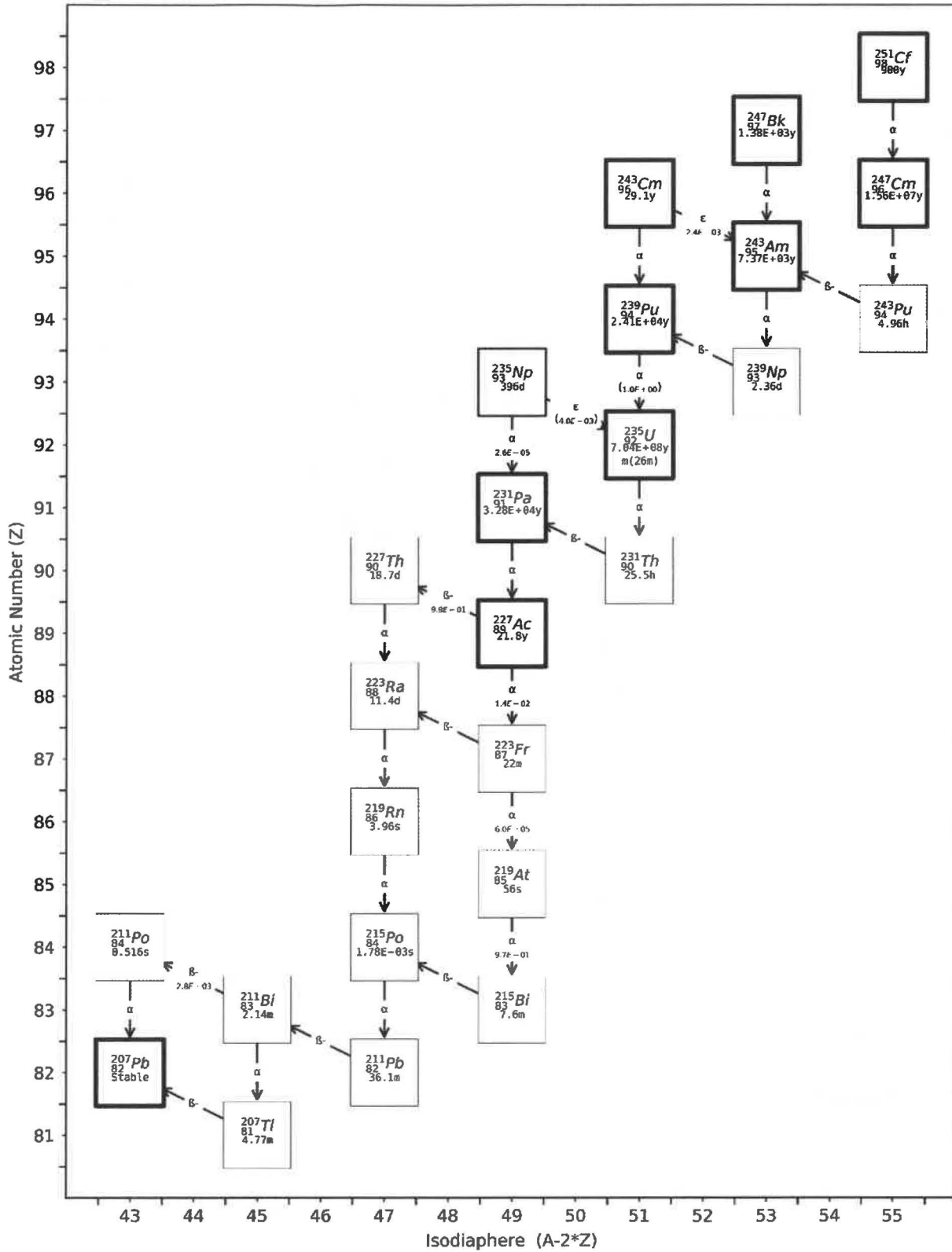


Figure A-2 – Actinium Series; includes branches starting from radionuclides with half-lives greater than 1 year

Information Only

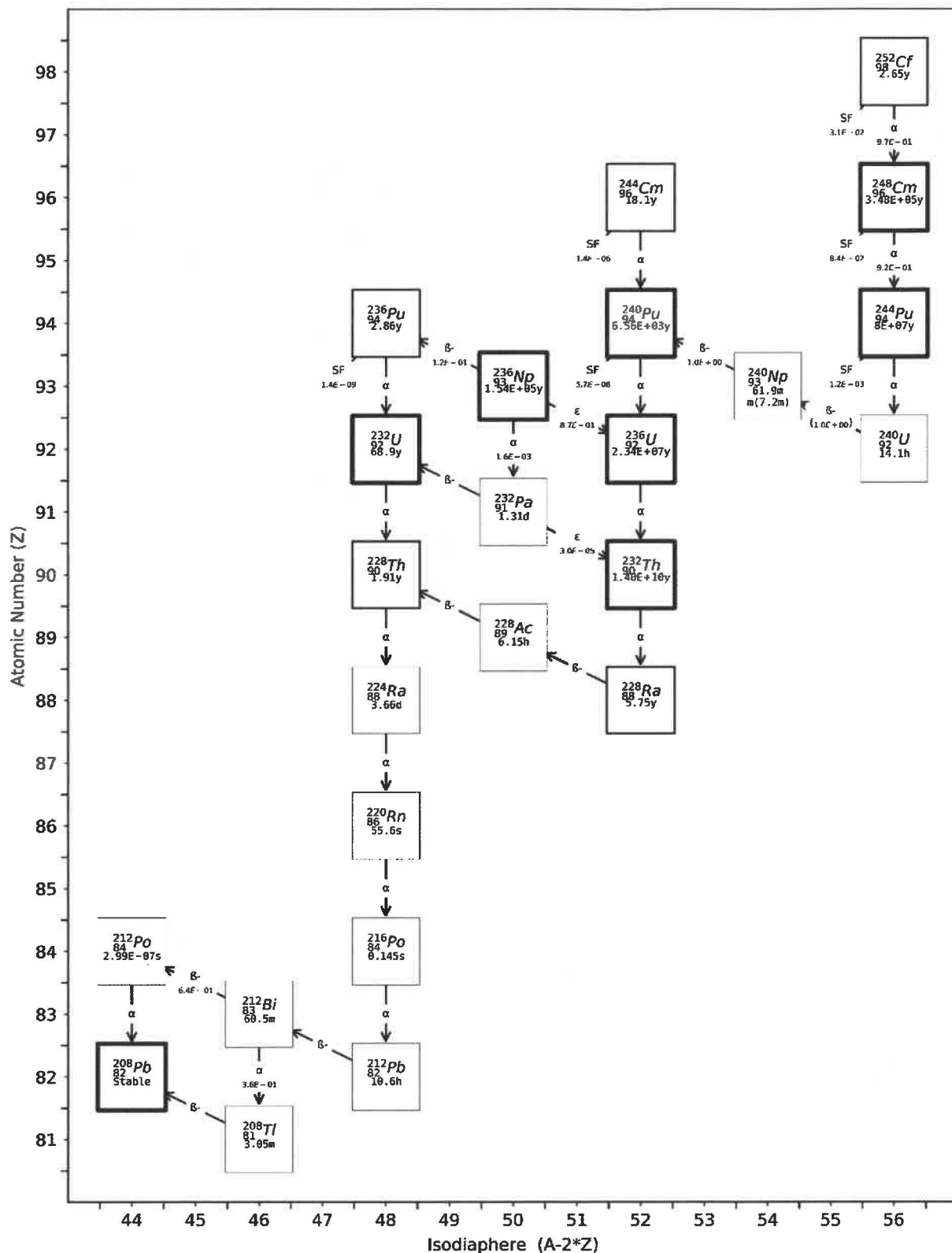


Figure A-3 Thorium Series; includes branches starting from radionuclides with half-lives greater than 1 year

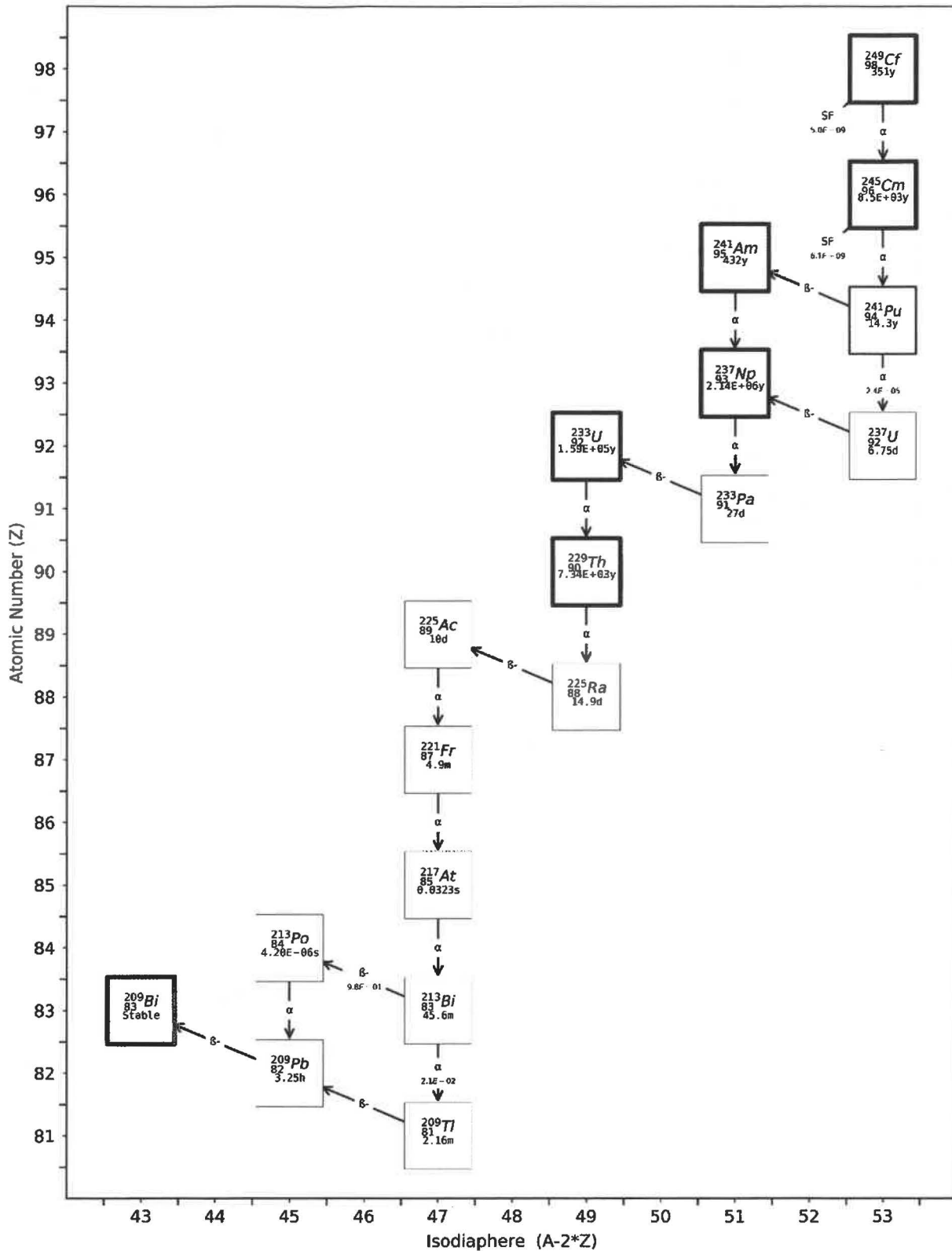


Figure A-4 Neptunium Series; includes branches starting from radionuclides with half-lives greater than 1 year

Information Only

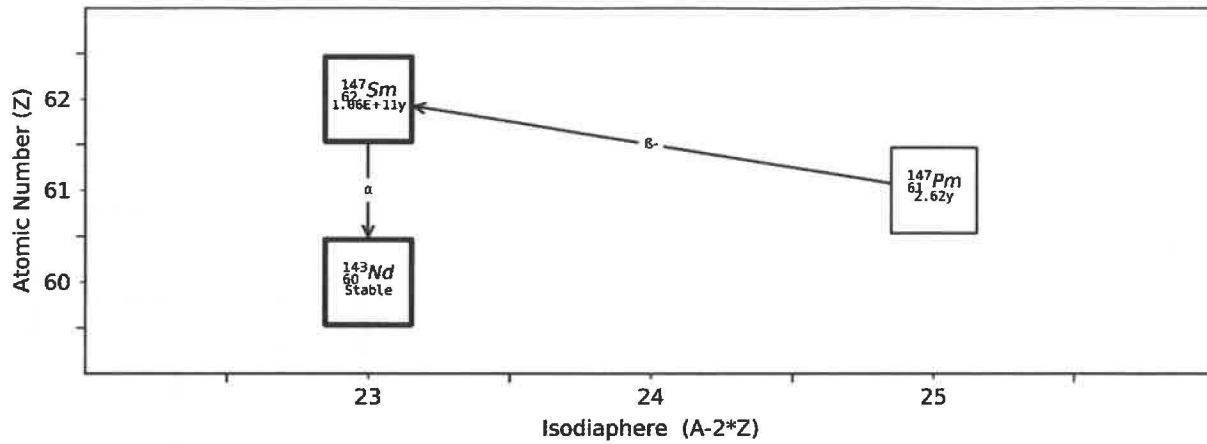


Figure A-5 – Decay chain for ^{147}Pm

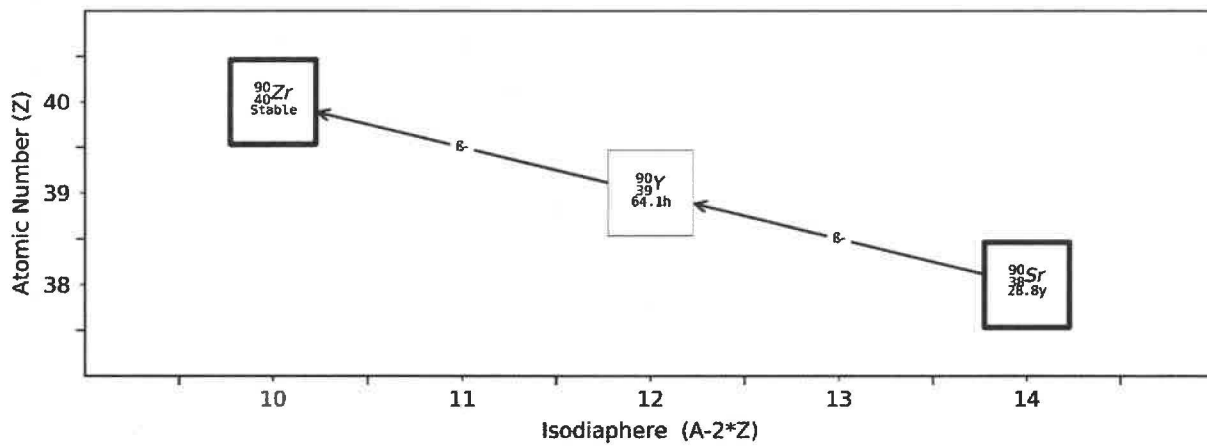


Figure A-6 – Decay chain for ^{90}Sr

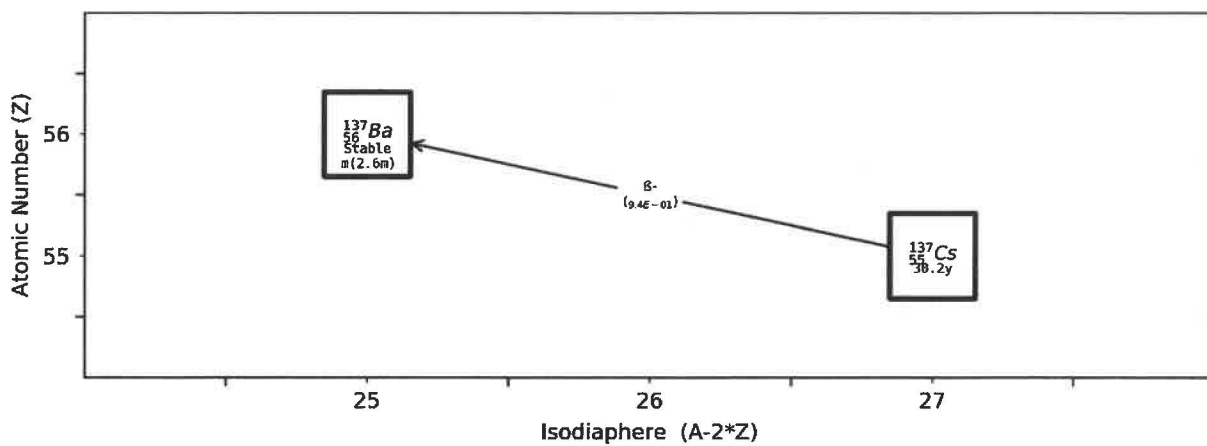


Figure A-7 – Decay chain for ^{137}Cs