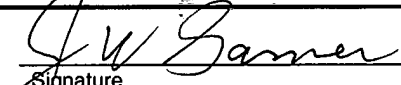

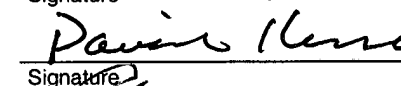
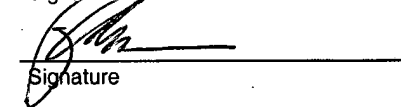


Appendix G

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

Does the user's manual contain as appropriate:

1. Software Name:	<u>PANEL</u>				
2. Software Version:	<u>4.02</u>				
3. Document Version:	<u>4.02</u>				
4. ERMS #:	<u>526652</u>				
5. A statement(s) of functional requirements (consistent with those in the RD) and system limitations?	<input checked="" type="checkbox"/> Yes	<input type="checkbox"/> No	<input type="checkbox"/> N/A	<input type="checkbox"/> N/R	
6. An explanation of the mathematical model and numerical models?	<input checked="" type="checkbox"/> Yes	<input type="checkbox"/> No	<input type="checkbox"/> N/A	<input type="checkbox"/> N/R	
7. Physical and mathematical assumptions?	<input checked="" type="checkbox"/> Yes	<input type="checkbox"/> No	<input type="checkbox"/> N/A	<input type="checkbox"/> N/R	
8. The capabilities and limitations inherent in the software?	<input checked="" type="checkbox"/> Yes	<input type="checkbox"/> No	<input type="checkbox"/> N/A	<input type="checkbox"/> N/R	
9. Instructions that describe the user's interaction with the software?	<input checked="" type="checkbox"/> Yes	<input type="checkbox"/> No	<input type="checkbox"/> N/A	<input type="checkbox"/> N/R	
10. The identification of input parameters, formats, and valid ranges?	<input checked="" type="checkbox"/> Yes	<input type="checkbox"/> No	<input type="checkbox"/> N/A	<input type="checkbox"/> N/R	
11. Messages initiated as a result of improper input and how the user can respond?	<input checked="" type="checkbox"/> Yes	<input type="checkbox"/> No	<input type="checkbox"/> N/A	<input type="checkbox"/> N/R	
12. The identification and description of output specifications and formats?	<input checked="" type="checkbox"/> Yes	<input type="checkbox"/> No	<input type="checkbox"/> N/A	<input type="checkbox"/> N/R	
13. A description of any required training necessary to use the software?	<input checked="" type="checkbox"/> Yes	<input type="checkbox"/> No	<input type="checkbox"/> N/A	<input type="checkbox"/> N/R	
14. The identification of components of the code that were not tested?	<input type="checkbox"/> Yes	<input type="checkbox"/> No	<input checked="" type="checkbox"/> N/A	<input type="checkbox"/> N/R	

15. <u>James Garner</u> Code Team/Sponsor (print)	 Signature	<u>4/25/03</u> Date
16. <u>Sean Dunagan</u> Technical Reviewer (print)	 Signature	<u>4/25/03</u> Date
17. <u>David Kessel</u> Responsible Manager (print)	 Signature	<u>4/29/03</u> Date
18. <u>Rodger Coman</u> SCM Coordinator (print)	 Signature	<u>4/25/03</u> Date

Key for check boxes above:

Check Yes for each item reviewed and found acceptable	Check No for each item which requires further work
Check N/A for items not applicable	Check N/R for items not reviewed (multiple technical reviews)

Information Only

WIPP PA

**User's Manual
for
PANEL (Version 4.02)**

Document Version 4.02

ERMS #526652

APRIL 25, 2003

Information Only

CONTENTS

1.0	Introduction	3
1.1	Software Identifier:.....	3
1.2	Points of Contact:	3
1.3	Description	4
1.4	Changes from panel 4.00 to 4.02.....	4
2.0	Functional Requirements.....	5
2.1	Functional Requirements.....	5
3.0	Required User Training and/or Background	6
4.0	Description of the Model and Methods	8
4.1	A Broad Description of the PA Model.....	8
4.2	Description of PANEL's Methods	10
4.3	Description of PANEL's Dissolution Model	11
4.4	Description of PANEL's Decay Model	12
4.5	PANEL's Release Calculation	14
4.6	PANEL's Run Sequence	16
5.0	Inherent Capabilities and Limitations of the Software.....	17
6.0	User Interactions with the Software	19
6.1	Exercising Panel in General	19
6.2	Exercising PANEL in an E2E1 type-1 Run.....	20
6.3	Exercising PANEL in a Decay-Only Type 2 Run	21
6.4	Exercising PANEL in a Concentration Type 3 Run.....	21
6.5	Exercising PANEL in a Radiolysis Type 4 Run.....	21
7.0	Description of PANEL's Input Files	22
8.0	Error Messages	23
9.0	Description of PANEL's Output Files	25
10.0	References	28
	APPENDIX A: EXAMPLE OF A MATSET INPUT FILE FOR A PANEL RUN	30

1.0 Introduction

This document is the User's Manual for the WIPP radioisotope-mobilization-and-decay code named PANEL (version number 4.02). It discusses the code, its execution, and its performance in the context of the Waste Isolation Pilot Project (WIPP) Performance Assessment (PA), and in that context only. The manual identifies the code, its authors and expert consultants (Section 1). It describes the code's WIPP-PA purposes and functions (Section 2), provides recommended user training (Section 3), outlines the code's theoretical basis and numerical methods (Section 4), its capabilities and limitations (Section 5), describes user interactions (Section 6), input files (Section 7), error messages (Section 8), and output files (Section 9), and provides examples of relevant input file in its Appendix .

1.1 Software Identifier:

Code Name: PANEL, a radioisotope-mobilization and decay code

WIPP Prefix: PNL

Version Number: 4.02

Date: 03/20/03 (which is the code's build date in the CMS system)

Platform: FORTRAN 77 for Open VMS AXP, ver. 6.1, on a DEC Alpha

1.2 Points of Contact:

Code Sponsor and Code Consultant:

Jim Garner
PIRU
(505) 284-2761 (Abq direct)
(505) 234-0078
jwgarne@sandia.gov

Code Tester:

Rodger Coman
Compaq Federal LLC
Sandia National Laboratories
4100 National Parks Highway
Carlsbad, N.M. 88220
(505) 234-0112
recoman@sandia.gov

Information Only

1.3 Description

PANEL takes brine flow and repository volume data from a CAMDAT database file and computes the amount of mobilized radioisotopes that leave the repository.

1.4 Changes from panel 4.00 to 4.02

There is a minor source term change in version 4.02. In version 4.00, there were microbial colloids computed for all realizations. In version 4.02, there is no microbial colloid component if the microbial degradation variable is zero. The variable signifies that there is no microbial activity for this PANEL run.

Also, PANEL version 4.02 adds the following Source Term variables to the CDB: LOGSOLM, FRCDIS, FRCHUM, FRCMIC, FRCINT, and FRCMIN. These six variables are added for materials AM, PU, U, TH, NP, PA, CF, CM, PM, AM241L, PU238L, PU239L, TH230L, and U234L. The last five materials are the material names for the lumped isotopes.

2.0 Functional Requirements

2.1 Functional Requirements

Given input data that (1) define the radioactive contents of the WIPP repository at time of decommissioning, (2) define the solubilities of all the elements within the repository that are to be mobilized for removal, and (3) describe (a) the volume of brine in the panel of interest, and (b) the rate at which brine is removed from that panel, PANEL computes the following at all future times up to 10,000 years:

- R.1 Compute the source term limits of elements stored within the repository that are to be mobilized for removal.
- R.2 Compute the concentrations of elements stored within the repository that are to be mobilized for removal (the concentration will be at the source term limit if the inventory is sufficient).
- R.3 Compute the mass of each radioisotope present in the repository by accounting for radioactive decay.
- R.4 Compute the amount of each radioisotope that transforms into a mobile phase.
- R.5 Compute the amount of each mobilized radioisotope that is transported by the brine flow and removed from the waste area.
- R.6 PANEL can input values for radionuclide half-lives and atomic weights from the input source CDB file.
- R.7 Input the time of intrusion on the command line and change the times of the flow data read from the input flow CDB file.
- R.8 - Read data from standard binary CAMDAT database files.
- R.9 - Produce a standard binary CAMDAT database file as output.
- R.10 - PANEL uses routines from, and therefore must be linked with, the following libraries: CAMDAT_LIB, CAMCON_LIB, and CAMSUPES_LIB.

PANEL has several external-interface requirements, including the ability (A) to read data from standard binary CAMDAT database files, (B) to produce a standard binary CAMDAT database file as output, and (C) to link to the following WIPP libraries: CAMDAT_LIB, CAMCON_LIB, and CAMSUPES_LIB.

3.0 Required User Training and/or Background

To exercise PANEL, users should have (1) basic knowledge of open VMS, (2) basic facility with Digital Command Language, (3) basic facility of Sandia's CAMDAT database, which is used in virtually every WIPP code (Rechard, 1992), and (4) operational familiarity with all of the support codes that must be exercised before and after PANEL is exercised. User's should also have (5) access to the WIPP cluster of Compaq Alpha computers with Open VMS AXP (ver. 6.1) operating system or their functional equivalents.

To manipulate and/or interpret the results of PANEL as it is exercised in WIPP PAs, user's should have (1) a basic understanding of the chemistry of radioactive decay, solution chemistry, colloid chemistry, and fluid flow in confined conduits, (2) a basic understanding of ordinary differential equations and integral calculus, and (3) a basic overview understanding of the WIPP PA process, including conceptual models, scenarios, inventories, release routes, uncertainty sampling, input-data vectors, and a general familiarity with the files and functions of the WIPP support codes that run prior to exercising PANEL, namely, GENMESH, MATSET, POSTLHS, and ALGEBRA . It is also useful to have basic familiarity with two upstream WIPP process codes, namely BRAGFLO and POSTBRAG . An annotated sketch of the PANEL code sequence involving the above codes is shown in Figure 1.

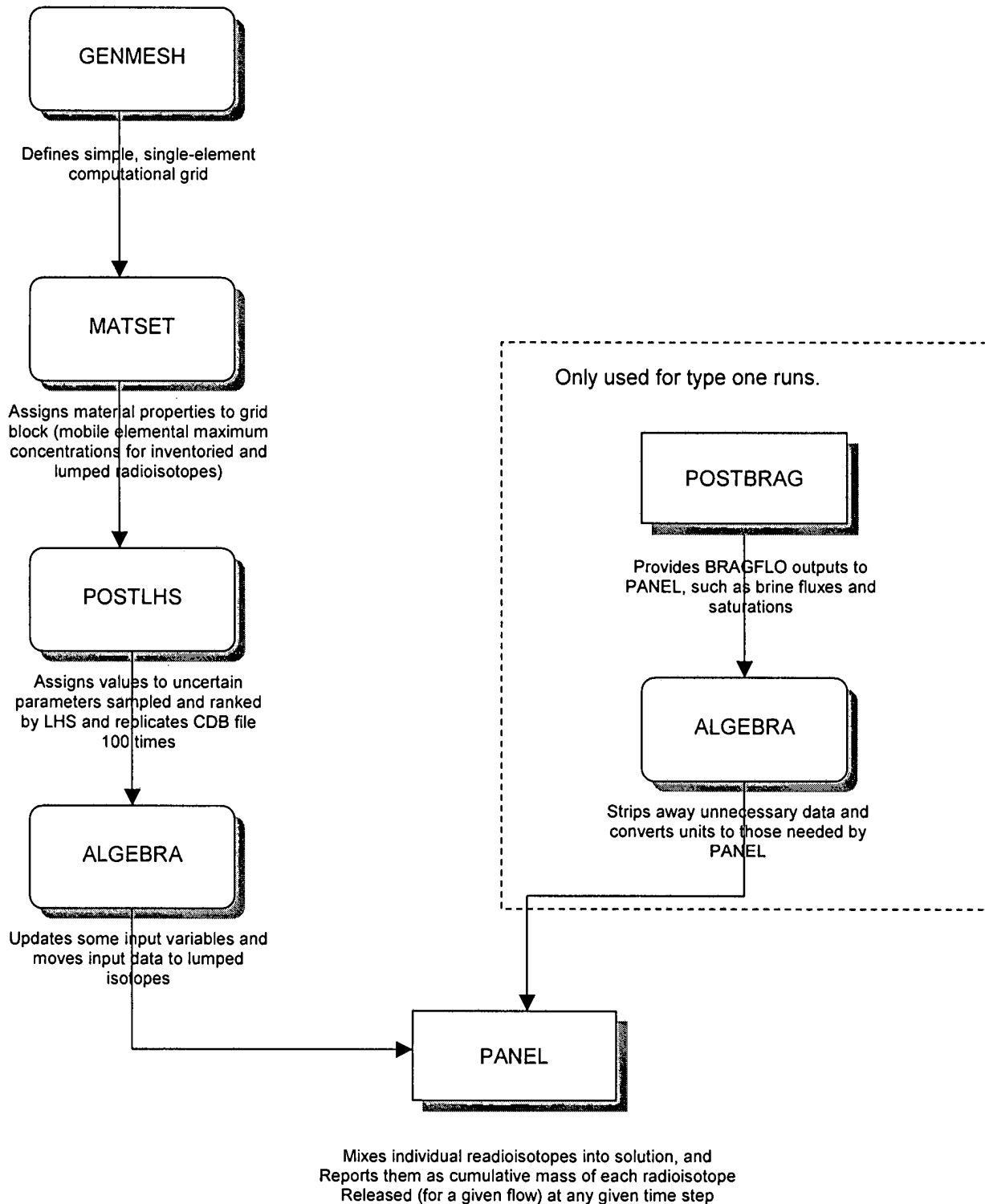


Figure 1: The run sequence for PANEL in a 2003 CRA PANEL run. Process codes are square and support codes are rounded..

4.0 Description of the Model and Methods

4.1 A Broad Description of the PA Model

PANEL has four roles in the WIPP PA system. The first is to compute the source term. This is the amount of radionuclides mobilized for a removal via a brine pathway. This source term is used by PANEL and code NUTS. PANEL then has three types of runs, done after the source term calculation. The DECAY run type does not use the source term or any flow from the repository. It only decays the radionuclide inventory for 10,000 years and outputs the results at various times. The CONCENTRATION run uses the source term and computes the amounts of radionuclides mobilized in a panel that contains 4,000 m³ of brine. The results are output at various times. The STANDARD run uses the source term and a flux input file that has both volume and brine outflow information. PANEL computes the amounts of radionuclides removed by these conditions.

PANEL's PA role is to estimate the mobilized radioactive contaminant load in the brine phase of the brine/gas mixture that seeps or flows through the repository's decommissioned waste panels. Mobilization by any process, for example dissolution or suspension on colloids, is modeled as taking place instantaneously. The contaminants introduced into the brine are the aged radioisotopes that are assumed to reside in the repository at the time of decommissioning plus any progeny of those radioisotopes that may have been produced through natural decomposition. Thus, a detailed inventory of the radioactive isotopes stored in the repository at the time of decommissioning must be provided to PANEL before it may be exercised.

PANEL plays no role in the physics of the fluid flow in or near the repository. The volume of brine within the repository and the volumetric flow rate out of the repository must be provided to PANEL by an independent physical-process code such as BRAGFLO. In this applications, values are retrieved from the controlled WIPP database.

In WIPP assessment scenarios, brine is assumed to enter the repository panels in either of two very different ways, namely: (a) by natural seepage from the surrounding Salado formation, and (b) by various locally-enhanced flows induced by hypothetical exploratory boreholes. In the case of undisturbed operation, Salado brine can seep through the disturbed rock zone from the surrounding undisturbed halite and marker beds. In the case of a repository breached by an exploratory borehole, Castile and/or Culebra brine could flow into and through the repository via the pipe-like channels created by the borehole(s). The most intense flow (of Castile brine) would occur if a borehole that penetrates a waste panel also penetrates a deep pressurized brine pocket, and some boreholes are assumed to do so.

The natural time scales associated with deep, tight-media, groundwater flows are typically centuries, and WIPP intrusion scenarios include temporal lapses of millennia prior to the hypothesized breaching of repository waste panels by boreholes. Moreover, EPA regulations extend to 10,000 years after decommissioning. On these time scales, radioisotopes of interest exhibit significant natural decay by which they transform to other radioactive and non-radioactive

isotopes and/or compounds in a well-established way (Kaplan, 1964). Thus, it is required to quantify the decay process and maintain a running record of the decayed contents of the repository as well as all the products of decomposition from the time of decommissioning onward to 10,000 years. PANEL does that.

In the context of the WIPP PA, PANEL has two principal areas of application. In the first, given the defining characteristics of the flow of uncontaminated brine into the repository's waste panels, PANEL is required to account for mobilization due to the source term of radioisotopes into the brine that wets the waste panels, and to calculate, given the fluid outflow rate, the exit rate (via the now contaminated brine flow) of each tracked isotope that was initially present in the repository, including the radioactive progeny and parents of those isotopes. The exit rate of contaminants depends on (i) the outflow rate of brine from the panel under consideration and (ii) the concentration of radioisotopes within the flowing brine, which depends on (iii) the volume of brine present in the repository at any given time and (iv) the inventory in the panel under consideration at that time. The first and third quantities must be provided in advance by, for example, BRAGFLO, which analyzes the 2-phase Darcy flow throughout the Castile, Salado, Rustler, and Dewey Lake Formations throughout the entire Land Withdrawal Act region. PANEL is required to calculate the second and fourth quantities at each of its timesteps, which are 50 years in duration.

The WIPP code NUTS calculates transport of radionuclides for most PA scenarios. However, for S6 scenarios in which 2 boreholes penetrate the same waste panel and the second one of them also penetrates a pressurized Castile brine pocket, PANEL calculates transport to the Culebra. PANEL's treatment of the flow field within the repository is much simpler than NUTS's treatment of it, but their treatment of chemical processes is identical except that PANEL considers 30 of the release-relevant radioisotopes, whereas NUTS treats only the 5 lumped equivalent isotopes.

In the second type of application, PANEL calculates the concentration of a contaminant load contained in the volume of brine (if any) that would be released directly to the surface in the form of a blowout.

To compute the initial inventory, PANEL assumes the repository comprises (i) 8 storage panels, each having a plan-view area of 11,640 m², (ii) a southern equivalent panel having an area of 8,820 m², and (iii) a northern equivalent panel having an area of 9,564 m² (WIPP PA Div., 1991, pages 3-5). These areas are used to scale the inventory linearly to the appropriate panel size. For WIPP regulatory runs, the default fraction has been set to represent one standard panel, that is, 11,640 m² divided by the net area of the repository (which is 111,504 m²), or 0.1044. This value is used unless a value is set in the MATSET run for PANEL.

4.2 Description of PANEL's Methods

PANEL is multi-purpose model. It is a radioisotope waste-mobilization model designed specifically to model waste mobilization in the WIPP's wetted repository waste panels. Also, PANEL is a radioactive-decay model and has the capability of tracking the repository's inventory as a function of time so as to account for (i) the decrease in mass of the isotopes initially placed there, and (ii) the corresponding increase in mass of their associated daughter, granddaughter, and subsequent decay products, which arise due to normal radioactive decay processes. Lastly, in the presence of the radiated products of radioactive decay, chemical compounds may disassociate through a process called radiolysis. PANEL is capable of calculating the amount of hydrogen gas produced in the repository as a function of time due to radiolysis by each isotope present in the repository. **The radiolysis capability of PANEL, called a type-4 run, is not used in PA regulatory calculations. It will not be discussed further herein.**

In WIPP applications, PANEL estimates the total radioisotope discharge from the repository that would result from various scenarios including one or more boreholes penetrating the Culebra, the Salado, the repository itself, and possibly a pressurized brine pocket in the Castile Formation beneath the Salado. Radioisotope mobilization and discharge from the repository depend in part on (i) the brine volume within the repository, and (ii) the outflow rate of brine from the repository. These are vital inputs for PANEL's isotope-transport calculation and are normally provided to PANEL by an independent WIPP flow code such as BRAGFLO

In the sections that follow, mobilization of isotopes will be discussed in detail. Efforts have been made to provide a unified approach to these two subjects. The general framework used is as follows:

In general, the "inventory" of the i^{th} element at the n^{th} timestep, $I_i(t_n)$, will mean the total amount of the i^{th} element in the repository at the time t_n , regardless of its form. Thus, elements in their original form, daughter elements arising from radioactive decay, dissolved elements, elements attached to colloids, and intrinsic colloids are all regarded as part of the inventory, provided they reside within the repository. They are removed from the "inventory" of a given element only if (i) they decay or (ii) they are mobilized and transported by means of a brine outflow to the exterior of the repository. In the latter case, they are assumed, in borehole scenarios, either to flow up the borehole toward the Culebra and higher-level Formations. They may disperse through the various porous media found in the vicinity of the repository, such as the disturbed rock zone and/or the anhydrite layers, but PANEL does not model the post-repository behavior of such transports.

If $C_{\text{max},i}^g$ is a generic maximum concentration (in moles/l) in brine of the i^{th} element due to some generic physical process (source term), then, at each timestep, PANEL will mobilize m_i^g moles of the i^{th} element into $V(t_n)$ liters of brine, the volume of brine residing in the repository at the n^{th} timestep. If PANEL is being used to support Culebra transport, $V(t_n)$ would be one of the input

data provided by BRAGFLO***. If PANEL is being used to support direct-release calculations, $V(t_n)$ is taken to be a constant 4000 cubic meters. If sufficient amounts of the i th element are available in the inventory, m_i^g will take on its maximum value, namely

$$m_{\max,i}^g = C_{\max,i}^g V(t_n)$$

If $m_{\max,i}^g$ moles of the i th element are not available in the inventory at the timestep in question, PANEL will mobilize a smaller amount, namely m_i^g , into the brine, where m_i^g is whatever amount is available at that timestep. That is,

$$m_i^g = I_i(t_n).$$

The resulting concentration of the i th element in the brine (in moles/l) would be $C_i^g = I_i / V$.

To summarize, if, at the end of the n th timestep, $I_i \geq (C_{\max,i}^g V)$, PANEL will have $(C_{\max,i}^g V)$ moles of the i th element in the brine. If $I_i < (C_{\max,i}^g V)$, PANEL will have I_i moles of the i th element in the brine.

The two principal mobilization mechanisms (associated with colloids and dissolution) are described in detail in terms of the above formulation in Section 4.3. The decay model is described in Section 4.4 and the actual release calculation is described in Section 4.5. The sequence of codes that is run in support of PANEL, including PANEL itself, is described in Section 4.6 and shown in Figure 1 (see Chapter 3).

4.3 Description of PANEL's Dissolution Model

PANEL's "dissolution" model is designed to estimate the net effects of dissolution but can be used for any type of mobilization that behaves mathematically like dissolution. In the source term part of PANEL, colloid mobilization has been combined with dissolution. The modified maximum solubilities or modified maximum concentrations are referred to herein as "enhanced" modified maximum solubilities or concentrations, since the effect of mobilized colloids is always to increase net effective solubility limits.

The dissolution part of PANEL's waste-mobilization-and-transport model is based on the following assumptions: (1) The concentration of each brine-dissolved element is uniform (i.e.,

*** Because the repository contains both brine and gas, the volume of liquid within the waste panels may vary. That is, the repository brine may have a free surface, and that free surface may rise or fall. Thus, the flow rate out of the repository need not equal the flow rate into the repository. It is (i) the brine outflow from the waste panels and (ii) the concentration of a radioisotope within that brine outflow that govern the amount of that isotope that will be delivered to the Culebra, to other fluid-bearing strata, or to the surface via a borehole at time of drilling. Strictly speaking, the timesteps used by BRAGFLO may be smaller than the 50-year timesteps used by PANEL. Consequently, BRAGFLO's $V(t)$ could vary over one of PANEL's timesteps. In that case, PANEL uses the BRAGFLO value of $V(t)$ that occurs at the end of its 50-year timestep.

constant) throughout a waste panel. (2) Mobilization is assumed to take place instantaneously and to maximum capacity, i.e., to saturation if inventory permits. (3) Supersaturation is disallowed. (4) When an element has several isotopes, the molar proportions of those isotopes dissolved in the brine are taken to be the same as the molar proportions in the total inventory contained in the waste panel.

The total enhanced concentration of the i^{th} element in the repository brine during the n^{th} timestep is given by $C^d_i(t_n)$, where

$$C^d_i(t_n) = \begin{cases} C^d_{\max,i} & , \text{ if } I_i(t_n) / V(t_n) \geq C^d_{\max,i} \\ I_i(t_n) / V(t_n) & , \text{ if } I_i(t_n) / V(t_n) < C^d_{\max,i} \end{cases}$$

and where

$$\begin{aligned} C^d_{\max,i} &= \text{enhanced maximum concentration of all elements } i, \\ I_i(t_n) &= \text{the inventory (mol) of the } i\text{th element at the } n^{\text{th}} \text{ timestep, and} \\ V(t_n) &= \text{volume (} l \text{) of brine contained in the repository during the } n^{\text{th}} \text{ timestep.} \end{aligned}$$

If PANEL is exercised in support of Culebra transport, the repository brine volume $V(t_n)$ is provided by BRAGFLO. Because BRAGFLO's timesteps are often smaller than PANEL's, PANEL uses the value of $V(t_n)$ reported at the end of its 50-year timestep. PANEL then converts $V(t_n)$ from units of m^3 to l and uses it in the equations above. The enhanced dissolution calculation is carried out element for element without regard to isotope. However, PANEL's results are reported on an isotope-for-isotope basis. The division of dissolved elements to their isotopes is according to the isotopic ratios in the inventory. Hence,

$$C^d_{i,j}(t_n) = C^d_i(t_n) [I_{i,j}(t_n) / I_i(t_n)] \quad ,$$

where all symbols are as previously defined, but with subscript j for isotopes. The inventory, $I_{i,j}$, continues to be time-dependent due to (i) removal from the repository by outflow of contaminated brine, and (ii) radioactive decay. The former effect is calculated by PANEL by correcting the inventory for the amount of isotope mobilized and removed by outflow. The latter effect is explained in Section 4.6 and requires application of Bateman's equations, which quantify both the decay of radioisotopes and the growth of daughter products.

4.4 Description of PANEL's Decay Model

Despite whatever else may be happening, every radioisotope in every decay chain is continually decaying to form its daughter product and, simultaneously, it may be continually growing through the decay of its parent isotope. The rates of decay and growth are different for different

isotopes, often quite different. The equations that quantify the decay-and-growth cycle of isotopes were first described by Bateman (1910) and traditionally bear his name.

Bateman's equations state that the rate at which the mass of a radioisotope decreases by natural radioactive decay is proportional to the present available mass of that radioisotope. In single decays, the constant of proportionality is the natural logarithm of 2 divided by the half-life of the isotope in question. If the isotope in question is other than the first isotope in the chain, its mass will also increase at a rate proportional to the present mass of its parent isotope. In simple decay chains, the constant of proportionality is the natural logarithm of 2 divided by the half-life of the parent. In multiple (i.e., bifurcated) chains, the decay algebra is slightly more complicated. However, the simple decay chains used in WIPP PAs have no bifurcations. PANEL's decay chains are listed in the block data GE_CHART given in PANEL's Implementation Document, and a printout of the products of decay appears in Appendix F.

In equation form, if M_i^* ($i = 1, 2, 3, \dots$) represents the present mass of the i th isotope in the repository in a 2-member chain, then

$$dM_i/dt = -\lambda_i M_i + \lambda_{i-1} M_{i-1},$$

where λ_i is $\ln(2)/T_i$, and T_i is the half-life of the i th isotope. For example, in a simple, direct, three-member chain, Bateman's equations would be written:

$$dM_1/dt = -\lambda_1 M_1$$

$$dM_2/dt = -\lambda_2 M_2 + \lambda_1 M_1$$

$$dM_3/dt = -\lambda_3 M_3 + \lambda_2 M_2.$$

These are linear ordinary differential equations with constant coefficients and well-posed initial conditions. Therefore, they have a unique, simple, well-known, closed-form solution. It involves (i) exponential functions, which are library functions on the WIPP DEC Alphas, and (ii) the various physical parameters of the problem. It is that solution that PANEL uses to age the inventory for decay. For the above three-element example, the closed-form solution is:

* M includes the amount m of the inventory that was mobilized as well as the remainder that has not been mobilized. That is, M includes *all* forms of all isotopes in the repository.

$$M_1(t) = [M_1(t=0)] [e^{-\lambda_1 t}]$$

$$M_2(t) = [M_2(t=0)] [e^{-\lambda_2 t}] + [\lambda_1 M_1(t=0)] [e^{-\lambda_1 t} - e^{-\lambda_2 t}] / [\lambda_2 - \lambda_1]$$

$$M_3(t) = [M_3(t=0)] [e^{-\lambda_3 t}] + [\lambda_2 M_2(t=0)] [e^{-\lambda_2 t} - e^{-\lambda_3 t}] / [\lambda_3 - \lambda_2] \\
+ \lambda_1 \lambda_2 M_1(t=0) \{e^{-\lambda_1 t} / [\lambda_2 - \lambda_1] [\lambda_3 - \lambda_1] + e^{-\lambda_2 t} / [\lambda_3 - \lambda_2] [\lambda_1 - \lambda_2] + e^{-\lambda_3 t} / [\lambda_1 - \lambda_3] [\lambda_2 - \lambda_3]\}$$

The closed-form solutions of Bateman's equations become algebraically more complex as the decay chain they treat becomes longer. However, they continue to involve only (1) physical parameters of the problem and (2) exponential functions of time (Kaplan [Chapter 10], 1964). PANEL computes only four members of a decay chain for a given time step.

PANEL uses the more complex analogue of the above results to age the inventory for decay before proceeding to the next timestep. In the equations above, the values of $M_i(t=0)$ are assigned according to the contents of the inventory at the beginning of the PANEL timestep t_n . The right-hand sides of Bateman's equations are then evaluated using $t = 50$ years and the physical constants of the problem. The results, $M_i(t)$, for $t = 50$ years, are the decay-corrected masses of each isotope at the end** of PANEL's timestep t_n . The inventory at each timestep t_n is corrected twice, (i) once for decay, and (ii) once for removal due to mobilization. It is then forwarded as the initial inventory for PANEL's next timestep, which starts at time t_{n+1} .

The above sections outline the methods by which isotopes are mobilized and decayed. However, PANEL's ultimate goal is to calculate, as a function of time, the net *releases* from the repository. The release calculation requires the net concentrations of isotopes within the repository as a function of time, which have been calculated above. It also requires repository brine-outflow data. The calculation that combines the two to form *releases* is described in the next section.

4.5 PANEL's Release Calculation

In WIPP PA performance scenarios, pressurized brine either flows upward from a deep brine pocket via an intrusion borehole or it seeps slowly through the Salado halite. A fraction of it enters a waste panel, flows through the waste, mobilizing radioisotopes as it does, and then flows either (1) upward to the Culebra via the same or a second intrusion borehole, (2) directly to the surface at the time of drilling via the intrusion borehole itself, or (3) along some other path. PANEL's job is to calculate the cumulative mass of radioisotopes mobilized at repository level and thereafter transported by the brine. The volume of brine removed from the repository during

** Actually, PANEL's decay calculations are centered within each 50-year timestep, the working value being taken as the average of the Bateman-decayed inventory at the beginning and end of the timestep. Thus, they are actually referred to 25, 75, 125, etc years after decommissioning, rather than 50, 100, 150, as described herein. The difference is unimportant in principle and inconsequential in fact.

PANEL's n^{th} timestep and transported to the Culebra is v_n (in l), a quantity that is provided in the output CDB of a WIPP flow code such as BRAGFLO, or by hypothesis, depending on the application at hand. The total amount of j^{th} isotope of the i^{th} element (in moles) transported with the brine is $C_{i,j}(t_n) v_n$, where $C_{i,j}(t_n)$ is the enhanced concentration (in moles/ l) of the j^{th} isotope of the i^{th} element in the repository during the n^{th} timestep due to *all* mobilization processes. It is useful to bear in mind that PANEL reports release results subdivided according to isotope but not mobilization process. However, the information needed to apportion the PANEL releases between the mobilization processes is contained in the computational database produced by PANEL. Before outputting its release data, PANEL first converts release units from moles back to kilograms, curies, and EPA units.

The amounts (in moles) of the j^{th} isotope of the i^{th} element mobilized and transported out of the repository during the n^{th} timestep due to source term mobilization is $[v_n C_{i,j}(t_n)]$, where $C_{i,j}$ was defined earlier and v_n is the volume of outflow during this timestep. Once these materials have exited the repository, the inventory must be revised to account for their removal before PANEL can proceed to the next timestep. PANEL must also age the revised inventory. Thus, PANEL calculates the inventory at the next timestep as:

$$I_{i,j}(t_{n+1}) = I_{i,j}(t_n) - [v_n C_{i,j}(t_n)] - D_{i,j}(t_n) + G_{i,j}(t_n) \quad ,$$

where $D_{i,j}(t_n)$ represents the total loss of the j^{th} isotope of the i^{th} element due to radioactive decay and $G_{i,j}(t_n)$ represents the gain from the parent.

The above discussion focused on PANEL's work *during* each timestep. However, PANEL does not report timestep-for-timestep results. Rather, it adds the release results of the present timestep to the sum of the release results for all prior timesteps and reports the sum. That is, it reports, at each timestep, the *cumulative* release $R_{i,j}(t_n)$ of the j^{th} radioisotope of element i from the repository. In mathematical terms, the cumulative release due to a generic process is written as follows:

$$R_{i,j}(t_n) = \int_0^{t_n} C_{i,j}(t)q(t)dt = \sum_{k=1}^n C_{i,j}(t_k)v_k(t_k)$$

where

- $C_{i,j}(t_k)$ is the individual concentration (in moles/ l) of the j^{th} isotope of the i^{th} element in the repository brine, due to the net effective mobilization processes,
- $q(t)$ is the rate (in l/s) at which brine *flows out* from the waste repository at time t . It is determined by BRAGFLO and forwarded to PANEL as an input on runs supporting Culebra transport, or assumed to be a minuscule amount ($10^{-5} \text{ m}^3/\text{yr}$) in runs supporting DBR_BRAGFLO calculations of direct release.

- $v_n(t_n)$ is the volume (in l) of brine ejected from the repository during PANEL's n th timestep and is calculated by PANEL using either (1) outflow data from BRAGFLO, or (2) the assumed rate.

4.6 PANEL's Run Sequence

To exercise PANEL as it is exercised in the WIPP PA, it is necessary to exercise a sequence of WIPP codes that support PANEL in various ways. Figure 1 (see Chapter 3.0) is an annotated depiction of that sequence for a PANEL run. The caption of Figure 1 explains the run-sequence differences required for BRAGFLO applications. Sample input files for the support code MATSET is provided in Appendices A of this User's Manual. The codes themselves are discussed in other documents supporting WIPP software QA.

5.0 Inherent Capabilities and Limitations of the Software

PANEL is capable of mobilizing and decaying all significant radioactive elements that are presently given in the repository's inventory, as it is specified on the controlled WIPP database. For the decay calculation, PANEL contains, internally, all the data necessary to age 30 WIPP isotopes, including the relevant system of Bateman solution equations, the decay chains, the half-lives, etc. To keep the mobilization calculation efficient, PANEL reads the mobilization parameters associated with six selected elements (Am, Cm, Np, Pu, Th, and U) that occur in various isotopic forms, which leads to mobilizations for 21 distinct chemical species. What PANEL does during each timestep is extremely simple, both physically and mathematically. The only differential equations it solves (Bateman's) are solved analytically and evaluated using library functions. Its mixing model is essentially algebraic within each timestep. It is straightforward and step like, exactly as was described in Section 4, above. PANEL's most advanced step is integrating its release results, which it accomplishes straightforwardly using right-hand numerical integration. Its limitations are only the validity of its assumptions, which are principally:

1. The mechanical mixing time and chemical reaction-rate times within the repository are small compared to characteristic flow times. Time scales (1) for hydrological flows and (2) for quiescent periods between exploratory borehole penetrations are so large that this assumption is not threatened. PANEL assumes all of the waste (i.e., the maximum possible amount) contained in a single waste panel is available for mobilization. It is a conservative estimate and actually represents an upper bound.

2. (A) The concentration of each brine-dissolved element is uniform (i.e., constant) throughout a waste panel. (B) The enhanced maximum concentration of each brine-dissolved-and-colloidally-mobilized element is dependent on (a) the valence state with which that element occurs in the repository and (b) the source of the brine, there being three principal sources, namely: brine from the Salado, brine from the Castile, and brine from the Culebra. Item 2B pertains more to ALGEBRA's pre-PANEL analysis than it does to PANEL itself. It is included here for completeness. (C) The fraction of each element that is permitted to dissolve into incoming brine is set *a priori* to the enhanced equivalent solubility limit for that element (that is, to the maximum possible value). Enhanced equivalent solubility data must be determined on the basis of reasonable chemical hypotheses and provided to PANEL. {In the 1996 CCA, these data were provided by ALGEBRA). The chemical basis for ALGEBRA's calculations are described in Section 7 of the SOTERM Appendix of the WIPP's 1996 Compliance Certification Application}. If insufficient material is available in the repository to reach the enhanced equivalent solubility limit, PANEL will mobilize whatever amount is available. The amounts of material available within the repository are estimated from inventory data. (D) Supersaturation is disallowed. (E) When an element has several isotopes, the molar proportions of those isotopes dissolved in the brine are taken to be the same as the molar proportions in the total inventory contained in the waste panel.

3. Mobilization by colloidally suspended particulate matter is treated in exactly the same way that dissolution is treated. Maximum concentrations for four different types of colloidal particulates are added to the maximum concentration for dissolution for each of the radioisotopes and oxidation states. The sum of the five maximum concentrations is then used in a single dissolution-like computation that estimates the net mobilization due to colloids and dissolution. {The chemical basis for these calculations is provided in Sections 6 and 7 of the SOTERM Appendix of the WIPP's 1996 Compliance Certification Application}. PANEL assumes (a) all isotopes present in the repository either form or sorb rapidly onto colloidal particulates, and all rapidly reach their assigned maximum capacities, so that (b) time dependency in colloidal formation and sorptive processes can be ignored. Item 3 pertains more to ALGEBRA's pre-PANEL analysis than it does to PANEL itself. It is included here for completeness.

4. In the past, PANEL has assumed the brine has access to the entire inventory, that is, to the entire contents of the repository. That is equivalent to assuming all the lower-level internal seals in the repository have failed well prior to the time of intrusion. In present applications, mobilization is limited to the particular waste panel that was penetrated. That is, internal seals are assumed to hold.

5. PANEL models the inventory as though it were distributed uniformly with regard to intensity and species throughout the entire repository. Thus, the full inventory is scaled linearly to a single panel's size. The possibility of inventory variability from one panel to another is not modeled.

6.0 User Interactions with the Software

In order to be executed, PANEL must have access, through CAMCON, to two previously created input data files. In WIPP PAs, these files take the form of CDB files (CAMCON Data Base) that were written as output files by the other WIPP PA codes that were exercised before PANEL in the PA code sequence.

As was said above, PANEL executes in four different ways, called run types, and performs four very different kinds of computations. Type-1 runs mobilize wastes and require externally-specified brine flows. Type-2 runs account for radioactive decay through Bateman's equations and require that the inventory be specified. Type 3 runs compute concentrations that are in the repository and remove no waste. **Type-4 runs account for radiolysis, and will not be used in regulatory calculations.** CMS regulatory runs are directed from a command file. To assist the user to understand the individual steps carried out by the command file, the two principal WIPP-type runs will be discussed below in detail from the user-interactive point of view, but first some general remarks that apply to all three run types.

6.1 Exercising Panel in General

To exercise PANEL in general, the user types the command line below at the VMS "\$" prompt, and follows it with a carriage return:

```
$ PANEL (arg1) (arg2) (arg3) (arg4) (arg5)
```

The five required command-line arguments are defined as follows:

- The value of arg1 depends on the type of run PANEL is making. For type-1 runs, arg1 is an "S" for "standard". For type-2 runs, arg1 is a "D" for "decay only". For type-3 runs, arg1 is a "CON" for "concentration. For type-4 runs, arg1 is an "R" for "radiolysis".
- arg2 is a CDB file from POSTLHS and then ALGEBRA containing sampled parameter values.
- arg3 is the output CDB files. It is not recommended, but users have limited freedom in naming these files, providing care is exercised to use proper format and compatible scenario and realization identification numbers. For example, this filename might use the format PANEL_Sx_S_Vyyy.CDB. The indices x take on the values 1, 2, ..., 6, and *must* correspond to the scenario being analyzed. The yyy are as before. If it is desired that the time of intrusion be shifted, this information is also included in arg3.

- arg4 is the input CDB file that specifies the repository brine volume and rate of brine outflow from the repository and must correspond to the scenario and vector numbers specified in the other input files. These files contain essential brine-flux data, and the user must know their BRAGFLO filenames. Examples are given in the subsections that follow. In WIPP PA runs, BRAGFLO's output files were passed through a preliminary ALGEBRA step that computed the necessary input variables (see Figure 1). Arg4 is "cancel" for decay and concentration runs.
- arg5 is PANEL's output debug file. The user is free to choose its name. An example is given in Appendix F.

Notice that PANEL does not have an input file *per se*. That is because there is nothing for the user to specify beyond the run type, which is chosen in arg1, above, and scenario, which is obtained from arg3. If time of intrusion is required, the time of intrusion is also obtained from arg3. All PANEL's input data derive from upstream codes and from the data distributions written on the controlled WIPP database. In that sense, arg2 serves as PANEL's input file in that it contains all the data previously written to the CDB file for the run in question. However, it isn't a control file in the usual sense, since control files are normally text files and (arg2) is in CDB format. GENMESH, MATSET, POSTLHS, and ALGEBRA are the four codes immediately upstream from PANEL. An examples of the input files for MATSET is in APPENDIX A.

6.2 Exercising PANEL in an E2E1 type-1 Run

In PA parlance, scenario number 6 corresponds to the E2E1 case in which a double intrusion occurs and floods at least one of the waste panels with pressurized brine. PANEL will be used to mobilize radioisotopes for all S6 runs. To exercise PANEL for that scenario and an unspecified realization number (i.e., input-vector number) yyy, enter the following command-line format at the VMS "\$" prompt:

```
$ PANEL S ALG_ST_CRA_R1_S6_Vyyy.CDB PANEL_S6_S_Vyyy.CDB -  
POSTALG_FLOW_S6_Vyyy.CDB PANEL_S6_S_Vyyy.DBG
```

That command line will exercise PANEL as a standard type-1 run for a scenario 6, which is an E2E1 double intrusion in which the first (E2) intrusion occurs at 1000 years and the second (E1) intrusion occurs at 2000 years after decommissioning. The brine-flux input-data CDB files PANEL requires are again recognized as BRAGFLO's output CDB files as modified by ALGEBRA.

If a different second time of intrusion is desired, it is necessary to add "_Tlxxxx" to the output file name. An example of wanting the second time of intrusion at 4000 years is:

```
$ PANEL S ALG_ST_CRA_R1_S6_Vyyy.CDB PANEL_S6_S_Vyyy.CDB -
```

POSTALG_FLOW_S6_TI4000_Vyyy.CDB PANEL_S6_TI4000_S_Vyyy.DBG

In this case, 2000 years would be added to all times on the BRAGFLO flow CDB.

6.3 Exercising PANEL in a Decay-Only Type 2 Run

To calculate the time history of a repository inventory when the inventory is influenced only by the effects of radioactive decomposition, which includes decreases in the masses of the given isotopes and increases in the masses of their daughter, granddaughter and succeeding products, enter the following command-line format at the VMS "\$" prompt.

```
$ PANEL D LHS_S1_S_Vyyy.CDB DECAY_S6_S_Vyyy.CDB CANCEL -  
_ $ DECAY_S6_S_Vyyy.DBG
```

The above command line will exercise PANEL in the decay mode (a type-2 run). Note that the scenario identification number is set at 06, as though this were an E2E1 run. That is a nomenclature formality. Any scenario number could have been used, since the decay process is wholly independent of scenario. The brine-flux input-data CDB file is canceled, which means PANEL defaults to internal values that specify no flow.

6.4 Exercising PANEL in a Concentration Type 3 Run

To calculate the time history of a repository concentrations when the inventory is influenced only by the effects of radioactive decomposition, which includes decreases in the masses of the given isotopes and increases in the masses of their daughter, granddaughter and succeeding products, enter the following command-line format at the VMS "\$" prompt

```
$ PANEL CON LHS_S1_S_Vyyy.CDB CON_S1_S_Vyyy.CDB CANCEL -  
_ $ CON_S1_S_Vyyy.DBG
```

The above command line will exercise PANEL in the concentration mode (a type-3 run). Note that the scenario identification number is set at 01, as though this were an undisturbed run. Scenarios 1,4, and 5 all compute Salado source term data and concentrations. Scenarios 2,3, and 6 all compute Castile source term data and concentrations.

6.5 Exercising PANEL in a Radiolysis Type 4 Run

Type-4 Radiolysis runs will not be exercised in any anticipated PA. Consequently, this topic will not be discussed herein.

7.0 Description of PANEL's Input Files

All PANEL's input data, except for run type, are read directly from CDB input files. Consequently, the user may not readily interact with or control these data. In essence, the input file for PANEL is the output CDB file from the post-POSTLHS ALGEBRA run. Examples of the input files for the five codes immediately upstream of PANEL are given in Appendices A, B, C, D, and E.

PANEL's input data include the quantities listed below. They are all read or derived from the controlled WIPP database and are, therefore, not available for user interaction.

Variable name	Description	Database Name
SECPY	The number of seconds in a year	GLOBAL YRSEC
XLOAD(IDION)	The initial inventory of the WIPP	***** INVCHD
		***** INVRHD ,

where ***** = PU242, etc.

Also, many input variables are read that are used to compute the source term. See the appendix that contain the MATSET input for all variables needed by PANEL

The ranges of validity of these parameters are not a user-relevant issue. The parameters are internally controlled and unavailable for user specification. Those parameters that are uncertain vary over ranges that are sampled by LHS. Parameter values that were used in a particular run are echoed in PANEL's DBG file for that run.

8.0 Error Messages

Because there is relatively little user interaction in PANEL's operation, there are relatively few places for errors to occur. Errors are, however, possible and lead directly to the generation of error messages. Most error messages inform the user of the general area in which the error occurred. The user is then expected to explore that area and make corrections accordingly. A brief list of possible error messages follows and includes comments on appropriate corrective actions.

- **INCORRECT FILE ASSIGNMENTS** • PANEL couldn't find and/or open the files specified in the command line. Troubleshoot.
- **PROBLEM WITH INPUT CDB** • PANEL doubts the POSTLHS output. Troubleshoot.
- **PROBLEM WITH OUTPUT CDB** • These are normally space problems. Troubleshoot.
- **SCENARIO NUMBER NOT FOUND IN FILE NAME** • Troubleshoot.
- **RUN NUMBER NOT FOUND IN FILE NAME** • Troubleshoot.
- **PROBLEM WITH FLUX CDB** • This problem could refer to the BRAGFLO output, the NUTS output, or, if ALGEBRA is used to preprocess flux input, to ALGEBRA output. Troubleshoot.
- **PROBLEM WITH DBOQAREC** • Problem with the output CDB QA records.
- **PROBLEM WITH DBOHEAD** • Problem starting the Output CDB.
- **PROBLEM WITH DBOCLOSE** • Problem ending the Output CDB.
- **DT PROBLEM** • Indicates a problem with PANEL's timestep. PANEL's usual timestep is 50 yr. However, if more than 10% of the brine volume exits during a single timestep, PANEL will reduce its next timestep by 50%. If the auto-reduction option operates several times in succession, PANEL will abort. In most cases, that would suggest a problem with the BRAGFLO input file.
- **DBOVAR ERROR N**, where N=0, 1, 2, 3, etc • Indicates a database output variable error. These are usually not run errors, but may occur, for example, if a variable is written to output but is not named.
- **PROBLEM N WITH FLUXIN.CDB**, where N=1, 2, 3 • Problems reading the brine flux inflow file.

- BRINEV=0, TFLUXOUT>0 • Problems reading the brine flux outflow file.
- PROBLEM 1A WITH FLUXIN.CDB • Problem reading the brine flux inflow file.
- INBHFLO, TIME PROBLEM • Indicates a problem in the borehole outflow. Normally, the BRAGFLO run would abort before 10,000 years.
- INDBIELBK • Indicates input element blocks exceed 100 in number. Normally there are 28 blocks in a WIPP run, so this error never arises.

9.0 Description of PANEL's Output Files

PANEL's only user-readable output file is its debug file, which echoes input data and repeats, in summary format, many of the data reported on PANEL's output CDB file. An example of a PANEL debug file is included in Appendix F. The quantities reported there are described below.

For a type 1 run, the standard run, the output variables are as follows:

History Variables (109):

BRNVOL00	SMFLOW00	SDETOTAL	SDMSR90	SDCSR90
SDESR90	SDMCS137	SDCCS137	SDECS137	SDMPB210
SDCPB210	SDEPB210	SDMRA226	SDCRA226	SDERA226
SDMRA228	SDCRA228	SDERA228	SDMTH229	SDCTH229
SDETH229	SDMTH230	SDCTH230	SDETH230	SDMTH232
SDCTH232	SDETH232	SDMPA231	SDCPA231	SDEPA231
SDMU233	SDCU233	SDEU233	SDMU234	SDCU234
SDEU234	SDMU235	SDCU235	SDEU235	SDMU236
SDCU236	SDEU236	SDMU238	SDCU238	SDEU238
SDMNP237	SDCNP237	SDENP237	SDMPU238	SDCPU238
SDEPU238	SDMPU239	SDCPU239	SDEPU239	SDMPU240
SDCPU240	SDEPU240	SDMPU241	SDCPU241	SDEPU241
SDMPU242	SDCPU242	SDEPU242	SDMPU244	SDCPU244
SDEPU244	SDMAM241	SDCAM241	SDEAM241	SDMCM244
SDCCM244	SDECM244	SDMCM248	SDCCM248	SDECM248
SDMCF252	SDCCF252	SDECF252	SDMPM147	SDCPM147
SDEPM147	SDMSM147	SDCSM147	SDESM147	SDMAM243
SDCAM243	SDEAM243	SDMCM243	SDCCM243	SDECM243
SDMCM245	SDCCM245	SDECM245	LDETOTAL	LDMAM241
LDCAM241	LDEAM241	LDMPU239	LDCPU239	LDEPU239
LDMPU238	LDCPU238	LDEPU238	LDMU234	LDCU234
LDEU234	LDMTH230	LDCTH230	LDETH230	

Key:

Prefixes

- SDE is summed discharged in EPA units
- SDM is summed discharged in mass (kg) units
- SDC is summed discharged in curies (ci)
- LDE is lumped discharge in EPA units
- LDM is lumped discharge in mass (kg) units
- LDC is lumped discharged in curies (ci)

Variable names

- BRNVOL00 is the brine volume (M³)
- SMFLOW00 is the integrated fluid discharge (M³)
- SDETOTAL is the summed release of all isotopes in EPA units
- LDETOTAL is the summed release of all lumped isotopes in EPA units

For a type 2 run, the decayed inventory run, the output variables are as follows:

History Variables (109):

BRNVOL00	SMFLOW00	SDETOTAL	SDMSR90	SDCSR90
SDESR90	SDMCS137	SDCCS137	SDECS137	SDMPB210
SDCPB210	SDEPB210	SDMRA226	SDCRA226	SDERA226
SDMRA228	SDCRA228	SDERA228	SDMTH229	SDCTH229
SDETH229	SDMTH230	SDCTH230	SDETH230	SDMTH232
SDCTH232	SDETH232	SDMPA231	SDCPA231	SDEPA231
SDMU233	SDCU233	SDEU233	SDMU234	SDCU234
SDEU234	SDMU235	SDCU235	SDEU235	SDMU236
SDCU236	SDEU236	SDMU238	SDCU238	SDEU238
SDMNP237	SDCNP237	SDENP237	SDMPU238	SDCPU238
SDEPU238	SDMPU239	SDCPU239	SDEPU239	SDMPU240
SDCPU240	SDEPU240	SDMPU241	SDCPU241	SDEPU241
SDMPU242	SDCPU242	SDEPU242	SDMPU244	SDCPU244
SDEPU244	SDMAM241	SDCAM241	SDEAM241	SDMCM244
SDCCM244	SDECM244	SDMCM248	SDCCM248	SDECM248
SDMCF252	SDCCF252	SDECF252	SDMPM147	SDCPM147
SDEPM147	SDMSM147	SDCSM147	SDESM147	SDMAM243
SDCAM243	SDEAM243	SDMCM243	SDCCM243	SDECM243
SDMCM245	SDCCM245	SDECM245	LDETOTAL	LDMAM241
LDCAM241	LDEAM241	LDMPU239	LDCPU239	LDEPU239
LDMPU238	LDCPU238	LDEPU238	LDMU234	LDCU234
LDEU234	LDMTH230	LDCTH230	LDETH230	

Key:

Prefixes

- SDE is the remaining inventory in EPA units
- SDM is the remaining inventory in mass (kg) units
- SDC is the remaining inventory in curies (ci)
- LDE is lumped remaining inventory in EPA units
- LDM is lumped remaining inventory in mass (kg) units
- LDC is lumped remaining inventory in curies (ci)

Variable names

- BRNVOL00 is the brine volume (M^3) (not used)
- SMFLOW00 is the integrated fluid discharge (M^3) (not used)
- SDETOTAL is the summed remaining inventory of all isotopes in EPA units
- LDETOTAL is the summed remaining inventory of all lumped isotopes in EPA units

Information Only

For a type 3 run, concentration, the output variables are as follows:

History Variables (109):

BRNVOL00	SMFLOW00	CNETOTAL	CNMSR90	CNCSR90
CNESR90	CNMCS137	CNCCS137	CNECS137	CNMPB210
CNCPB210	CNEPB210	CNMRA226	CNCRA226	CNERA226
CNMRA228	CNCRA228	CNERA228	CNMTH229	CNCTH229
CNETH229	CNMTH230	CNCTH230	CNETH230	CNMTH232
CNCTH232	CNETH232	CNMPA231	CNCPA231	CNEPA231
CNMU233	CNCU233	CNEU233	CNMU234	CNCU234
CNEU234	CNMU235	CNCU235	CNEU235	CNMU236
CNCU236	CNEU236	CNMU238	CNCU238	CNEU238
CNMNP237	CNCNP237	CNENP237	CNMPU238	CNCPU238
CNEPU238	CNMPU239	CNCPU239	CNEPU239	CNMPU240
CNCPU240	CNEPU240	CNMPU241	CNCPU241	CNEPU241
CNMPU242	CNCPU242	CNEPU242	CNMPU244	CNCPU244
CNEPU244	CNMAM241	CNCAM241	CNEAM241	CNMCM244
CNCCM244	CNECM244	CNMCM248	CNCCM248	CNECM248
CNMGF252	CNCCF252	CNECF252	CNMMP147	CNCPM147
CNEPM147	CNMSM147	CNCSM147	CNESM147	CNMAM243
CNCAM243	CNEAM243	CNMCM243	CNCCM243	CNECM243
CNMCM245	CNCCM245	CNECM245		
LCETOTAL	CLMAM241			
CLCAM241	CLEAM241	CLMPU239	CLCPU239	CLEPU239
CLMPU238	CLCPU238	CLEPU238	CLMU234	CLCU234
CLEU234	CLMTH230	CLCTH230	CLETH230	

Key:

Prefixes

- CNE is the concentration in EPA units per m^3
- CNM is the concentration in mass (kg) units per m^3
- CNC is the concentration in curies (ci) per m^3
- CLE is lumped concentration in EPA units per m^3
- CLM is lumped concentration in mass (kg) units per m^3
- CLC is lumped concentration in curies (ci) per m^3

Variable names

- BRNVOL00 is the brine volume (M^3)
- SMFLOW00 is the integrated fluid discharge (M^3) (not used)
- CNETOTAL is the summed concentration of all isotopes in EPA units per m^3
- LCETOTAL is the summed concentration of all lumped isotopes in EPA units per m^3

Information Only

10.0 References

Bateman, H. (1910) The Solution of a System of Differential Equations Occurring in the Theory of Radio-active Transformations, *Proc. Cambridge Phil. Soc.* **16**, 423.

Kaplan, Irving (1964) *Nuclear Physics*, 2nd Ed. (Chapter 10), Addison-Wesley Publishing Co, Reading, Mass.

Rechard, R. P., ed. (1992). *User's Reference Manual for CAMCON: Compliance Assessment Methodology Controller; Version 3.0*. SAND90 - 1983. Sandia National Laboratories, Albuquerque NM.

Rechard, R. P. , A. P. Gilkey, H. J. Iuzzolino, D. K. Rudeen, and K. A. Byle. (1993). *Programmer's Manual for CAMCON: Compliance Assessment Methodology Controller*. SAND90 - 1984. Sandia National Laboratories, Albuquerque NM.

WIPP PA Division (1991) *Preliminary Comparison with 40 CFR 191, Subpart B for the Waste Isolation Pilot Plant, December 1991*. Volume 3. Eds, R. P. Richard, A. C. Peterson, J. D. Schreibner, H. J. Iuzzolino, M. S. Tierney, and J. S. Sandha. SAND91 - 0893/3. Sandia National Laboratories, Albuquerque, NM.

WIPP PA Department (1992). *Preliminary Performance Assessment for the Waste Isolation Pilot Plant, December 1992. Volume 1: Third Comparison with 40 CFR 191, Subpart B*. SAND92 - 0700/1. Sandia National Laboratories, Albuquerque NM.

WIPP PA Department (1992). *Preliminary Performance Assessment for the Waste Isolation Pilot Plant, December 1992. Volume 2: Technical Basis*. SAND92 - 0700/2. Sandia National Laboratories, Albuquerque NM

WIPP PA Department (1992). *Preliminary Performance Assessment for the Waste Isolation Pilot Plant, December 1992. Volume 3: Model Parameters*. SAND92 - 0700/3. Sandia National Laboratories, Albuquerque NM.

WIPP PA Department (1992). *Preliminary Performance Assessment for the Waste Isolation Pilot Plant, December 1992. Volume 4: Uncertainty and Sensitivity Analyses for 40 CFR 191, Subpart B*. SAND92 - 0700/4. Sandia National Laboratories, Albuquerque NM.

WIPP PA Department (1992). *Preliminary Performance Assessment for the Waste Isolation Pilot Plant, December 1992. Volume 5: Uncertainty and Sensitivity Analyses of Gas and Brine Migration for Undisturbed Performance*. SAND92 - 0700/5. Sandia National Laboratories,

Albuquerque NM.

Information Only

APPENDIX A: EXAMPLE OF A MATSET INPUT FILE FOR A PANEL RUN

MATSET INPUT FILE

```
!=====
! TITLE:    MATSET input file for PANEL (CRA for SOURCE term in PANEL runs)
! ANALYSTS: C. T. STOCKMAN, J. W. GARNER
! CREATED:  Feb 17, 2003
! A modification of the 1996 CCA Source Term MATSET input file
! PURPOSE:  PREPARE INPUT CDB FOR PANEL
!=====
!
!*HEADING
RUN=0
SCALE=SOURCE
SCENARIO=00
TITLE=SOURCE TERM
!
!*PRINT_ASSIGNED_VALUES
!
!*UNITS=SI
!
!*CREATE_BLOCK
BLOCKID=    2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, &
            16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, &
            31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, &
            46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60, &
            61, 62, 63, 64, 65
!*RETRIEVE*NAME
COORDINATE, DIM=3, NAMES=X, Y, Z
MATERIAL,    1=GLOBAL, 2=REFCON, &
            3=AM241, 4=AM243, 5=CF252, 6=CM243, 7=CM244, 8=CM245, &
            9=CM248, 10=CS137, 11=NP237, 12=PA231, 13=PB210, 14=PM147, &
            15=PU238, 16=PU239, 17=PU240, 18=PU241, 19=PU242, 20=PU244, &
            21=RA226, 22=RA228, 23=SR90, 24=TH229, 25=TH230, &
            26=TH232, 27=U233, 28=U234, 29=U235, 30=U236, 31=U238, &
            32=AM, 33=CF, 34=CM, 35=CS, 36=NP, 37=PA, 38=PB, 39=PM, 40=PU, &
            41=RA, 42=SR, 43=TH, 44=U, &
            45=SOLMOD3, 46=SOLMOD4, 47=SOLMOD5, 48=SOLMOD6, &
            49=PHUMOX3, 50=PHUMOX4, 51=PHUMOX5, 52=PHUMOX6, &
            53=SOLAM3, 54=SOLPU3, 55=SOLPU4, 56=SOLTH4, 57=SOLU4, 58=SOLU6, &
            59=AM241L, 60=PU238L, 61=PU239L, 62=TH230L, 63=U234L, 64=BOREHOLE, &
            65=WAS AREA
!*MATERIALS 59-63 ARE LUMPED PARAMETERS FOR NUTS
!
PROPERTY    MATERIAL=WAS AREA,    NAMES =PROBDEG
PROPERTY    MATERIAL=Global,      NAMES =OXSTAT
PROPERTY    MATERIAL=REFCON,      NAMES =YRSEC, INVSCALE
!*ISOTOPES
PROPERTY    MATERIAL=Am241,        NAMES =InvCHD, InvRHD, ATWEIGHT, HALFLIFE, EPAREL
PROPERTY    MATERIAL=Am243,        NAMES =InvCHD, InvRHD, ATWEIGHT, HALFLIFE, EPAREL
PROPERTY    MATERIAL=Cf252,        NAMES =InvCHD, InvRHD, ATWEIGHT, HALFLIFE, EPAREL
PROPERTY    MATERIAL=Cm243,        NAMES =InvCHD, InvRHD, ATWEIGHT, HALFLIFE, EPAREL
PROPERTY    MATERIAL=Cm244,        NAMES =InvCHD, InvRHD, ATWEIGHT, HALFLIFE, EPAREL
PROPERTY    MATERIAL=Cm245,        NAMES =InvCHD, InvRHD, ATWEIGHT, HALFLIFE, EPAREL
PROPERTY    MATERIAL=Cm248,        NAMES =InvCHD, InvRHD, ATWEIGHT, HALFLIFE, EPAREL
PROPERTY    MATERIAL=Cs137,        NAMES =InvCHD, InvRHD, ATWEIGHT, HALFLIFE, EPAREL
PROPERTY    MATERIAL=Np237,        NAMES =InvCHD, InvRHD, ATWEIGHT, HALFLIFE, EPAREL
PROPERTY    MATERIAL=Pa231,        NAMES =InvCHD, InvRHD, ATWEIGHT, HALFLIFE, EPAREL
PROPERTY    MATERIAL=Pb210,        NAMES =InvCHD, InvRHD, ATWEIGHT, HALFLIFE, EPAREL
```

```
PROPERTY MATERIAL=Pm147, NAMES =InvCHD, InvRHD, ATWEIGHT, HALFLIFE, EPAREL
PROPERTY MATERIAL=Pu238, NAMES =InvCHD, InvRHD, ATWEIGHT, HALFLIFE, EPAREL
PROPERTY MATERIAL=Pu239, NAMES =InvCHD, InvRHD, ATWEIGHT, HALFLIFE, EPAREL
PROPERTY MATERIAL=Pu240, NAMES =InvCHD, InvRHD, ATWEIGHT, HALFLIFE, EPAREL
PROPERTY MATERIAL=Pu241, NAMES =InvCHD, InvRHD, ATWEIGHT, HALFLIFE, EPAREL
PROPERTY MATERIAL=Pu242, NAMES =InvCHD, InvRHD, ATWEIGHT, HALFLIFE, EPAREL
PROPERTY MATERIAL=Pu244, NAMES =InvCHD, InvRHD, ATWEIGHT, HALFLIFE, EPAREL
PROPERTY MATERIAL=Ra226, NAMES =InvCHD, InvRHD, ATWEIGHT, HALFLIFE, EPAREL
PROPERTY MATERIAL=Ra228, NAMES =InvCHD, InvRHD, ATWEIGHT, HALFLIFE, EPAREL
PROPERTY MATERIAL=Sr90 , NAMES =InvCHD, InvRHD, ATWEIGHT, HALFLIFE, EPAREL
PROPERTY MATERIAL=Th229, NAMES =InvCHD, InvRHD, ATWEIGHT, HALFLIFE, EPAREL
PROPERTY MATERIAL=Th230, NAMES =InvCHD, InvRHD, ATWEIGHT, HALFLIFE, EPAREL
PROPERTY MATERIAL=Th232, NAMES =InvCHD, InvRHD, ATWEIGHT, HALFLIFE, EPAREL
PROPERTY MATERIAL=U233, NAMES =InvCHD, InvRHD, ATWEIGHT, HALFLIFE, EPAREL
PROPERTY MATERIAL=U234, NAMES =InvCHD, InvRHD, ATWEIGHT, HALFLIFE, EPAREL
PROPERTY MATERIAL=U235, NAMES =InvCHD, InvRHD, ATWEIGHT, HALFLIFE, EPAREL
PROPERTY MATERIAL=U236, NAMES =InvCHD, InvRHD, ATWEIGHT, HALFLIFE, EPAREL
PROPERTY MATERIAL=U238, NAMES =InvCHD, InvRHD, ATWEIGHT, HALFLIFE, EPAREL
! LUMPED ISOTOPES
PROPERTY MATERIAL=AM241L, NAMES =InvCHD, InvRHD
PROPERTY MATERIAL=PU238L, NAMES =InvCHD, InvRHD, LSOLDIFF
PROPERTY MATERIAL=PU239L, NAMES =InvCHD, InvRHD
PROPERTY MATERIAL=TH230L, NAMES =InvCHD, InvRHD, LSOLDIFF
PROPERTY MATERIAL=U234L, NAMES =InvCHD, InvRHD, LSOLDIFF
! ELEMENTS
PROPERTY MATERIAL=AM, NAMES =CONCMIN, CONCINT, CAPHUM, CAPMIC, PROPMIC
PROPERTY MATERIAL=NP, NAMES =CONCMIN, CONCINT, CAPHUM, CAPMIC, PROPMIC
PROPERTY MATERIAL=PU, NAMES =CONCMIN, CONCINT, CAPHUM, CAPMIC, PROPMIC
PROPERTY MATERIAL=TH, NAMES =CONCMIN, CONCINT, CAPHUM, CAPMIC, PROPMIC
PROPERTY MATERIAL=U, NAMES =CONCMIN, CONCINT, CAPHUM, CAPMIC, PROPMIC
! OXIDATION STATES
PROPERTY MATERIAL=SOLMOD3, NAMES =SOLSIM, SOLCIM
PROPERTY MATERIAL=SOLMOD4, NAMES =SOLSIM, SOLCIM
PROPERTY MATERIAL=SOLMOD5, NAMES =SOLSIM, SOLCIM
PROPERTY MATERIAL=SOLMOD6, NAMES =SOLSIM, SOLCIM
PROPERTY MATERIAL=PHUMOX3, NAMES =PHUMSIM, PHUMCIM
PROPERTY MATERIAL=PHUMOX4, NAMES =PHUMSIM, PHUMCIM
PROPERTY MATERIAL=PHUMOX5, NAMES =PHUMSIM, PHUMCIM
PROPERTY MATERIAL=PHUMOX6, NAMES =PHUMSIM, PHUMCIM
! SOLUBILITIES
PROPERTY MATERIAL=SOLAM3, NAMES =SOLSIM, SOLCIM
PROPERTY MATERIAL=SOLPU3, NAMES =SOLSIM, SOLCIM
PROPERTY MATERIAL=SOLPU4, NAMES =SOLSIM, SOLCIM
PROPERTY MATERIAL=SOLTH4, NAMES =SOLSIM
PROPERTY MATERIAL=SOLU4, NAMES =SOLSIM
PROPERTY MATERIAL=SOLU6, NAMES =SOLSIM, SOLCIM
! WASTE UNIT FACTOR
PROPERTY MATERIAL=BOREHOLE, NAMES=WUF
! =====
! *SDB ANALYSIS=CCA
PROPERTY MATERIAL=BOREHOLE, NAMES=WUF
PROPERTY MATERIAL=AM241, NAMES=INVRHD
PROPERTY MATERIAL=CF252, NAMES=INVRHD
PROPERTY MATERIAL=CM245, NAMES=INVCHD
PROPERTY MATERIAL=AM241L, NAMES=INVCHD, INVRHD
PROPERTY MATERIAL=PU238, NAMES=INVCHD
PROPERTY MATERIAL=PU238L, NAMES=INVCHD, INVRHD
PROPERTY MATERIAL=PU239L, NAMES=INVCHD, INVRHD
PROPERTY MATERIAL=TH230, NAMES=INVCHD
PROPERTY MATERIAL=TH230L, NAMES=INVCHD, INVRHD
PROPERTY MATERIAL=U234, NAMES=INVCHD
PROPERTY MATERIAL=U234L, NAMES=INVCHD, INVRHD
*SET*VALUES
! INVSCALE NEEDED UNTIL ADDED TO DATA BASE
! PROPERTY MATERIAL=REFCON, NAMES*VALUE: INVSCALE=.1044
```



```
PROPERTY MATERIAL=REFCON, NAMES*VALUE: INVSCALE=1.
PROPERTY MATERIAL=BOREHOLE, NAMES*VALUE: WUF=2.97
! PROPERTY MATERIAL=PU238L, NAMES*VALUE: LSOLDIFF=2.17519
PROPERTY MATERIAL=PU238L, NAMES*VALUE: LSOLDIFF=2.16910
! PROPERTY MATERIAL=TH230L, NAMES*VALUE: LSOLDIFF=2.900
PROPERTY MATERIAL=TH230L, NAMES*VALUE: LSOLDIFF=3.88641
! PROPERTY MATERIAL=U234L, NAMES*VALUE: LSOLDIFF=2.550
PROPERTY MATERIAL=U234L, NAMES*VALUE: LSOLDIFF=3.76045
! ADD TEMPORARY INVENTORY VALUES HERE
PROPERTY MATERIAL=Am241, NAMES*VALUE: InvCHD=4.78e5 ,InvRHD=3.96e4
PROPERTY MATERIAL=Am243, NAMES*VALUE: InvCHD=3.33e1 ,InvRHD=7.58e-1
PROPERTY MATERIAL=Cf252, NAMES*VALUE: InvCHD=6.40e-5 ,InvRHD=5.61e-6
PROPERTY MATERIAL=Cm243, NAMES*VALUE: InvCHD=1.82e-1 ,InvRHD=2.31e-1
PROPERTY MATERIAL=Cm244, NAMES*VALUE: InvCHD=4.82e3 ,InvRHD=1.05e2
PROPERTY MATERIAL=Cm245, NAMES*VALUE: InvCHD=1.36e-2 ,InvRHD=1.09e-2
PROPERTY MATERIAL=Cm248, NAMES*VALUE: InvCHD=2.16e-6 ,InvRHD=1.89e-7
PROPERTY MATERIAL=Cs137, NAMES*VALUE: InvCHD=6.93e3 ,InvRHD=1.77e5
PROPERTY MATERIAL=Np237, NAMES*VALUE: InvCHD=1.13e1 ,InvRHD=1.01e0
PROPERTY MATERIAL=Pa231, NAMES*VALUE: InvCHD=1.96e0 ,InvRHD=6.86e-4
PROPERTY MATERIAL=Pb210, NAMES*VALUE: InvCHD=7.90e0 ,InvRHD=1.62e-5
PROPERTY MATERIAL=Pm147, NAMES*VALUE: InvCHD=4.13e-4 ,InvRHD=8.05e-2
PROPERTY MATERIAL=Pu238, NAMES*VALUE: InvCHD=1.53e6 ,InvRHD=3.48e3
PROPERTY MATERIAL=Pu239, NAMES*VALUE: InvCHD=7.77e5 ,InvRHD=5.64e3
PROPERTY MATERIAL=Pu240, NAMES*VALUE: InvCHD=1.32e5 ,InvRHD=1.82e3
PROPERTY MATERIAL=Pu241, NAMES*VALUE: InvCHD=5.17e5 ,InvRHD=1.49e5
PROPERTY MATERIAL=Pu242, NAMES*VALUE: InvCHD=2.16e1 ,InvRHD=5.02e-1
PROPERTY MATERIAL=Pu244, NAMES*VALUE: InvCHD=1.41e-6 ,InvRHD=1.56e-3
PROPERTY MATERIAL=Ra226, NAMES*VALUE: InvCHD=1.00e1 ,InvRHD=5.55e-5
PROPERTY MATERIAL=Ra228, NAMES*VALUE: InvCHD=7.65e0 ,InvRHD=3.36e-1
PROPERTY MATERIAL=Sr90 , NAMES*VALUE: InvCHD=2.82e4 ,InvRHD=1.18e5
PROPERTY MATERIAL=Th229, NAMES*VALUE: InvCHD=6.13e0 ,InvRHD=1.83e-1
PROPERTY MATERIAL=Th230, NAMES*VALUE: InvCHD=2.26e-1 ,InvRHD=7.24e-3
PROPERTY MATERIAL=Th232, NAMES*VALUE: InvCHD=6.63e0 ,InvRHD=2.91e-1
PROPERTY MATERIAL=U233, NAMES*VALUE: InvCHD=1.43e3 ,InvRHD=4.38e1
PROPERTY MATERIAL=U234, NAMES*VALUE: InvCHD=3.64e2 ,InvRHD=2.35e1
PROPERTY MATERIAL=U235, NAMES*VALUE: InvCHD=1.38e0 ,InvRHD=9.79e-1
PROPERTY MATERIAL=U236, NAMES*VALUE: InvCHD=2.60e-1 ,InvRHD=1.48e0
PROPERTY MATERIAL=U238, NAMES*VALUE: InvCHD=2.46e1 ,InvRHD=5.69e2
```

! *END

!-----

--

END OF APPENDIX A

Information Only