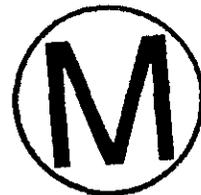

**Title 40 CFR Part 191
Compliance Certification
Application
for the
Waste Isolation Pilot Plant**

Appendix PANEL



**United States Department of Energy
Waste Isolation Pilot Plant**

**Carlsbad Area Office
Carlsbad, New Mexico**

WIPP PA User's Manual for PANEL



WIPP PA

User's Manual

for

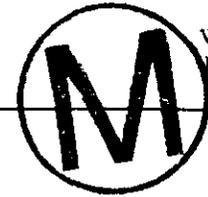
PANEL (Version 3.60)



Document Version 1.00

WPO #37361

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1.0 INTRODUCTION

This document is the User's Manual for the WIPP radioisotope-mobilization-and-decay code named PANEL (version number 3.60). It discusses the code, its execution, and its performance in the context of the 1996 Waste Isolation Pilot Project (WIPP) Compliance Certification Application (CCA) 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, output, and debug files in its Appendices as well as calculations of interest (distributed throughout).

1.1 Software Identifier:

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

WIPP Prefix:

~~PNE~~ PANEL JWB 9-4-96

Version Number: 3.60

Date: 10/May/96 (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:

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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 The mass of each radioisotope present in the repository by accounting for radioactive decay.
- R.2 The amount of each radioisotope that transforms into a mobile phase.
- R.3 The amount of each mobilized radioisotope that is transported by the brine flow and removed from the waste area.

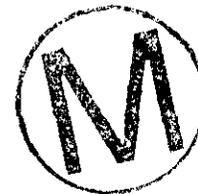
PANEL has several external-interface requirements, including the ability (A) to read data from standard binary CAMDAT database files, (B) to produce a standard binary CAMDAT database file as output, and (C) to link to the following WIPP libraries: CAMDAT_LIB, CAMCON_LIB, and CAMSUPES_LIB.



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 DEC Alpha microcomputers with an 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, as they apply in the mathematical formulation of physical principles and especially of conservation of mass*, 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 (WIPP PA Dept [5 Volumes], 1992). It is also useful to have basic familiarity with two upstream WIPP process codes, namely BRAGFLO and DBR_BRAGFLO**. An annotated sketch of the PANEL code sequence involving the above codes is shown in Figure 1.



* Strictly speaking, the system is not mass conserving. Radioactive decay involves the loss of mass, although it is insignificant for assessment purposes. Still, PANEL conserves the number of atoms of radioactive material during the decay process. Accordingly, PANEL's principal computational units are moles. Upon completing its work, PANEL converts its release units from moles back to kilograms for its Culebra applications. For DBR_BRAGFLO applications, a final ALGEBRA step converts output units to Normalized EPA units per cubic meter of outflow. Note also that PANEL treats both alpha and beta decay.

** In other CCA code documentation, these two codes are sometimes referred to by their CMS version numbers, which are BRAGFLO 4.00 and BRAGFLO 4.01, respectively. The two BRAGFLO codes are quite similar in their internal structure, but quite different in their purposes, applications, and run sequences.

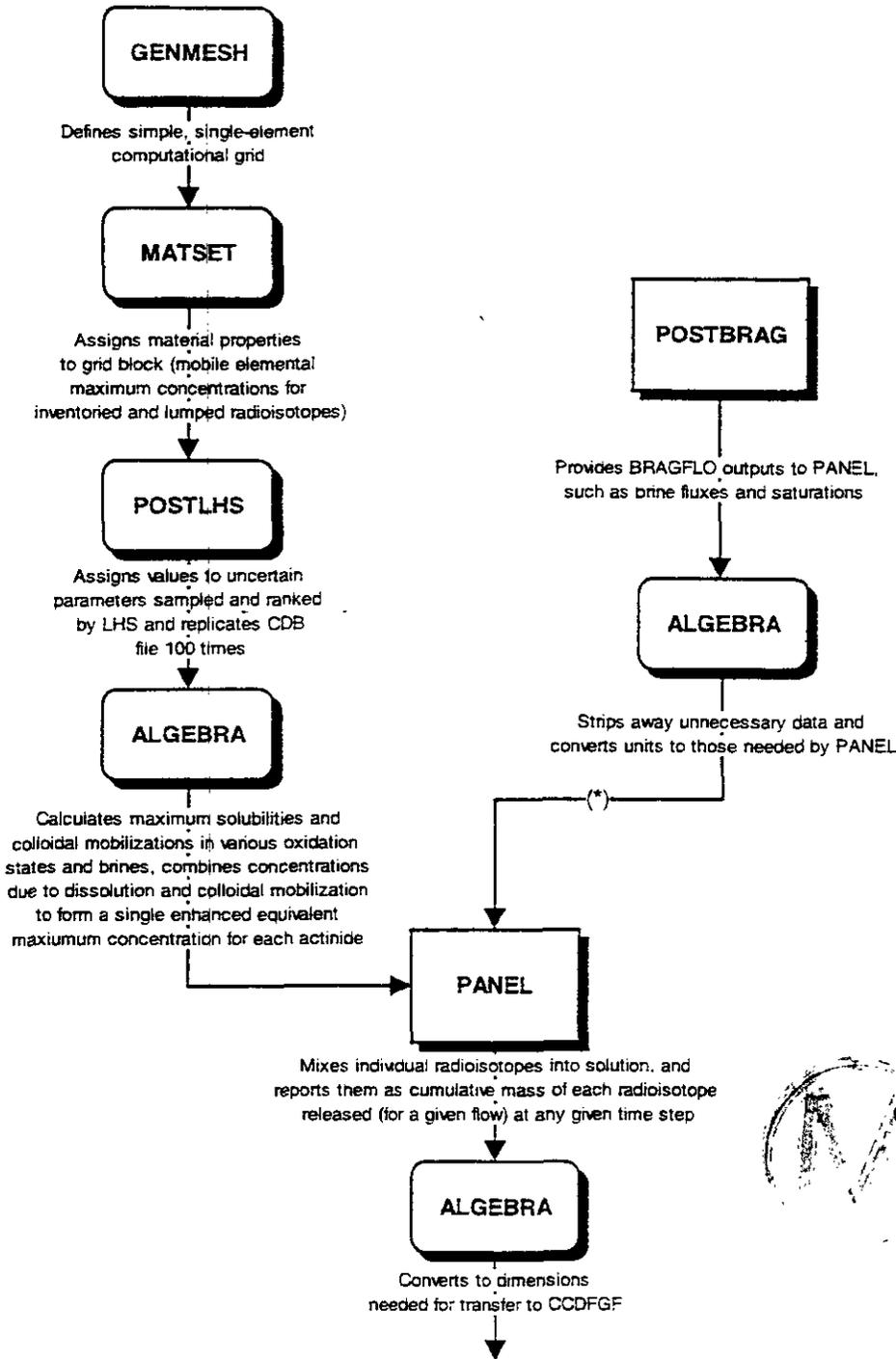


Figure 1: The run sequence for PANEL in a 1996 CCA BRAGFLO run. Process codes are square and support codes are rounded. The asterisk represents the location of an additional ALGEBRA application that is required in DBR_BRAGFLO runs to replace POSTBRAGFLO's data with hypothetical flow-rate and brine-volume data.

4.0 DESCRIPTION OF THE MODEL AND METHODS

4.1 A Broad Description of the CCA Model

PANEL's CCA 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 DBR_BRAGFLO direct-release applications, both data are provided by hypothesis. In both applications, values are retrieved from the controlled WIPP data base.

In CCA 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 CCA, 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 dissolution and colloidal suspension 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 the time. The first and third quantities must be provided in advance by, for example, BRAGFLO, which analyses 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. The WIPP code NUTS is charged to perform that very calculation for most CCA 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 is directed to perform the calculation. 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. PANEL is afforded that versatility because it exercises quickly, run time being a factor on account of the large number of cases that are required. PANEL can also serve as an internal consistency check for NUTS by providing reasonable upper-bound limits.

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In the second type of application, PANEL calculates the contaminant load contained in the volume of brine (if any) that would be released directly to the surface in the form of a mixture with the liquid slurry drillers use to cool and lubricate drill bits, and to remove borehole debris. Such releases would occur at the time of drilling as a result of pressure relief and are possible only if repository pore pressures exceed 8MPa. In this application, PANEL uses ALGEBRA to retrieve (1) a fixed assumed repository brine volume and (2) an assumed repository outflow rate that is very small but non zero. PANEL's release rates are divided by the assumed flow rate to compute mobilized mass per unit volume of brine for each radioisotope considered. Thus, PANEL's final result of radioisotope released per volume of brine released is actually independent of the assumed flow rate. The volume of brine that is released (if any) must be provided by another code, which was DBR_BRAGFLO in the 1996 CCA.



In both of the above applications, the outflow rate of the brine and the volume of brine present in the repository at any given time are required by PANEL to calculate and report its principal results, namely, the total transport, up to the present timestep, of each of 21** selected (decayed) radioisotopes that exist within the repository.

Because of natural decay processes, it is entirely possible to find compounds in the effluent that were not present in the initial repository inventory.

* PANEL treats 30 of the 33 radioisotopes singled out as potentially important in the 1996 CCA, the other 3 being insignificant. One of the 30, SM147, is absent from the initial inventory. It appears only as a decay product, which explains why the initial conditions in Appendix F are 29-rows long. SM147 ingrowth is calculated and reported, but, like 8 other isotopes, SM147 is neither mobilized nor released. Thus, PANEL mobilizes and releases 21 radioisotopes.

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** In 1996 CCA runs, PANEL transports the 21 isotopes of 6 elements (Am, Cm, Np, Pu, Th, & U), the choice being based on their significance in earlier assessments. PANEL is able to mobilize any number of radioisotopes if it undergoes minor revisions, recompiling, and reQAing.

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. In past PAs, PANEL's runs assumed the contents of the *entire* repository inventory were available for release into whatever brine was present. In no PA is the fraction of the repository that is available to brine flow adjustable as an input parameter. It is hard-wired into the code and is not, therefore, readily adjustable by the user. For 1996 CCA regulatory runs, the 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.

4.2 Description of PANEL's Methods

PANEL is triple-purpose model. First, it is a radioisotope waste-mobilization model designed specifically to model waste mobilization in the WIPP's wetted repository waste panels. Secondly, 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. In PANEL, these three kinds of computations are called runs of type 1, 2, and 3, respectively. **The radiolysis capability of PANEL, called a type-3 run, is not used in CCA regulatory calculations. It is unavailable to CCA users and will not be discussed further herein.**

In WIPP type-1 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 (a) an independent WIPP flow code such as BRAGFLO in groundwater applications, and (b) by hypothesis in DBR_BRAGFLO direct-release applications.



* PANEL's releases are from the interior of the WIPP repository (i.e., from within its waste panels) to the exterior of the waste panels, but no further. PANEL does not profess to describe the transport of radioisotopes or brine through the porous media surrounding the waste panels. That task is performed by other WIPP codes such as NUTS or the SECO suite of codes. However, because the flow associated with DBR_BRAGFLO direct-release applications is relatively rapid (time scale of days) PANEL's results apply directly in that case.

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 (a) to flow up the borehole toward the Culebra** and higher level Formations, or (b) to flow up the borehole and directly to the surface at time of drilling in DBR_BRAGFLO direct-release applications. In either case, 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 $C_{\max,i}^E$ is a generic maximum concentration (in moles/l) in brine of the i th element due to some generic physical process (dissolution or mobilization associated with colloids), then, at each timestep, PANEL will mobilize m_i^E 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 in the 1996 CCA). If sufficient amounts of the i th element are available in the inventory, m_i^E will take on its maximum value, namely

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

If $m_{\max,i}^E$ 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^E , into the brine, where m_i^E is whatever amount is available at that timestep. That is,

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

** Within the Culebra, their further transport is modeled by the SECO suite of WIPP codes.

*** 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.



The resulting concentration of the i th element in the brine (in moles/l) would be $C_i^e = I_i / V$. To summarize, if, at the end of the n th timestep, $I_i \geq (C_{\max,i}^e V)$, PANEL will have $(C_{\max,i}^e V)$ moles of the i th element in the brine. If $I_i < (C_{\max,i}^e V)$, 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 Sections 4.3, 4.4, and 4.5. The decay model is described in Section 4.6 and the actual release calculation is described in Section 4.7. The sequence of codes that is run in support of PANEL, including PANEL itself, is described in Section 4.8 and shown in Figure 1 (see Chapter 3).

4.3 Description of PANEL's Colloidal-Suspension Model

In CCA applications, mobilization associated with suspended colloids has been combined with mobilization due to dissolution. That approach is justified because dispersion and sorption are the only physical processes that could cause significant differences in the transport models used for dissolved versus colloidal species, and since dispersion and adsorption are not modeled by PANEL, the transport models that apply to the two species will be identical. The merging of the treatment of mobilization of dissolved and colloidal species is performed prior to PANEL in an ALGEBRA calculation known as "SOTERM" for "solubility term." In that application, four types of colloid-related mobilization are considered, as follows: (i) condensation of hydrolyzed actinide ions into intrinsic colloids, and sorption onto already existent colloidal materials of (ii) humic, (iii) microbial, and (iv) mineral origin. Maximum concentrations for the four different types of colloidal particulates are combined with the maximum concentration for dissolution for each of the radioisotopes. A maximum concentration associated with the five processes together is then used in a single dissolution-like computation that estimates the net mobilization due to colloid mobilization and dissolution. That calculation is described in the next section.

PANEL contains another different colloid-transport model that is based on the assumptions of (1) rapid sorption onto mobile colloids, (2) the same sorption concentrations for all radioisotopes, and (3) consideration of two sizes of colloidal particulates, namely small and large, with different sorption capacities for each. **However, that model is not included with PANEL for CCA applications and is therefore not included in PANEL's QAed software documentation.** For information and completeness, that model is described in Appendix G, at the end of this User's Manual. Note that several of the defunct data columns reported in PANEL's DBG file (Appendix F) relate to this model.

4.4 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 CCA calculations, colloid mobilization has been combined with dissolution by adding the maximum concentration from colloidal forms to the maximum concentrations due to 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., 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

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

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,

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

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.

4.5 Accounting for Valence State During Dissolution

PANEL includes a random sampling scheme that apportions the amount of each element present in a repository into its various possible oxidation states. **This option is not used in the CCA calculations, will not be available to CCA users, and is not intended to be part of PANEL's QAed software documentation.** However, a description of the oxidation-state sampling option is included in Appendix H of this User's Manual. It is included for completeness and information.

4.6 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 radioisotopes 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 radioisotope 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:

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

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

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



* 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.

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:

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

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

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

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 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.

4.7 PANEL's Release Calculation

Following WIPP PA performance scenarios (WIPP PA Dept., 1992), 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

** 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.



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 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 the SOTERM ALGEBRA run. Before forwarding its release data, PANEL first converts release units from moles back to kilograms. It does so by multiplying each release by $W_{i,j}/1000$, where $W_{i,j}$ is the molecular weight of the j th isotope of the i th element in grams/mole, and 1000 is the number of grams in a kilogram. In support of direct-release calculations, the cumulative kg release of each isotope from PANEL is converted by a post-PANEL ALGEBRA run to concentration data by forming the difference of the time integral of the calculated release divided by the difference of the time integral of the assumed outflow rate, these calculations being based on the minuscule assumed flow rate of roughly 10^{-5} cubic meters per year. ALGEBRA then converts the units to Normalized EPA release units per cubic meter and sums the isotopes in preparation for multiplication by DBR_BRAGFLO's direct-release volumetric-brine-output estimates, which are reported in cubic meters. The resultant product is, of course, in normalized EPA release units.

In general, BRAGFLO does not provide v_n . Rather, it provides the brine outflow rate $q(t_n)$ (in m^3/s), and quite often it reports q at timesteps t_n to t_{n+1} that may be a good deal smaller than PANEL's timesteps t_n to t_{n+1} . To rectify the mismatch, PANEL (i) converts BRAGFLO's brine outflow rates to l/s , and then (ii) computes v_n by integrating q over one of PANEL's timesteps. The computation is by right-hand integration, and looks like

$$v_n(t_n) = \sum_{m: t_m=t_n}^{t_m=t_{n+1}} [q(t_{m+1})] [t_{m+1} - t_m] .$$

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 dissolution and colloidal mobilization is $[v_n C_{i,j}(t_n)]$, where $C_{i,j}$ was defined earlier. 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:

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

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} m³/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.

4.8 PANEL's Run Sequence

To exercise PANEL as it was exercised in the 1996 CCA, 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 run in support of a groundwater release through the Culebra (SECOTP and CCDF_GF). The caption of Figure 1 explains the run-sequence differences required for DBR_BRAGFLO applications. Sample input files for the five support codes of the sequence are provided in Appendices A through E of this User's Manual. The codes themselves are discussed in other documents supporting WIPP CCA 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 data base. 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 (see Figure 1 in Chapter 3). 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 colloiddally 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.

LHS, for Latin Hypercube Sampling, is such a code and leads to the production of numerous CDB files, one for each of the collections of sampled input data called input vectors. The number of samples is normally determined by an optimization scheme that balances the need for statistical confidence (which favors larger samples) against resource costs (which favor smaller samples). The exact number of samples required for the 1996 CCA is fixed at 100. PANEL's calculations will therefore be executed in sets having 100 runs each, and many more if one includes replication runs. This multiplicity of runs is intended to assure (a) representative and (b) adequate sampling. Because of it, reasonable measures were applied to make PANEL as efficient as possible in terms of run time. In the 1996 CCA runs, PANEL did not receive its sampled data directly from LHS. Rather, as shown in Figure 1, LHS's sampled data were passed through an ALGEBRA step, which modifies some of the chemical data so as to generate enhanced equivalent solubility limits (see Chapter 4 herein, and Section 7 of the SOTERM Appendix of the WIPP's 1996 Compliance Certification Application).

As was said above, PANEL executes in three different ways, called run types, and performs three very different kinds of computations. Type-1 runs mobilize wastes (by dissolution and colloidal mobilization) 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 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 an "R" for "radiolysis".

- arg2 is any one of PANEL's sampled input CDB files. Typically, they are named* LHS_S1_S_Vyyy, where yyy is a variable index that identifies the realization. In CCA calculations, yyy would vary from 001 to 100. The file actually employed in 1996 CCA runs was named ALG_ST_CCA_Rz_Sx_Vyyy.CDB, where z (= 1, 2, or 3) is the replicate number and x (= 1,2, ..., 6) is the scenario number.
- arg3 is any one of PANEL's sampled 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.
- arg4 is the sampled input CDB file that specifies the repository brine volume and rate of brine outflow from the repository and must correspond to the scenario and realization 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 1996 CCA runs, BRAGFLO's output files were passed through a preliminary ALGEBRA step that simplified them so as to enhance run speed (see Figure 1).
- 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. All PANEL's input data derive from upstream codes and from the data distributions written on the controlled WIPP data base. 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. Examples of their input control files for PANEL runs are reproduced in APPENDICES A, B, C, and D. Appendix D applies to the source-term ALGEBRA run, which is quite different from the ALGEBRA run described in the following section.



6.2 Exercising ALGEBRA to Prepare PANEL's Input Flow Data CDB File

It is possible to streamline PANEL somewhat by exercising ALGEBRA in a mode that strips the arg4 BRAGFLO CDB file of unnecessary information and, thereby, decreases run time. The change in run time is small, but it accumulates during multiple runs. This step is a housekeeping chore and does not affect PANEL's operations or foundations in any way. However, as it is included in 1996 CCA regulatory calculations, it is described in this User's Manual. The entire input file required by this application of ALGEBRA is included in Appendix E.

* The filenames used in this section will work, however, they differ from the filenames employed by the CMS that controls CCA runs. CMS filenames appear in the examples in the appendices of this manual. Also, the letter R, which in past PAs signified "realization," has been replaced by V for "vector." R now signifies "replicate."

The Appendix-E ALGEBRA input file is actually more complex than is absolutely required by PANEL, which uses only two of the many POSTBRAG output variables the input file calls, namely: variable #30, BRNVOL_W, and variable #78, BNBHUDRZ. However, it is the ALGEBRA file that was used in the 1996 CCA calculations and it is therefore listed in Appendix E. Variable #30 is volume of brine in the repository during the present timestep. Variable #78 is the cumulative brine outflow up the borehole.

In the paragraph that follows, the command line that exercises the necessary ALGEBRA application is given.

If the file named BRAGFLO_FLOW_S6_V064.CDB is POSTBRAGFLO's output CDB, and if its ALGEBRA-revised version is named BRAGFLO_ALG_FLOW_S6_V064.CDB, then the command line to exercise ALGEBRA on BRAGFLO's output in preparation for exercising PANEL is as follows:

```
$ ALGEBRA -<CR>
_ $ BRAGFLO_FLOW_S6_V064.CDB -<CR>
_ $ BRAGFLO_ALG_FLOW_S6_V064.CDB -<CR>
_ $ POSTALG_CCA_186.INP -<CR>
_ $ CANCEL <CR>
```

where <CR> means strike the "carriage return", and where the debug file has been canceled. The third file in the sequence, POSTALG_CCA_186.INP, is the ALGEBRA input control file that was actually used in 1996 CCA runs. It resides on the WIPP Alphas in the file U1:[JDMILLE.CCA.POSTALG] and is listed in full in Appendix E.

6.3 Exercising PANEL in an Undisturbed Type-1 Run

To exercise PANEL in a standard brine-flux type-1 run, enter the following command-line format at the VMS "\$" prompt:

```
$ PANEL S ALG_ST_CCA_R1_S1_Vyyy.CDB PANEL_S1_S_Vyyy.CDB -
_ $ BRAGFLO_ALG_FLOW_S1_Vyyy.CDB PANEL_S1_S_Vyyy.DBG
```

This command will exercise PANEL in the standard (type-1) manner for events associated with scenario number 1, which is the identification number for the undisturbed state. The brine-flux input-data CDB file is recognized as BRAGFLO's output file for an "undisturbed" scenario number and unspecified realization number. The hyphen at the end of the command line is the digital-command-language symbol for "continued on the next line". In CCA runs, PANEL will not be applied to undisturbed runs.



6.4 Exercising PANEL in an E2E1 type-1 Run

In CCA 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 1996 CCA 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_CCA_R1_S6_Vyyy.CDB PANEL_S6_S_Vyyy.CDB -  
_ $ BRAGFLO_ALG_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.

6.5 Exercising PANEL in a Decay-Only 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.

6.6 Exercising PANEL in a Radiolysis Run

Type-3 radiolysis runs will not be exercised in the CCA 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 data base and are, therefore, not available for user interaction.

Variable name	Description	Database Name	
SECPY	The number of seconds in a year	GLOBAL	YRSEC
SOL(3,IELE)	Base-10 log of actinide's solubility in m/l	**	LOGSOLM
XLOAD(IDION)	The initial inventory of the WIPP	*****	INVCHD
		*****	INVRHD ,

where ** = AM, CM, NP, PU, TH, & U , and
 ***** = PU242, etc.

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 specified by a scrupulously controlled scientific procedure (WIPP PA Div., 1991; and WIPP PA Dept, Vol. 3, 1992). Parameter values that were used in a particular run are echoed in PANEL's DBG file for that run. A sample PANEL DBG file is included in Appendix F.



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.
- INBHFO, 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.

PANEL writes 92 history variables to the data base at each timestep. Those variables are listed below in tabular format and are defined in the paragraphs immediately below the list.

History Variables:

BRNVOL00	SMFLOW00	SD0SR90	SL0SR90	SS0SR90
SD0CS137	SL0CS137	SS0CS137	SD0PB210	SL0PB210
SS0PB210	SD0RA226	SL0RA226	SS0RA226	SD0RA228
SL0RA228	SS0RA228	SD0TH229	SL0TH229	SS0TH229
SD0TH230	SL0TH230	SS0TH230	SD0TH232	SL0TH232
SS0TH232	SD0PA231	SL0PA231	SS0PA231	SD0U233
SL0U233	SS0U233	SD0U234	SL0U234	SS0U23
SD0U235	SL0U235	SS0U235	SD0U236	SL0U236
SS0U236	SD0U238	SL0U238	SS0U238	SD0NP237
SL0NP237	SS0NP237	SD0PU238	SL0PU238	SS0PU238
SD0PU239	SL0PU239	SS0PU239	SD0PU240	SL0PU240
SS0PU240	SD0PU241	SL0PU241	SS0PU241	SD0PU242
SL0PU242	SS0PU242	SD0PU244	SL0PU244	SS0PU244
SD0AM241	SL0AM241	SS0AM241	SD0CM244	SL0CM244
SS0CM244	SD0CM248	SL0CM248	SS0CM248	SD0CF252
SL0CF252	SS0CF252	SD0PM147	SL0PM147	SS0PM147
SD0SM147	SL0SM147	SS0SM147	SD0AM243	SL0AM243
SS0AM243	SD0CM243	SL0CM243	SS0CM243	SD0CM245
SL0CM245	SS0CM245			

In the above listing, the 00 in the BRNVOL00 and the SMFLOW00 variables, and the 0 used as the third character in all the other history variables are indices intended to identify the waste panel that was assumed to be breached. Since 1991, all PA calculations have been full-repository runs. That is, the entire contents of the repository were assumed to be wetted by the inflowing brine, which, in previous PANEL runs, meant using the panel index numbers 0, and 00. In CCA runs, the panel index numbers will continue to be set at 0 and 00, however, in CCA runs, 0 will mean any *one* of the standard-sized waste panels (area = 11,640 m², or roughly one-tenth of the repository's total volume).

BRNVOL00 is the Brine Volume in the repository for the present run in cubic meters.

SMFLOW00 in the time-integrated rate of outflow of brine from the repository up the intrusion borehole in cubic meters.

For type-1 runs:

SD0***** is the time-integrated mass in kilograms of isotope ***** discharged in solution from the panel.

SLO***** is the time-integrated mass in kilograms of isotope ***** discharged on large colloids⁺.

SS0***** is the time-integrated mass in kilograms of isotope ***** discharged on small colloids⁺.

For type-2 runs:

SD0***** is the current inventory of isotope ***** in Curies.

Type-3 runs are not included in the CCA PA and therefore are not discussed herein.

9.1 Tips for Using type-1 Outputs

PANEL routinely outputs release data for 21 radioisotopes. However, the transport codes that read these data as input data may accommodate an even smaller number of radioisotopes. If the transport code that follows PANEL is not transporting a certain radioisotope, say R, it is *not* sufficient simply to delete PANEL's R releases from the computation. That is because the transport code may be considering R's daughter, D, or R's granddaughter, GD. If so, the mass flux and the integrated mass of R should be accounted for and added to PANEL's calculated mass fluxes and integrated masses of D and/or GD. That can be accomplished exactly if the downstream code has complete Bateman-decay capability (in which case, R would act as a source term in D's or GD's transport equation). If it does not, the effect can be approximated as outlined below.

For example, suppose the transport code is not considering radioisotope PU242, but is considering U238. To account for the U238 produced by decomposition of PU242, one might add SD0PU242 to SD0U238, add SLOPU242 to SLOU238, and add SS0PU242 to SS0U238. This correction is crude but conservative.

Alternatively, one might add the integrated release of R in kilograms to the release of D or GD (also in kilograms) in such a way that the total amount of radioactivity (in Curies) is maintained. For example: one might add SD0PU242*HLPU239/HLPU242 to SD0PU239, where HL***** represents the half-life of a radioisotope named *****. The same correction would be applied to the releases associated with PANEL's colloidal mobilization module when it is enabled (it was disabled in the 1996 CCA).

⁺ In the 1996 CCA, SLO and SS0 are both zero because colloidal mobilization was combined with mobilization due to dissolution (see Chapter 4). That is, PANEL's internal colloidal-mobilization code was disabled.

10.0 REFERENCES

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APPENDIX A: EXAMPLE OF A GENMESH INPUT FILE FOR A PANEL RUN.

GENMESH INPUT FILE

```
=====
! FILETYPE: GENMESH input text file
! TITLE: Simple GENMESH to set up Source Term CDB
! ANALYSTS: Christine Stockman
! DATE: May 31, 1996
=====
!
!
*SETUP
  DIM=      3
  ORIGIN= 0.0, 0.0, 0.0
  IJKMAX= 2, 2, 2
*GRID
! ===== X direction =====
  DEL, COORD=X, DEL= 1.00, INRANGE= 1, 2, FACTOR= 1.0
! ===== Y direction =====
  DEL, COORD=Y, DEL= 1.00, INRANGE= 1, 2, FACTOR= 1.0
! ===== Z direction =====
  DEL, COORD=Z, DEL= 1.00, INRANGE= 1, 2, FACTOR= 1.0
!
*REGIONS
  REGION= 1, IRANGE= 1,2, JRANGE= 1,2 KRANGE= 1, 2
! =====
*END
```



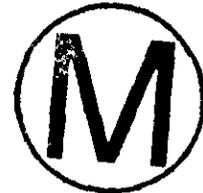
END OF APPENDIX A



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

MATSET INPUT FILE

```
!=====
! TITLE:      SOURCE TERM 1996: The WIPP PA CCA Calculation
! ANALYSTS:   C. T. STOCKMAN, J. W. GARNER
! CREATED:    MAY 31, 1996
! MODIFIED:
! PURPOSE:    PREPARE SOURCE TERM CDB FOR NUTS, 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, 67
!
! *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:AM241, 60=PU238L:PU238, 61=PU239L:PU239, &
!                62=TH230L:TH230, 63=U234L:U234, &
!                64=AML, 65=PUL, 66=THL, 67=UL
! MATERIALS 61-69 ARE LUMPED PARAMETERS FOR NUTS
!
! PROPERTY, MATERIAL=Global, NAMES =OXSTAT
! PROPERTY, MATERIAL=REFCON, NAMES =YRSEC
! ISOTOPES
! PROPERTY MATERIAL=Am241, NAMES =InvCHD, InvRHD, ATWEIGHT, HALFLIFE
! PROPERTY MATERIAL=Am243, NAMES =InvCHD, InvRHD, ATWEIGHT, HALFLIFE
! PROPERTY MATERIAL=Cf252, NAMES =InvCHD, InvRHD, ATWEIGHT, HALFLIFE
! PROPERTY MATERIAL=Cm243, NAMES =InvCHD, InvRHD, ATWEIGHT, HALFLIFE
! PROPERTY MATERIAL=Cm244, NAMES =InvCHD, InvRHD, ATWEIGHT, HALFLIFE
! PROPERTY MATERIAL=Cm245, NAMES =InvCHD, InvRHD, ATWEIGHT, HALFLIFE
! PROPERTY MATERIAL=Cm248, NAMES =InvCHD, InvRHD, ATWEIGHT, HALFLIFE
! PROPERTY MATERIAL=Cs137, NAMES =InvCHD, InvRHD, ATWEIGHT, HALFLIFE
! PROPERTY MATERIAL=Np237, NAMES =InvCHD, InvRHD, ATWEIGHT, HALFLIFE
! PROPERTY MATERIAL=Pa231, NAMES =InvCHD, InvRHD, ATWEIGHT, HALFLIFE
```



PROPERTY	MATERIAL=Pb210,	NAMES =InvCHD, InvRHD, ATWEIGHT, HALFLIFE
PROPERTY	MATERIAL=Pm147,	NAMES =InvCHD, InvRHD, ATWEIGHT, HALFLIFE
PROPERTY	MATERIAL=Pu238,	NAMES =InvCHD, InvRHD, ATWEIGHT, HALFLIFE
PROPERTY	MATERIAL=Pu239,	NAMES =InvCHD, InvRHD, ATWEIGHT, HALFLIFE
PROPERTY	MATERIAL=Pu240,	NAMES =InvCHD, InvRHD, ATWEIGHT, HALFLIFE
PROPERTY	MATERIAL=Pu241,	NAMES =InvCHD, InvRHD, ATWEIGHT, HALFLIFE
PROPERTY	MATERIAL=Pu242,	NAMES =InvCHD, InvRHD, ATWEIGHT, HALFLIFE
PROPERTY	MATERIAL=Pu244,	NAMES =InvCHD, InvRHD, ATWEIGHT, HALFLIFE
PROPERTY	MATERIAL=Ra226,	NAMES =InvCHD, InvRHD, ATWEIGHT, HALFLIFE
PROPERTY	MATERIAL=Ra228,	NAMES =InvCHD, InvRHD, ATWEIGHT, HALFLIFE
PROPERTY	MATERIAL=Sr90,	NAMES =InvCHD, InvRHD, ATWEIGHT, HALFLIFE
PROPERTY	MATERIAL=Th229,	NAMES =InvCHD, InvRHD, ATWEIGHT, HALFLIFE
PROPERTY	MATERIAL=Th230,	NAMES =InvCHD, InvRHD, ATWEIGHT, HALFLIFE
PROPERTY	MATERIAL=Th232,	NAMES =InvCHD, InvRHD, ATWEIGHT, HALFLIFE
PROPERTY	MATERIAL=U233,	NAMES =InvCHD, InvRHD, ATWEIGHT, HALFLIFE
PROPERTY	MATERIAL=U234,	NAMES =InvCHD, InvRHD, ATWEIGHT, HALFLIFE
PROPERTY	MATERIAL=U235,	NAMES =InvCHD, InvRHD, ATWEIGHT, HALFLIFE
PROPERTY	MATERIAL=U236,	NAMES =InvCHD, InvRHD, ATWEIGHT, HALFLIFE
PROPERTY	MATERIAL=U238,	NAMES =InvCHD, InvRHD, ATWEIGHT, HALFLIFE



PROPERTY	MATERIAL=AM241L,	NAMES =InvCHD, InvRHD, ATWEIGHT, HALFLIFE
PROPERTY	MATERIAL=PU238L,	NAMES =InvCHD, InvRHD, ATWEIGHT, HALFLIFE
PROPERTY	MATERIAL=PU239L,	NAMES =InvCHD, InvRHD, ATWEIGHT, HALFLIFE
PROPERTY	MATERIAL=TH230L,	NAMES =InvCHD, InvRHD, ATWEIGHT, HALFLIFE
PROPERTY	MATERIAL=U234L,	NAMES =InvCHD, InvRHD, ATWEIGHT, HALFLIFE

! ELEMENTS

PROPERTY	MATERIAL=AM,	NAMES =CONCMIN, CONCINT, CAPHUM, CAPMIC, PROPMIC
PROPERTY	MATERIAL=CF,	NAMES =LOGSOLM
PROPERTY	MATERIAL=CM,	NAMES =LOGSOLM
PROPERTY	MATERIAL=SR,	NAMES =LOGSOLM
PROPERTY	MATERIAL=CS,	NAMES =LOGSOLM
PROPERTY	MATERIAL=NP,	NAMES =CONCMIN, CONCINT, CAPHUM, CAPMIC, PROPMIC
PROPERTY	MATERIAL=PA,	NAMES =LOGSOLM
PROPERTY	MATERIAL=PB,	NAMES =LOGSOLM
PROPERTY	MATERIAL=PM,	NAMES =LOGSOLM
PROPERTY	MATERIAL=PU,	NAMES =CONCMIN, CONCINT, CAPHUM, CAPMIC, PROPMIC
PROPERTY	MATERIAL=RA,	NAMES =LOGSOLM
PROPERTY	MATERIAL=TH,	NAMES =CONCMIN, CONCINT, CAPHUM, CAPMIC, PROPMIC
PROPERTY	MATERIAL=U,	NAMES =CONCMIN, CONCINT, CAPHUM, CAPMIC, PROPMIC

PROPERTY	MATERIAL=PUL,	NAMES =LOGSOLM
PROPERTY	MATERIAL=AML,	NAMES =LOGSOLM
PROPERTY	MATERIAL=UL,	NAMES =LOGSOLM
PROPERTY	MATERIAL=THL,	NAMES =LOGSOLM

! OXIDATION STATES

PROPERTY	MATERIAL=SOLMOD3,	NAMES =SOLSIM, SOLCIM, SOLSOM, SOLCOM
PROPERTY	MATERIAL=SOLMOD4,	NAMES =SOLSIM, SOLCIM, SOLSOM, SOLCOM
PROPERTY	MATERIAL=SOLMOD5,	NAMES =SOLSIM, SOLCIM, SOLSOM, SOLCOM
PROPERTY	MATERIAL=SOLMOD6,	NAMES =SOLSIM, SOLCIM, SOLSOM, SOLCOM
PROPERTY	MATERIAL=PHUMOX3,	NAMES =PHUMSIM, PHUMCIM
PROPERTY	MATERIAL=PHUMOX4,	NAMES =PHUMSIM, PHUMCIM
PROPERTY	MATERIAL=PHUMOX5,	NAMES =PHUMSIM, PHUMCIM
PROPERTY	MATERIAL=PHUMOX6,	NAMES =PHUMSIM, PHUMCIM

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

```
!=====
*SET*VALUES
!LOGSOLM=0 ARE NEEDED AS PLACE HOLDERS FOR ELEMENTS THAT WILL HAVE THEIR
!SOLUBILITIES CONSTRUCTED
PROPERTY MATERIAL=CF, NAMES*VALUE: LOGSOLM=0.
PROPERTY MATERIAL=CM, NAMES*VALUE: LOGSOLM=0.
PROPERTY MATERIAL=PA, NAMES*VALUE: LOGSOLM=0.
PROPERTY MATERIAL=PM, NAMES*VALUE: LOGSOLM=0.
!
PROPERTY MATERIAL=AML, NAMES*VALUE: LOGSOLM=0.
PROPERTY MATERIAL=THL, NAMES*VALUE: LOGSOLM=0.
PROPERTY MATERIAL=PUL, NAMES*VALUE: LOGSOLM=0.
PROPERTY MATERIAL=UL, NAMES*VALUE: LOGSOLM=0.
!
*END
!-----
```



END OF APPENDIX B

APPENDIX C: EXAMPLE OF A POSTLHS INPUT FILE FOR A PANEL RUN

POSTLHS INPUT FILE

! TITLE: POSTLHS input file == POSTLHS_S00.INP
! ANALYST: J.W.GARNER - 5/29/92

! DESCRIPTION: NAS FALL,1992 SCENARIO

*END

END OF APPENDIX C

APPENDIX D: EXAMPLE OF ALGEBRA'S POST-POSTLHS SOURCE-TERM INPUT FILE

A detailed explanation of the chemical basis for this input file may be found in Section 7 of the SOTERM Appendix of the WIPP's 1996 Compliance Certification Application.

SOURCE TERM ALGEBRA INPUT FILE

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



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



```
TOTSOL = MAKEPROP (IFLT0 (CAPMIC [B:44] -TOT, MIN (TOTNM+CAPMIC [B:44], TOT), TOT))
MIC= MAKEPROP (IFLT0 (CAPMIC [B:44] -TOT, TOTSOL-TOTNM, MIC1))
LOGSOLM=MAKEPROP (LOG10 (TOTSOL))
FRCDIS=MAKEPROP (DIS/TOTSOL)
FRCHUM=MAKEPROP (HUM/TOTSOL)
FRCMIC=MAKEPROP (MIC/TOTSOL)
FRCINT=MAKEPROP (CONCINT [B:44] /TOTSOL)
FRCMIN=MAKEPROP (CONCMIN [B:44] /TOTSOL)
!NOW CHECK OX
LIMIT BLOCK 44
LOGSOLM=MAKEPROP (IFGT0 (OX, LOGSOLM [B:58], LOGSOLM [B:57]))
FRCDIS =MAKEPROP (IFGT0 (OX, FRCDIS [B:58], FRCDIS [B:57]))
FRCHUM =MAKEPROP (IFGT0 (OX, FRCHUM [B:58], FRCHUM [B:57]))
FRCINT =MAKEPROP (IFGT0 (OX, FRCINT [B:58], FRCINT [B:57]))
FRCMIN =MAKEPROP (IFGT0 (OX, FRCMIN [B:58], FRCMIN [B:57]))
FRCMIC =MAKEPROP (IFGT0 (OX, FRCMIC [B:58], FRCMIC [B:57]))
!
!NP
!PUT LOGSOLM ETC INTO SOLNP UNTIL CHECK OXIDATION STATE, THEN PUT INTO NP
!NP=36, SOLMOD4=46, PHUMOX4=50, SOLMOD5=47, PHIMOX5=51
LIMIT BLOCKS 36
DISNP4=MAKEPROP (SOLSIM [B:46])
HUMNP4=MAKEPROP (MIN (CAPHUM [B:36], SOLSIM [B:46] *PHUMSIM [B:50]))
MNP4=MAKEPROP (SOLSIM [B:46] *PROPMIC [B:36])
TNMNP4=MAKEPROP (DISNP4+HUMNP4+CONCINT [B:36]+CONCMIN [B:36])
TOT4=MAKEPROP (TNMNP4+MNP4)
TOTNP4 = MAKEPROP (IFLT0 (CAPMIC -TOT4, MIN (TNMNP4+CAPMIC, TOT4), TOT4))
MICNP4=MAKEPROP (IFLT0 (CAPMIC -TOT4, TOTNP4 -TNMNP4, MNP4))
!
DISNP5=MAKEPROP (SOLSIM [B:47])
HUMNP5=MAKEPROP (MIN (CAPHUM [B:36], SOLSIM [B:47] *PHUMSIM [B:51]))
MNP5=MAKEPROP (SOLSIM [B:47] *PROPMIC [B:36])
TNMNP5=MAKEPROP (DISNP5+HUMNP5+CONCINT [B:36]+CONCMIN [B:36])
TOT5=MAKEPROP (TNMNP5+MNP5)
TOTNP5 = MAKEPROP (IFLT0 (CAPMIC -TOT5, MIN (TNMNP5+CAPMIC, TOT5), TOT5))
MICNP5=MAKEPROP (IFLT0 (CAPMIC -TOT5, TOTNP5 -TNMNP5, MNP5))
LOGSOLM=MAKEPROP (IFGT0 (OX, LOG10 (TOTNP5), LOG10 (TOTNP4)))
FRCDIS =MAKEPROP (IFGT0 (OX, DISNP5/TOTNP5, DISNP4/TOTNP4))
FRCHUM =MAKEPROP (IFGT0 (OX, HUMNP5/TOTNP5, HUMNP4/TOTNP4))
FRCMIC =MAKEPROP (IFGT0 (OX, MICNP5/TOTNP5, MICNP4/TOTNP4))
FRCINT =MAKEPROP (IFGT0 (OX, CONCINT [B:36] /TOTNP5, CONCINT [B:36] /TOTNP4))
FRCMIN =MAKEPROP (IFGT0 (OX, CONCMIN [B:36] /TOTNP5, CONCMIN [B:36] /TOTNP4))
!
!PA
!PA=37, NP=36
LIMIT BLOCKS 37
LOGSOLM=MAKEPROP (LOGSOLM [B:36])
!
!CF, CM, PM SET TO AM=32
LIMIT BLOCKS 33, 34, 39
LOGSOLM=MAKEPROP (LOGSOLM [B:32])
!
!NOW TO LUMP FOR NUTS
!NOW INVENTORY ARE FOR SINGLE SPEICES, NEED TO ADD IN TH229, U233,
!Pu241, Pu240, Pu242
!
!use most conservative method: if added species is shorter-lived, add curies
!if added species is longer-lived, add curies scaled by halflives (add grams)
!
!U234L=63, U234=28, U233=27
```



```
LIMIT BLOCK 63
INVCHD=MAKEPROP (INVCHD[B:28]+INVCHD[B:27])
INVRHD=MAKEPROP (INVRHD[B:28]+INVRHD[B:27])
!
!TH230L=62, TH229=24, TH230=25
LIMIT BLOCK 62
INVCHD=MAKEPROP (INVCHD[B:25]+INVCHD[B:24])
INVRHD=MAKEPROP (INVRHD[B:25]+INVRHD[B:24])
!
!AM241L=59, AM241=3, PU241=18
!DECAY ALL PU241 TO AM241 AND ADD THIS IN TO AM241
!SO CONVERT CI PU241 TO KG PU241, CONVERT TO KG AM241, CONVERT BACK TO CI
AM241
!THIS IS DONE USING RATIO OF HALFLIFES
LIMIT BLOCK 59
INVCHD=MAKEPROP (INVCHD[B:3]+INVCHD[B:18]*HALFLIFE[B:18]/HALFLIFE[B:3])
INVRHD=MAKEPROP (INVRHD[B:3]+INVRHD[B:18]*HALFLIFE[B:18]/HALFLIFE[B:3])
!
!PU239L=61, PU239=16, PU240=17, PU242=19
LIMIT BLOCK 61
LIFERATO = HALFLIFE[B:19]/HALFLIFE[B:16]
INVCHD=MAKEPROP (INVCHD[B:16]+INVCHD[B:17]+INVCHD[B:19]*LIFERATO)
INVRHD=MAKEPROP (INVRHD[B:16]+INVRHD[B:17]+INVCHD[B:19]*LIFERATO)
!
!REDUCE SOLUBILITIES BY RATIO'S WITH OTHER ISOTOPES
!AML=64, PUL=65, THL=66, UL=67: AM=32, PU=40, TH=43, U=44
LIMIT BLOCK 64
LOGSOLM=MAKEPROP (LOGSOLM[B:32])
FRCDIS=MAKEPROP (FRCDIS[B:32])
FRCHUM=MAKEPROP (FRCHUM[B:32])
FRCMIC=MAKEPROP (FRCMIC[B:32])
FRCINT=MAKEPROP (FRCINT[B:32])
FRCMIC=MAKEPROP (FRCMIC[B:32])
LIMIT BLOCK 65
LOGSOLM=MAKEPROP (LOGSOLM[B:40])
FRCDIS=MAKEPROP (FRCDIS[B:40])
FRCHUM=MAKEPROP (FRCHUM[B:40])
FRCMIC=MAKEPROP (FRCMIC[B:40])
FRCINT=MAKEPROP (FRCINT[B:40])
FRCMIC=MAKEPROP (FRCMIC[B:40])
LIMIT BLOCK 66
LOGSOLM=MAKEPROP (LOGSOLM[B:43]-3)
FRCDIS=MAKEPROP (FRCDIS[B:43])
FRCHUM=MAKEPROP (FRCHUM[B:43])
FRCMIC=MAKEPROP (FRCMIC[B:43])
FRCINT=MAKEPROP (FRCINT[B:43])
FRCMIC=MAKEPROP (FRCMIC[B:43])
LIMIT BLOCK 67
LOGSOLM=MAKEPROP (LOGSOLM[B:44]-2)
FRCDIS=MAKEPROP (FRCDIS[B:44])
FRCHUM=MAKEPROP (FRCHUM[B:44])
FRCMIC=MAKEPROP (FRCMIC[B:44])
FRCINT=MAKEPROP (FRCINT[B:44])
FRCMIC=MAKEPROP (FRCMIC[B:44])
!
END
```

END OF APPENDIX D

APPENDIX E: EXAMPLE OF ALGEBRA'S POST-POSTBRAGFLO INPUT FILES: USED TO PREPARE BRINE INPUT DATA FOR PANEL.

This file is more complex than is required for PANEL's needs. PANEL reads only variables #30 and # 78, which are explained on the file.

```
!=====
!
! ALGEBRA file for calculating BRAGFLO sensitivity analysis parameters
!
! Based on file: POSTALG_CCA_180.INP (Parameters 1-180) plus 6 additional
!
! 07 June 1996 - 186 variables
!
! Authors: Joel D. Miller, SNL Org. 9363
!          David A. Mc Arthur, Org. 9363
!
!=====
! Eliminate excess output
!
DELETE ALL
!
! Calculate general parameters
!
GRIDVOL = DEL_X * DEL_Y * THICK
!
!*****
!*****
!
! Remaining inventories of steel and cellulose (kg)
!
! Param 001: Remaining mass of steel -----> FE_KG
! Param 002: Remaining mass of cellulose -----> CELL_KG
!
! Remaining inventories of steel and cellulose (%/100)
!
! Param 003: Remaining fraction of steel -----> FE_REM
! Param 004: Remaining fraction of cellulose --> CELL_REM
!
! Cumulative gas generation in waste disposal regions (moles)
!
! Param 005: by corrosion -----> FE_MOLE
! Param 006: by humid microbial -----> CELL_M_H
! Param 007: by inundated microbial --> CELL_M_I
! Param 008: by total microbial -----> CELL_MOL, C_M_HI_T
! Param 010: Total gas generation -----> GAS_MOLE
!
! Cumulative gas generation in waste disposal regions (moles/drum)
!
! Param 011: by corrosion -----> FE_MOL_D
! Param 012: by humid microbial -----> CEL_MH_D
! Param 013: by inundated microbial --> CEL_MI_D
! Param 014: by total microbial -----> CELMOL_D, C_MHIT_D
! Param 016: Total gas generation -----> GASMOL_D
!
! Cumulative gas generation in waste disposal regions (m**3)
!
! Param 017: by corrosion -----> GAS_FE_V
! Param 018: by humid microbial -----> GAS_CMH
```



```
! Param 019: by inundated microbial --> GAS_CMI
! Param 020: by total microbial -----> GAS_C_V, C_MHIT_V
! Param 022: Total gas generation ----> GAS_VOL
!
!*****
!
! Limit calculation to areas with waste (WAS_AREA + REPOSIT)
!
LIMIT ELEMENT 596 TO 625
!
! Define molecular weights of iron, cellulosics, water and brine (kg/mol)
!
MW_FE      = 0.055847
MW_CELL    = 0.03002628
MW_H2O     = 0.01801534
MW_BRINE   = 0.022653859
!
! Calculate mass inventories (kg) remaining
!
FE_KG      = SUM(GRIDVOL*FECONC)
CELL_KG    = SUM(GRIDVOL*CELLCONC)
!
! Maximum Fe and bio is at time = 0.0
!
MXFE       = ENVMAX(FE_KG)
MXCELL     = ENVMAX(CELL_KG)
!
! Calculate masses consumed and divide by initial amount to get fractions gone
! Subtract fraction gone from one to get fractions remaining
!
FE_REM     = 1.0 - ((MXFE - FE_KG)/MXFE)
CELL_REM   = 1.0 - ((MXCELL - CELL_KG)/MXCELL)
!
! Calculate total moles of gas (H2) generated from corrosion of Fe
!
FE_MOLE    = (MXFE - FE_KG)/MW_FE*(4.0-STOICOR[B:12])/3.0
!
! Calculate total moles of gas (H2) generated from biodegradation of cellulosics
!
CELL_MOL   = (MXCELL - CELL_KG)/MW_CELL*STOIMIC[B:12]
!
! Total moles of gas generated
!
GAS_MOLE   = FE_MOLE + CELL_MOL
!
! Determine humid and inundated biodegradation components
!
! Inundated rate GRATI (moles/s)
!
SATBR      = 1.0 - SATGAS
SATFAC     = 1.0 - EXP(-1000*SATBR)
LSAT       = SATBR + SAT_WICK[B:12]*(SATFAC)
LSAT       = IFGTO(LSAT-1,1,LSAT)
GRATI      = KBGSI[B:12]*(LSAT)*STOIMIC[B:12]*GRIDVOL
!
! Humid rate GRATH (moles/s)
!
GSAT       = SATGAS - SAT_WICK[B:12]*SATFAC
GSAT       = IFLT0(GSAT,0.0,GSAT)
GRATH      = KBGSH[B:12]*(GSAT)*STOIMIC[B:12]*GRIDVOL
!
! Determine the time interval DT by integrating a non-zero function
!
! This is necessary because the input .cdb file has history variables and
! associated history time steps, which prevents using DT = TIME-TIME[T:-1]
!
```



```
! VAL(I) = (VAL(I-1) + D(VAL)/DT)*DT where VAL is the integral of DENGAS
! DENGAS is the gas density and is always greater than zero
!
DENGASC = INTRIGHT(DENGAS)
DT      = (DENGASC - DENGASC[T:-1])/DENGAS
!
! Calculate kg/m**3 of cellulose consumed as if rate is valid for entire
! time interval (DT)
!
KGC1    = KBGSI[B:12]*LSAT*MW_CELL*DT
KGCH    = KBGSH[B:12]*GSAT*MW_CELL*DT
KGTOT   = KGC1 + KGCH
!
! Adjust GRATI and GRATH for step when CELLCONC goes to zero
! Note: KGTOT may be equal to zero if KBGSI and KBGSH are both zero
! so to avoid dividing by zero set DENOM equal to 1, which is
! acceptable since the coding below will use the true branch
! for calculating GRATI and GRATIH
!
DENOM    = IFEQ0(KGTOT,1,KGTOT)
SLOPE    = CELLCONC[T:-1]/DENOM
GRATI    = IFGT0(CELLCONC,GRATI,GRATI*SLOPE)
GRATH    = IFGT0(CELLCONC,GRATH,GRATH*SLOPE)
!
! Sum up humid and inundated over panel elements, add together for total
!
GRATHT   = SUM(GRATH)
GRATIT   = SUM(GRATI)
GRATIH   = GRATIT + GRATHT
!
! Integrate humid, inundated, and total (note C_M_HI_T should equal CELL_MOL)
!
CELL_M_H = INTRIGHT(GRATHT)
CELL_M_I = INTRIGHT(GRATIT)
C_M_HI_T = INTRIGHT(GRATIH)
!
! Clean up output--limit to requested quantities, delete temporary variables
! that are not used in another calculation later
!
DELETE MW_FE, MW_CELL, MW_H2O, MW_BRINE, MXFE, MXCELL
DELETE GRATHT, GRATIT, GRATIH, GRATI, GRATH, SATBR, DT, SATFAC
DELETE LSAT, GSAT, DENGASC, KGC1, KGCH, KGTOT, DENOM, SLOPE
!
!*****
!
! Convert to units of moles per drum by dividing by total number of drums
!
FE_MOL_D = FE_MOLE / DRUMTOT[B:12]
CEL_MH_D = CELL_M_H / DRUMTOT[B:12]
CEL_MI_D = CELL_M_I / DRUMTOT[B:12]
CELMOL_D = CELL_MOL / DRUMTOT[B:12]
C_MHIT_D = C_M_HI_T / DRUMTOT[B:12]
GASMOL_D = GAS_MOLE / DRUMTOT[B:12]
!
!*****
!
! Convert to volumetric units (m**3) using PV=nRT at reference P & T
!
! T = 300.15 K
! P = 101325.00 Pa = 101325 N/(m**2)
! R = 8.3145 J/(mol*K) = 8.3145 (N*m)/(mol*K)
! V = n*(R*T/P) m**3 = n moles * 0.024630 (m**3)/mole
!
GAS_FE_V = 0.02463 * FE_MOLE
GAS_CMH = 0.02463 **CELL_M_H
GAS_CMI = 0.02463 * CELL_M_I
```



```
GAS_C_V = 0.02463 * CELL_MOL
C_MHIT_V = 0.02463 * C_M_HI_T
GAS_VOL = 0.02463 * GAS_MOLE
!
!*****
!
!*****
!*****
!
! Volume-averaged pressure (Pa)
!
! Param 023: for region 23 (waste panel,      block 12) --> WAS_PRES
! Param 024: for region 24 (rest of repository, block 13) --> REP_PRES
! Param 025: for region 26 (operation region,  block 21) --> OPS_PRES
! Param 026: for region 27 (experimental region, block 22) --> EXP_PRES
! Param 027: for regions 23+24 -----> W_R_PRES
! Param 028: for region 30 (brine pocket,     block 11) --> B_P_PRES
!
!*****
!
! WAS_AREA
!
LIMIT ELEMENT 596 TO 616
!
! Total volume of waste area
!
R12VOL = SUM(GRIDVOL)
!
! Add up brine pressures weighted by element volume
!
R12PRES = SUM(GRIDVOL*PRESBRIN)
!
! Determine average pressure in waste area
!
WAS_PRES = R12PRES/R12VOL
!
!*****
!
! REPOSIT
!
LIMIT ELEMENT 617 TO 625
R13VOL = SUM(GRIDVOL)
R13PRES = SUM(GRIDVOL*PRESBRIN)
REP_PRES = R13PRES/R13VOL
!
!*****
!
! OPS_AREA
!
LIMIT ELEMENT 626 TO 631
R21VOL = SUM(GRIDVOL)
R21PRES = SUM(GRIDVOL*PRESBRIN)
OPS_PRES = R21PRES/R21VOL
!
!*****
!
! EXP_AREA
!
LIMIT ELEMENT 632 TO 637
R22VOL = SUM(GRIDVOL)
R22PRES = SUM(GRIDVOL*PRESBRIN)
EXP_PRES = R22PRES/R22VOL
!
!*****
!
! Average brine pressure in waste area and rest of repository
```



```
!  
W_R_PRES = (R12PRES + R13PRES)/(R12VOL + R13VOL)  
!  
!*****  
!  
! Brine pocket  
!  
LIMIT ELEMENT 1007 TO 1023  
R30VOL = SUM(GRIDVOL)  
R30PRES = SUM(GRIDVOL*PRESBRIN)  
B_P_PRES = R30PRES/R30VOL  
!  
!*****  
!  
! Clean up output--limit to requested quantities (regional volumes used below)  
!  
DELETE R12PRES, R13PRES, R21PRES, R22PRES, R30PRES  
!  
!*****  
!*****  
!  
! Param 029: Total pore volume in repository (m**3) --> PORVOL_T  
!  
!*****  
!  
! WAS_AREA + REPOSIT -  
!  
LIMIT ELEMENT 596 TO 625  
!  
! Pore volume = porosity (m**3 void/m**3 rock) * volume  
!  
PORVOL_T = SUM(POROS*GRIDVOL)  
!  
!*****  
!*****  
!  
! Brine volume in repository (m**3)  
!  
! Param 030: for region 23 (waste panel, block 12) --> BRNVOL_W  
! Param 031: for region 24 (rest of repository, block 13) --> BRNVOL_R  
! Param 032: for regions 23+24 -----> BRNVOL_T  
! Param 033: for region 26 (operations, block 21) --> BRNVOL_O  
! Param 034: for region 27 (experimental region, block 22) --> BRNVOL_E  
! Param 035: for regions 23+24+26+27 -----> BRNVOL_A  
!  
!*****  
!  
! WAS_AREA  
!  
LIMIT ELEMENT 596 TO 616  
!  
! Brine volume = porosity * volume * brine saturation  
! Brine saturation = 1.0 - SATGAS  
!  
BRNVOL_W = SUM(POROS*GRIDVOL*(1.0-SATGAS))  
!  
!*****  
!  
! REPOSIT  
!  
LIMIT ELEMENT 617 TO 625  
!  
BRNVOL_R = SUM(POROS*GRIDVOL*(1.0-SATGAS))  
!  
!*****  
!  
!
```



```
! WAS_AREA + REPOSIT
!
BRNVOL_T = BRNVOL_W + BRNVOL_R
!
!*****
!
! OPS_AREA
!
LIMIT ELEMENT 626 TO 631
!
BRNVOL_O = SUM(POROS*GRIDVOL*(1.0-SATGAS))
!
!*****
!
! EXP_AREA
!
LIMIT ELEMENT 632 TO 637
!
BRNVOL_E = SUM(POROS*GRIDVOL*(1.0-SATGAS))
!
!*****
!
! All repository regions
!
BRNVOL_A = BRNVOL_T + BRNVOL_O + BRNVOL_E
!
!*****
!*****
!
! Volume-averaged gas saturation (dimensionless)
!
!   Param 036: for region 23 (waste panel,      block 12) --> WAS_SATG
!   Param 037: for region 24 (rest of repository, block 13) --> REP_SATG
!   Param 038: for region 26 (operation region,  block 21) --> OPS_SATG
!   Param 039: for region 27 (experimental region, block 22) --> EXP_SATG
!   Param 040: for regions 23+24 -----> W_R_SATG
!   Param 041: for region 30 (brine pocket,     block 11) --> B_P_SATG
!
!*****
!
! WAS_AREA
!
LIMIT ELEMENT 596 TO 616
!
! Add up gas saturation weighted by element volume
!
R12SATG = SUM(GRIDVOL*SATGAS)
!
! Determine average gas saturation in waste area
!
WAS_SATG = R12SATG/R12VOL
!
!*****
!
! REPOSIT
!
LIMIT ELEMENT 617 TO 625
R13SATG = SUM(GRIDVOL*SATGAS)
REP_SATG = R13SATG/R13VOL
!
!*****
!
! OPS_AREA
!
LIMIT ELEMENT 626 TO 631
R21SATG = SUM(GRIDVOL*SATGAS)
```

```
OPS_SATG = R21SATG/R21VOL
!
!*****
!
! EXP_AREA
!
LIMIT ELEMENT 632 TO 637
R22SATG = SUM(GRIDVOL*SATGAS)
EXP_SATG = R22SATG/R22VOL
!
!*****
!
! Average gas saturation in waste area and rest of repository
W_R_SATG = (R12SATG + R13SATG)/(R12VOL + R13VOL)
!
!*****
!
! Brine pocket
!
LIMIT ELEMENT 1007 TO 1023
R30SATG = SUM(GRIDVOL*SATGAS)
B_P_SATG = R30SATG/R30VOL
!
!*****
!
! Clean up output--limit to requested quantities
!
DELETE R12SATG, R13SATG, R21SATG, R22SATG, R30SATG
DELETE R12VOL, R13VOL, R21VOL, R22VOL, R30VOL
!
!*****
!*****
!
! Volume-averaged brine saturation (dimensionless)
!
!   Param 042: for region 23 (waste panel,          block 12) --> WAS_SATB
!   Param 043: for region 24 (rest of repository,  block 13) --> REP_SATB
!   Param 044: for region 26 (operation region,    block 21) --> OPS_SATB
!   Param 045: for region 27 (experimental region, block 22) --> EXP_SATB
!   Param 046: for regions 23+24 -----> W_R_SATB
!   Param 047: for region 30 (brine pocket,        block 11) --> B_P_SATB
!
!*****
!
! WAS_AREA
!
WAS_SATB = 1.0 - WAS_SATG
!
!*****
!
! REPOSIT
!
REP_SATB = 1.0 - REP_SATG
!
!*****
!
! OPS_AREA
!
OPS_SATB = 1.0 - OPS_SATG
!
!*****
!
! EXP_AREA
!
EXP_SATB = 1.0 - EXP_SATG
```



```
!
!*****
!
! Average brine saturation in waste area and rest of repository
!
W_R_SATB = 1.0 - W_R_SATG
!
!*****
!
! Brine pocket
!
B_P_SATB = 1.0 - B_P_SATG
!
!*****
!*****
!*****
!
! Volume-averaged porosity (m**3 void/m**3 rock)
!
!   Param 048: for region 23 (waste panel,      block 12) --> WAS_POR
!   Param 049: for region 24 (rest of repository, block 13) --> REP_POR
!   Param 050: for region 26 (operation region,  block 21) --> OPS_POR
!   Param 051: for region 27 (experimental region, block 22) --> EXP_POR
!   Param 052: for regions 23+24 -----> W_R_POR
!
!*****
!
! WAS_AREA
!
LIMIT ELEMENT 596 TO 616
!
WAS_POR = SUM(GRIDVOL*POROS) / SUM(GRIDVOL)
!
!*****
!
! REPOSIT
!
LIMIT ELEMENT 617 TO 625
!
REP_POR = SUM(GRIDVOL*POROS) / SUM(GRIDVOL)
!
!*****
!
! OPS_AREA
!
LIMIT ELEMENT 626 TO 631
!
OPS_POR = SUM(GRIDVOL*POROS) / SUM(GRIDVOL)
!
!*****
!
! EXP_AREA
!
LIMIT ELEMENT 632 TO 637
!
EXP_POR = SUM(GRIDVOL*POROS) / SUM(GRIDVOL)
!
!*****
!
! Average porosity in waste area and rest of repository
!
LIMIT ELEMENT 596 TO 625
!
W_R_POR = SUM(GRIDVOL*POROS) / SUM(GRIDVOL)
!
```

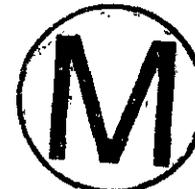


```
!*****  
!  
!*****  
!*****  
!  
! Param 053: Brine consumed (m**3) --> BRN_RMV  
!  
LIMIT ELEMENT OFF  
!  
! Add up consumption rates (resulting units are kg/s)  
!  
BRN_CR = SUM(BRINRATE*GRIDVOL)  
!  
! Integrate result to get kg of brine consumed  
!  
BRN_CON = INTRIGHT(BRN_CR)  
!  
! Convert to volumetric amount (m**3) by  
! dividing by brine density (kg/m**3) at reference conditions  
!  
BRN_RMV = -1.0*BRN_CON/1220.0  
!  
! Delete temporary variables  
!  
DELETE BRN_CR, BRN_CON  
!  
!*****  
!  
!*****  
!  
! Cumulative brineflow (m**3)  
!  
! Param 054: Total brineflow into repository -----> BRNREPTC  
! Param 055: Total brineflow into waste panel -----> BRNWPIC  
! Param 056: Total brineflow into rest of repository --> BRNRRIC  
! Param 057: Total brineflow into operations region ---> BRNORIC  
! Param 058: Total brineflow into experimental area ---> BRNEAIC  
! Param 059: Net brineflow out of repository -----> BRNREPOC  
! Param 060: Net brineflow out of waste panel -----> BRNWP0C  
! Param 061: Net brineflow out of rest of repository --> BRNRR0C  
! Param 062: Net brineflow out of operations region ---> BRNOR0C  
! Param 063: Net brineflow out of experimental area ---> BRNEA0C  
! Param 064: Net brineflow into repository -----> BRNREPNC  
! Param 065: Net brineflow into waste panel -----> BRNWPNC  
! Param 066: Net brineflow into rest of repository ----> BRNRRNC  
! Param 067: Net brineflow into operations regions ----> BRNORNc  
! Param 068: Net brineflow into experimental area ----> BRNEANC  
! Param 069: Brineflow up shaft (@element 661) -----> BRNSHUPC  
! Param 070: Brineflow up shaft (@element 666) -----> BRNSHUPR  
! Param 071: Brineflow up shaft (@element 669) -----> BRNSHUPS  
! Param 072: Brineflow up borehole (@element 599) -----> BRNBHUPP  
! Param 073: Brineflow up borehole (@element 471) -----> BRNBHUPC  
! Param 074: Brineflow up borehole (@element 713) -----> BRNBHRCC  
! Param 075: Brineflow up borehole (@element 841) -----> BRNBHRUC  
! Param 076: Brineflow up borehole (@element 937) -----> BRNBHRSC  
! Param 077: Brineflow up borehole (@element 439) -----> BNBHLDRZ  
! Param 078: Brineflow up borehole (@element 575) -----> BNBHUDRZ  
!  
!*****  
!  
! Total cumulative brineflow into repository  
!  
! Accumulate x-direction inward flows from left side of repository  
!  
BRNREPIX = IFGT0(FLOWBRX[E:596],FLOWBRX[E:596],0.0)
```

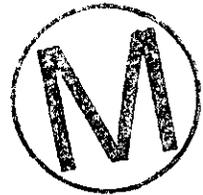


```
BRNREPIX = BRNREPIX + IFGT0(FLOWBRX[E:603],FLOWBRX[E:603],0.0)
BRNREPIX = BRNREPIX + IFGT0(FLOWBRX[E:610],FLOWBRX[E:610],0.0)
!
!   Add x-direction inward flow contributions from right side
!
BRNREPIX = BRNREPIX + IFLT0(FLOWBRX[E:641],-1.0*FLOWBRX[E:641],0.0)
BRNREPIX = BRNREPIX + IFLT0(FLOWBRX[E:642],-1.0*FLOWBRX[E:642],0.0)
BRNREPIX = BRNREPIX + IFLT0(FLOWBRX[E:643],-1.0*FLOWBRX[E:643],0.0)
!
!   Accumulate y-direction inward flows from bottom of repository
!
BRNREPIY =          IFGT0(FLOWBRY[E:596],FLOWBRY[E:596],0.0)
BRNREPIY = BRNREPIY + IFGT0(FLOWBRY[E:597],FLOWBRY[E:597],0.0)
BRNREPIY = BRNREPIY + IFGT0(FLOWBRY[E:598],FLOWBRY[E:598],0.0)
BRNREPIY = BRNREPIY + IFGT0(FLOWBRY[E:599],FLOWBRY[E:599],0.0)
BRNREPIY = BRNREPIY + IFGT0(FLOWBRY[E:600],FLOWBRY[E:600],0.0)
BRNREPIY = BRNREPIY + IFGT0(FLOWBRY[E:601],FLOWBRY[E:601],0.0)
BRNREPIY = BRNREPIY + IFGT0(FLOWBRY[E:602],FLOWBRY[E:602],0.0)
BRNREPIY = BRNREPIY + IFGT0(FLOWBRY[E:638],FLOWBRY[E:638],0.0)
BRNREPIY = BRNREPIY + IFGT0(FLOWBRY[E:617],FLOWBRY[E:617],0.0)
BRNREPIY = BRNREPIY + IFGT0(FLOWBRY[E:618],FLOWBRY[E:618],0.0)
BRNREPIY = BRNREPIY + IFGT0(FLOWBRY[E:619],FLOWBRY[E:619],0.0)
!
!   Add Y-direction inward flow contributions from top side
!
BRNREPIY = BRNREPIY + IFLT0(FLOWBRY[E:468],-1.0*FLOWBRY[E:468],0.0)
BRNREPIY = BRNREPIY + IFLT0(FLOWBRY[E:469],-1.0*FLOWBRY[E:469],0.0)
BRNREPIY = BRNREPIY + IFLT0(FLOWBRY[E:470],-1.0*FLOWBRY[E:470],0.0)
BRNREPIY = BRNREPIY + IFLT0(FLOWBRY[E:471],-1.0*FLOWBRY[E:471],0.0)
BRNREPIY = BRNREPIY + IFLT0(FLOWBRY[E:472],-1.0*FLOWBRY[E:472],0.0)
BRNREPIY = BRNREPIY + IFLT0(FLOWBRY[E:473],-1.0*FLOWBRY[E:473],0.0)
BRNREPIY = BRNREPIY + IFLT0(FLOWBRY[E:474],-1.0*FLOWBRY[E:474],0.0)
BRNREPIY = BRNREPIY + IFLT0(FLOWBRY[E:475],-1.0*FLOWBRY[E:475],0.0)
BRNREPIY = BRNREPIY + IFLT0(FLOWBRY[E:476],-1.0*FLOWBRY[E:476],0.0)
BRNREPIY = BRNREPIY + IFLT0(FLOWBRY[E:477],-1.0*FLOWBRY[E:477],0.0)
BRNREPIY = BRNREPIY + IFLT0(FLOWBRY[E:478],-1.0*FLOWBRY[E:478],0.0)
!
!   Sum x- and y-direction inward flows, then integrate over time
!
BRNREPT  = BRNREPIX + BRNREPIY
BRNREPTC = INTRIGHT(BRNREPT)
!
!   Delete flow rate temporary variables
!
DELETE BRNREPT, BRNREPIX, BRNREPIY
!
!*****
!
! Total cumulative brine flow into waste panel
!
!   Left side
!
BRNWPI   =          IFGT0(FLOWBRX[E:596],FLOWBRX[E:596],0.0)
BRNWPI   = BRNWPI + IFGT0(FLOWBRX[E:603],FLOWBRX[E:603],0.0)
BRNWPI   = BRNWPI + IFGT0(FLOWBRX[E:610],FLOWBRX[E:610],0.0)
!
!   Right side
!
BRNWPI   = BRNWPI + IFLT0(FLOWBRX[E:638],-1.0*FLOWBRX[E:638],0.0)
BRNWPI   = BRNWPI + IFLT0(FLOWBRX[E:639],-1.0*FLOWBRX[E:639],0.0)
BRNWPI   = BRNWPI + IFLT0(FLOWBRX[E:640],-1.0*FLOWBRX[E:640],0.0)
!
!   Bottom
!
BRNWPI   = BRNWPI + IFGT0(FLOWBRY[E:596],FLOWBRY[E:596],0.0)
BRNWPI   = BRNWPI + IFGT0(FLOWBRY[E:597],FLOWBRY[E:597],0.0)
```

```
BRNWPI = BRNWPI + IFGT0 (FLOWBRY[E:598],FLOWBRY[E:598],0.0)
BRNWPI = BRNWPI + IFGT0 (FLOWBRY[E:599],FLOWBRY[E:599],0.0)
BRNWPI = BRNWPI + IFGT0 (FLOWBRY[E:600],FLOWBRY[E:600],0.0)
BRNWPI = BRNWPI + IFGT0 (FLOWBRY[E:601],FLOWBRY[E:601],0.0)
BRNWPI = BRNWPI + IFGT0 (FLOWBRY[E:602],FLOWBRY[E:602],0.0)
!
!   Top
!
BRNWPI = BRNWPI + IFLT0 (FLOWBRY[E:468],-1.0*FLOWBRY[E:468],0.0)
BRNWPI = BRNWPI + IFLT0 (FLOWBRY[E:469],-1.0*FLOWBRY[E:469],0.0)
BRNWPI = BRNWPI + IFLT0 (FLOWBRY[E:470],-1.0*FLOWBRY[E:470],0.0)
BRNWPI = BRNWPI + IFLT0 (FLOWBRY[E:471],-1.0*FLOWBRY[E:471],0.0)
BRNWPI = BRNWPI + IFLT0 (FLOWBRY[E:472],-1.0*FLOWBRY[E:472],0.0)
BRNWPI = BRNWPI + IFLT0 (FLOWBRY[E:473],-1.0*FLOWBRY[E:473],0.0)
BRNWPI = BRNWPI + IFLT0 (FLOWBRY[E:474],-1.0*FLOWBRY[E:474],0.0)
!
!   Integrate for cumulative, delete flow rate
!
BRNWPIC = INTRIGHT(BRNWPI)
DELETE BRNWPI
!
!*****
!
! Total cumulative brine flow into rest of repository
!
!   Left side
!
BRNRRI = IFGT0 (FLOWBRX[E:617],FLOWBRX[E:617],0.0)
BRNRRI = BRNRRI + IFGT0 (FLOWBRX[E:620],FLOWBRX[E:620],0.0)
BRNRRI = BRNRRI + IFGT0 (FLOWBRX[E:623],FLOWBRX[E:623],0.0)
!
!   Right side
!
BRNRRI = BRNRRI + IFLT0 (FLOWBRX[E:641],-1.0*FLOWBRX[E:641],0.0)
BRNRRI = BRNRRI + IFLT0 (FLOWBRX[E:642],-1.0*FLOWBRX[E:642],0.0)
BRNRRI = BRNRRI + IFLT0 (FLOWBRX[E:643],-1.0*FLOWBRX[E:643],0.0)
!
!   Bottom
!
BRNRRI = BRNRRI + IFGT0 (FLOWBRY[E:617],FLOWBRY[E:617],0.0)
BRNRRI = BRNRRI + IFGT0 (FLOWBRY[E:618],FLOWBRY[E:618],0.0)
BRNRRI = BRNRRI + IFGT0 (FLOWBRY[E:619],FLOWBRY[E:619],0.0)
!
!   Top
!
BRNRRI = BRNRRI + IFLT0 (FLOWBRY[E:476],-1.0*FLOWBRY[E:476],0.0)
BRNRRI = BRNRRI + IFLT0 (FLOWBRY[E:477],-1.0*FLOWBRY[E:477],0.0)
BRNRRI = BRNRRI + IFLT0 (FLOWBRY[E:478],-1.0*FLOWBRY[E:478],0.0)
!
!   Integrate for cumulative, delete flow rate
!
BRNRRI = INTRIGHT(BRNRRI)
DELETE BRNRRI
!
!*****
!
! Total cumulative brine flow into operations region
!
!   Left side
!
BRNORI = IFGT0 (FLOWBRX[E:626],FLOWBRX[E:626],0.0)
BRNORI = BRNORI + IFGT0 (FLOWBRX[E:628],FLOWBRX[E:628],0.0)
BRNORI = BRNORI + IFGT0 (FLOWBRX[E:630],FLOWBRX[E:630],0.0)
!
!   Right side
!
```



```
BRNORI = BRNORI + IFLT0 (FLOWBRX[E:646],-1.0*FLOWBRX[E:646],0.0)
BRNORI = BRNORI + IFLT0 (FLOWBRX[E:647],-1.0*FLOWBRX[E:647],0.0)
BRNORI = BRNORI + IFLT0 (FLOWBRX[E:648],-1.0*FLOWBRX[E:648],0.0)
!
!   Bottom
!
BRNORI = BRNORI + IFGT0 (FLOWBRY[E:626],FLOWBRY[E:626],0.0)
BRNORI = BRNORI + IFGT0 (FLOWBRY[E:627],FLOWBRY[E:627],0.0)
!
!   Top
!
BRNORI = BRNORI + IFLT0 (FLOWBRY[E:480],-1.0*FLOWBRY[E:480],0.0)
BRNORI = BRNORI + IFLT0 (FLOWBRY[E:481],-1.0*FLOWBRY[E:481],0.0)
!
!   Integrate for cumulative, delete flow rate
!
BRNORIC = INTRIGHT(BRNORI)
DELETE BRNORI
!
!*****
!
! Total cumulative brine flow into experimental area
!
!   Left side
!
BRNEAI = -IFGT0 (FLOWBRX[E:632],FLOWBRX[E:632],0.0)
BRNEAI = BRNEAI + IFGT0 (FLOWBRX[E:634],FLOWBRX[E:634],0.0)
BRNEAI = BRNEAI + IFGT0 (FLOWBRX[E:636],FLOWBRX[E:636],0.0)
!
!   Right side
!
BRNEAI = BRNEAI + IFLT0 (FLOWBRX[E:148],-1.0*FLOWBRX[E:148],0.0)
BRNEAI = BRNEAI + IFLT0 (FLOWBRX[E:156],-1.0*FLOWBRX[E:156],0.0)
BRNEAI = BRNEAI + IFLT0 (FLOWBRX[E:164],-1.0*FLOWBRX[E:164],0.0)
!
!   Bottom
!
BRNEAI = BRNEAI + IFGT0 (FLOWBRY[E:632],FLOWBRY[E:632],0.0)
BRNEAI = BRNEAI + IFGT0 (FLOWBRY[E:633],FLOWBRY[E:633],0.0)
!
!   Top
!
BRNEAI = BRNEAI + IFLT0 (FLOWBRY[E:524],-1.0*FLOWBRY[E:524],0.0)
BRNEAI = BRNEAI + IFLT0 (FLOWBRY[E:525],-1.0*FLOWBRY[E:525],0.0)
!
!   Integrate for cumulative, delete flow rate
!
BRNEAIC = INTRIGHT(BRNEAI)
DELETE BRNEAI
!
!*****
!
! Net cumulative brineflow into repository = flow in minus flow out
! (brine consumed by waste corrosion neglected since brine consumption
! rate not available as history variable in bragflow output database)
!
! Accumulate x-direction outward flows from left side of repository
!
BRNREPOX = IFLT0 (FLOWBRX[E:596],-1.0*FLOWBRX[E:596],0.0)
BRNREPOX = BRNREPOX + IFLT0 (FLOWBRX[E:603],-1.0*FLOWBRX[E:603],0.0)
BRNREPOX = BRNREPOX + IFLT0 (FLOWBRX[E:610],-1.0*FLOWBRX[E:610],0.0)
!
! Add x-direction outward flow contributions from right side
!
BRNREPOX = BRNREPOX + IFGT0 (FLOWBRX[E:641],FLOWBRX[E:641],0.0)
BRNREPOX = BRNREPOX + IFGT0 (FLOWBRX[E:642],FLOWBRX[E:642],0.0)
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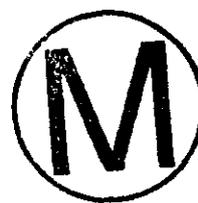


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BRNREPOX = BRNREPOX + IFGT0 (FLOWBRX[E:643],FLOWBRX[E:643],0.0)
!
! Accumulate y-direction outward flows from bottom of repository
!
BRNREPOY = IFLT0 (FLOWBRY[E:596],-1.0*FLOWBRY[E:596],0.0)
BRNREPOY = BRNREPOY + IFLT0 (FLOWBRY[E:597],-1.0*FLOWBRY[E:597],0.0)
BRNREPOY = BRNREPOY + IFLT0 (FLOWBRY[E:598],-1.0*FLOWBRY[E:598],0.0)
BRNREPOY = BRNREPOY + IFLT0 (FLOWBRY[E:599],-1.0*FLOWBRY[E:599],0.0)
BRNREPOY = BRNREPOY + IFLT0 (FLOWBRY[E:600],-1.0*FLOWBRY[E:600],0.0)
BRNREPOY = BRNREPOY + IFLT0 (FLOWBRY[E:601],-1.0*FLOWBRY[E:601],0.0)
BRNREPOY = BRNREPOY + IFLT0 (FLOWBRY[E:602],-1.0*FLOWBRY[E:602],0.0)
BRNREPOY = BRNREPOY + IFLT0 (FLOWBRY[E:638],-1.0*FLOWBRY[E:638],0.0)
BRNREPOY = BRNREPOY + IFLT0 (FLOWBRY[E:617],-1.0*FLOWBRY[E:617],0.0)
BRNREPOY = BRNREPOY + IFLT0 (FLOWBRY[E:618],-1.0*FLOWBRY[E:618],0.0)
BRNREPOY = BRNREPOY + IFLT0 (FLOWBRY[E:619],-1.0*FLOWBRY[E:619],0.0)
!
! Add Y-direction outward flow contributions from top side
!
BRNREPOY = BRNREPOY + IFGT0 (FLOWBRY[E:468],FLOWBRY[E:468],0.0)
BRNREPOY = BRNREPOY + IFGT0 (FLOWBRY[E:469],FLOWBRY[E:469],0.0)
BRNREPOY = BRNREPOY + IFGT0 (FLOWBRY[E:470],FLOWBRY[E:470],0.0)
BRNREPOY = BRNREPOY + IFGT0 (FLOWBRY[E:471],FLOWBRY[E:471],0.0)
BRNREPOY = BRNREPOY + IFGT0 (FLOWBRY[E:472],FLOWBRY[E:472],0.0)
BRNREPOY = BRNREPOY + IFGT0 (FLOWBRY[E:473],FLOWBRY[E:473],0.0)
BRNREPOY = BRNREPOY + IFGT0 (FLOWBRY[E:474],FLOWBRY[E:474],0.0)
BRNREPOY = BRNREPOY + IFGT0 (FLOWBRY[E:475],FLOWBRY[E:475],0.0)
BRNREPOY = BRNREPOY + IFGT0 (FLOWBRY[E:476],FLOWBRY[E:476],0.0)
BRNREPOY = BRNREPOY + IFGT0 (FLOWBRY[E:477],FLOWBRY[E:477],0.0)
BRNREPOY = BRNREPOY + IFGT0 (FLOWBRY[E:478],FLOWBRY[E:478],0.0)
!
! Sum x- and y-direction outward flows, then integrate over time
!
BRNREPO = BRNREPOX + BRNREPOY
BRNREPOC = INTRIGHT(BRNREPO)
!
! Subtract outflow from inflow to obtain net inflow
!
BRNREPNC = BRNREPTC - BRNREPOC
!
! Delete flow rate temporary variables
!
DELETE BRNREPO, BRNREPOX, BRNREPOY
!
!*****
!
! Net cumulative brine flow into waste panel = flow in minus flow out
!
! Left side outward flows
!
BRNWPO = IFLT0 (FLOWBRX[E:596],-1.0*FLOWBRX[E:596],0.0)
BRNWPO = BRNWPO + IFLT0 (FLOWBRX[E:603],-1.0*FLOWBRX[E:603],0.0)
BRNWPO = BRNWPO + IFLT0 (FLOWBRX[E:610],-1.0*FLOWBRX[E:610],0.0)
!
! Right side
!
BRNWPO = BRNWPO + IFGT0 (FLOWBRX[E:638],FLOWBRX[E:638],0.0)
BRNWPO = BRNWPO + IFGT0 (FLOWBRX[E:639],FLOWBRX[E:639],0.0)
BRNWPO = BRNWPO + IFGT0 (FLOWBRX[E:640],FLOWBRX[E:640],0.0)
!
! Bottom
!
BRNWPO = BRNWPO + IFLT0 (FLOWBRY[E:596],-1.0*FLOWBRY[E:596],0.0)
BRNWPO = BRNWPO + IFLT0 (FLOWBRY[E:597],-1.0*FLOWBRY[E:597],0.0)
BRNWPO = BRNWPO + IFLT0 (FLOWBRY[E:598],-1.0*FLOWBRY[E:598],0.0)
BRNWPO = BRNWPO + IFLT0 (FLOWBRY[E:599],-1.0*FLOWBRY[E:599],0.0)
BRNWPO = BRNWPO + IFLT0 (FLOWBRY[E:600],-1.0*FLOWBRY[E:600],0.0)
```

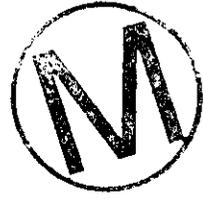


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BRNWPO = BRNWPO + IFLT0 (FLOWBRY[E:601], -1.0*FLOWBRY[E:601], 0.0)
BRNWPO = BRNWPO + IFLT0 (FLOWBRY[E:602], -1.0*FLOWBRY[E:602], 0.0)
!
!   Top
!
BRNWPO = BRNWPO + IFGT0 (FLOWBRY[E:468], FLOWBRY[E:468], 0.0)
BRNWPO = BRNWPO + IFGT0 (FLOWBRY[E:469], FLOWBRY[E:469], 0.0)
BRNWPO = BRNWPO + IFGT0 (FLOWBRY[E:470], FLOWBRY[E:470], 0.0)
BRNWPO = BRNWPO + IFGT0 (FLOWBRY[E:471], FLOWBRY[E:471], 0.0)
BRNWPO = BRNWPO + IFGT0 (FLOWBRY[E:472], FLOWBRY[E:472], 0.0)
BRNWPO = BRNWPO + IFGT0 (FLOWBRY[E:473], FLOWBRY[E:473], 0.0)
BRNWPO = BRNWPO + IFGT0 (FLOWBRY[E:474], FLOWBRY[E:474], 0.0)
!
!   Integrate for cumulative outward flow, delete flow rate
!
BRNWPOC = INTRIGHT(BRNWPO)
DELETE BRNWPO
!
!   Subtract outflow from inflow to obtain net inflow
!
BRNWPNC = BRNWPIC - BRNWPOC
!
!*****
!
! Total cumulative brine flow out of rest of repository
!
!   Left side outward flows
!
BRNRRO =          IFLT0 (FLOWBRX[E:617], -1.0*FLOWBRX[E:617], 0.0)
BRNRRO = BRNRRO + IFLT0 (FLOWBRX[E:620], -1.0*FLOWBRX[E:620], 0.0)
BRNRRO = BRNRRO + IFLT0 (FLOWBRX[E:623], -1.0*FLOWBRX[E:623], 0.0)
!
!   Right side
!
BRNRRO = BRNRRO + IFGT0 (FLOWBRX[E:641], FLOWBRX[E:641], 0.0)
BRNRRO = BRNRRO + IFGT0 (FLOWBRX[E:642], FLOWBRX[E:642], 0.0)
BRNRRO = BRNRRO + IFGT0 (FLOWBRX[E:643], FLOWBRX[E:643], 0.0)
!
!   Bottom
!
BRNRRO = BRNRRO + IFLT0 (FLOWBRY[E:617], -1.0*FLOWBRY[E:617], 0.0)
BRNRRO = BRNRRO + IFLT0 (FLOWBRY[E:618], -1.0*FLOWBRY[E:618], 0.0)
BRNRRO = BRNRRO + IFLT0 (FLOWBRY[E:619], -1.0*FLOWBRY[E:619], 0.0)
!
!   Top
!
BRNRRO = BRNRRO + IFGT0 (FLOWBRY[E:476], FLOWBRY[E:476], 0.0)
BRNRRO = BRNRRO + IFGT0 (FLOWBRY[E:477], FLOWBRY[E:477], 0.0)
BRNRRO = BRNRRO + IFGT0 (FLOWBRY[E:478], FLOWBRY[E:478], 0.0)
!
!   Integrate for cumulative outward flow, delete flow rate
!
BRNRROC = INTRIGHT(BRNRRO)
DELETE BRNRRO
!
!   Subtract outflow from inflow to obtain net inflow
!
BRNRROC = BRNRROC - BRNRROC
!
!*****
!
! Total cumulative brine flow out of operations region
!
!   Left side outward flows
!
BRNORO =          IFLT0 (FLOWBRX[E:626], -1.0*FLOWBRX[E:626], 0.0)
```

```
BRNORO = BRNORO + IFLT0 (FLOWBRX[E:628],-1.0*FLOWBRX[E:628],0.0)
BRNORO = BRNORO + IFLT0 (FLOWBRX[E:630],-1.0*FLOWBRX[E:630],0.0)
!
!   Right side
!
BRNORO = BRNORO + IFGT0 (FLOWBRX[E:646],FLOWBRX[E:646],0.0)
BRNORO = BRNORO + IFGT0 (FLOWBRX[E:647],FLOWBRX[E:647],0.0)
BRNORO = BRNORO + IFGT0 (FLOWBRX[E:648],FLOWBRX[E:648],0.0)
!
!   Bottom
!
BRNORO = BRNORO + IFLT0 (FLOWBRY[E:626],-1.0*FLOWBRY[E:626],0.0)
BRNORO = BRNORO + IFLT0 (FLOWBRY[E:627],-1.0*FLOWBRY[E:627],0.0)
!
!   Top
!
BRNORO = BRNORO + IFGT0 (FLOWBRY[E:480],FLOWBRY[E:480],0.0)
BRNORO = BRNORO + IFGT0 (FLOWBRY[E:481],FLOWBRY[E:481],0.0)
!
!   Integrate for cumulative outward flow, delete flow rate
!
BRNOROC = INTRIGHT(BRNORO)
DELETE BRNORO
!
!   Subtract outflow from inflow to obtain net inflow
!
BRNORNC = BRNORIC - BRNOROC
!
!*****
!
! Total cumulative brine flow out of experimental area:
!
!   Left side outward flows
!
BRNEAO = IFLT0 (FLOWBRX[E:632],-1.0*FLOWBRX[E:632],0.0)
BRNEAO = BRNEAO + IFLT0 (FLOWBRX[E:634],-1.0*FLOWBRX[E:634],0.0)
BRNEAO = BRNEAO + IFLT0 (FLOWBRX[E:636],-1.0*FLOWBRX[E:636],0.0)
!
!   Right side
!
BRNEAO = BRNEAO + IFGT0 (FLOWBRX[E:148],FLOWBRX[E:148],0.0)
BRNEAO = BRNEAO + IFGT0 (FLOWBRX[E:156],FLOWBRX[E:156],0.0)
BRNEAO = BRNEAO + IFGT0 (FLOWBRX[E:164],FLOWBRX[E:164],0.0)
!
!   Bottom
!
BRNEAO = BRNEAO + IFLT0 (FLOWBRY[E:632],-1.0*FLOWBRY[E:632],0.0)
BRNEAO = BRNEAO + IFLT0 (FLOWBRY[E:633],-1.0*FLOWBRY[E:633],0.0)
!
!   Top
!
BRNEAO = BRNEAO + IFGT0 (FLOWBRY[E:524],FLOWBRY[E:524],0.0)
BRNEAO = BRNEAO + IFGT0 (FLOWBRY[E:525],FLOWBRY[E:525],0.0)
!
!   Integrate for cumulative outward flow, delete flow rate
!
BRNEAOC = INTRIGHT(BRNEAO)
DELETE BRNEAO
!
!   Subtract outflow from inflow to obtain net inflow
!
BRNEANC = BRNEAIC - BRNEAOC
!
!*****
!
! Cumulative brineflow up through shaft (past Salado/Rustler Interface)
```



```
!  
BRNSHUP = IFGT0 (FLOWBRY[E:661],FLOWBRY[E:661],0.0)  
BRNSHUPC = INTRIGHT (BRNSHUP)  
!  
!*****  
!  
! Cumulative brineflow up through shaft (past Rustler)  
!  
BRNSUPR = IFGT0 (FLOWBRY[E:666],FLOWBRY[E:666],0.0)  
BRNSHUPR = INTRIGHT (BRNSUPR)  
!  
!*****  
!  
! Cumulative brineflow up through shaft (to surface)  
!  
BRNSUPS = IFGT0 (FLOWBRY[E:669],FLOWBRY[E:669],0.0)  
BRNSHUPS = INTRIGHT (BRNSUPS)  
!  
!*****  
!  
! Cumulative brineflow up borehole (into panel)  
!  
BRNBBUP = IFGT0 (FLOWBRY[E:599],FLOWBRY[E:599],0.0)  
BRNBHUPP = INTRIGHT (BRNBBUP)  
!  
!*****  
!  
! Cumulative brineflow up borehole (measured at repository top boundary)  
!  
BRNBHUP = IFGT0 (FLOWBRY[E:471],FLOWBRY[E:471],0.0)  
BRNBHUPC = INTRIGHT (BRNBHUP)  
!  
!*****  
!  
! Cumulative brineflow up borehole (measured at Rustler/Culebra interface)  
!  
BRNBHRC = IFGT0 (FLOWBRY[E:713],FLOWBRY[E:713],0.0)  
BRNBHRCC = INTRIGHT (BRNBHRC)  
!  
!*****  
!  
! Cumulative brineflow up borehole (past Rustler)  
!  
BRNBHRU = IFGT0 (FLOWBRY[E:841],FLOWBRY[E:841],0.0)  
BRNBHRUC = INTRIGHT (BRNBHRU)  
!  
!*****  
!  
! Cumulative brineflow up borehole (to surface)  
!  
BRNBHRS = IFGT0 (FLOWBRY[E:937],FLOWBRY[E:937],0.0)  
BRNBHRSC = INTRIGHT (BRNBHRS)  
!  
!*****  
!  
! Cumulative brineflow up borehole (into lower DRZ below waste panel)  
!  
BNBHLDR = IFGT0 (FLOWBRY[E:439],FLOWBRY[E:439],0.0)  
BNBHLDRZ = INTRIGHT (BNBHLDR)  
!  
!*****  
!  
! Cumulative brineflow up borehole (at top of DRZ region)  
!  
BNBHUDR = IFGT0 (FLOWBRY[E:575],FLOWBRY[E:575],0.0)  
BNBHUDRZ = INTRIGHT (BNBHUDR)
```



```
!  
!*****  
!  
! Clean up output--limit to requested quantities  
!  
DELETE BRNSHUP, BRNSUPR, BRNSUPS, BNBHLDR, BNBHUOR  
DELETE BRNBUP, BRNBHUP, BRNBHRC, BRNBHRU, BRNBHRS  
!  
!*****  
!*****  
!  
! Total brineflow out of marker beds toward repository (m**3)  
!  
!   Param 079: MB 138,           North --> BRM38NIC  
!   Param 080: Anhydrite A&B, North --> BRAABNIC  
!   Param 081: MB 139,           North --> BRM39NIC  
!   Param 082: MB 138,           South --> BRM38SIC  
!   Param 083: Anhydrite A&B, South --> BRAABSIC  
!   Param 084: MB 139,           South --> BRM39SIC  
!   Param 085: all marker beds -----> BRAALIC  
!  
!*****  
!  
! Total inward brineflow from MB 138, north (right) side  
!  
BRNM38NI = IFLT0(FLOWBRX[E:588],-1.0*FLOWBRX[E:588],0.0)  
BRM38NIC = INTRIGHT(BRNM38NI)  
!  
!*****  
!  
! Total inward brineflow from Anhydrite A&B, north (right) side  
!  
BRNAABNI = IFLT0(FLOWBRX[E:556],-1.0*FLOWBRX[E:556],0.0)  
BRAABNIC = INTRIGHT(BRNAABNI)  
!  
!*****  
!  
! Total inward brineflow from MB 139, north (right) side  
!  
BRNM39NI = IFLT0(FLOWBRX[E:540],-1.0*FLOWBRX[E:540],0.0)  
BRM39NIC = INTRIGHT(BRNM39NI)  
!  
!*****  
!*****  
!  
! Total inward brineflow from MB 138, south (left) side  
!  
BRNM38SI = IFGT0(FLOWBRX[E:572],FLOWBRX[E:572],0.0)  
BRM38SIC = INTRIGHT(BRNM38SI)  
!  
!*****  
!  
! Total inward brineflow from Anhydrite A&B, south (left) side  
!  
BRNAABSI = IFGT0(FLOWBRX[E:482],FLOWBRX[E:482],0.0)  
BRAABSIC = INTRIGHT(BRNAABSI)  
!  
!*****  
!  
! Total inward brineflow from MB 139, south (left) side  
!  
BRNM39SI = IFGT0(FLOWBRX[E:436],FLOWBRX[E:436],0.0)  
BRM39SIC = INTRIGHT(BRNM39SI)  
!  
!*****  
!
```



```
! Total inward brineflow from all anhydrite layers
!  
BRAALIC = BRM38NIC + BRAABNIC + BRM39NIC + BRM38SIC + BRAABSIC + BRM39SIC
!  
!*****  
!  
! Clean up output--limit to requested quantities
!  
DELETE BRNM38NI, BRNAABNI, BRNM39NI, BRNM38SI, BRNAABSI, BRNM39SI
!  
!*****  
!*****  
!  
! Total brineflow into marker beds away from repository (m**3)
!  
!   Param 086: MB 138,      North --> BRM38NOC
!   Param 087: Anhydrite A&B, North --> BRAABNOC
!   Param 088: MB 139,      North --> BRM39NOC
!   Param 089: MB 138,      South --> BRM38SOC
!   Param 090: Anhydrite A&B, South --> BRAABSOC
!   Param 091: MB 139,      South --> BRM39SOC
!   Param 092: all marker beds -----> BRAALOC
!  
!*****  
!  
! Total brineflow into MB 138 away from repository, north (right) side
!  
BRNM38NO = IFGT0(FLOWBRX[E:588],FLOWBRX[E:588],0.0)
BRM38NOC = INTRIGHT(BRNM38NO)
!  
!*****  
!  
! Total brineflow into Anhydrite A&B away from repository, north side
!  
BRNAABNO = IFGT0(FLOWBRX[E:556],FLOWBRX[E:556],0.0)
BRAABNOC = INTRIGHT(BRNAABNO)
!  
!*****  
!  
! Total brineflow into MB 139 away from repository, north (right) side
!  
BRNM39NO = IFGT0(FLOWBRX[E:540],FLOWBRX[E:540],0.0)
BRM39NOC = INTRIGHT(BRNM39NO)
!  
!*****  
!*****  
!  
! Total brineflow into MB 138 away from repository, south (left) side
!  
BRNM38SO = IFLT0(FLOWBRX[E:572],-1.0*FLOWBRX[E:572],0.0)
BRM38SOC = INTRIGHT(BRNM38SO)
!  
!*****  
!  
! Total brineflow into Anhydrite A&B away from repository, south side
!  
BRNAABSO = IFLT0(FLOWBRX[E:482],-1.0*FLOWBRX[E:482],0.0)
BRAABSOC = INTRIGHT(BRNAABSO)
!  
!*****  
!  
! Total brineflow into MB 139 away from repository, south (left) side
!  
BRNM39SO = IFLT0(FLOWBRX[E:436],-1.0*FLOWBRX[E:436],0.0)
BRM39SOC = INTRIGHT(BRNM39SO)
!
```

```
!*****  
!  
! Total outward brineflow into all anhydrite layers  
!  
BRAALOC = BRM38NOC + BRAABNOC + BRM39NOC + BRM38SOC + BRAABSOC + BRM39SOC  
!  
!*****  
!  
! Clean up output--limit to requested quantities  
!  
DELETE BRNM38NO, BRNAABNO, BRNM39NO, BRNM38SO, BRNAABSO, BRNM39SO  
!  
!*****  
!*****  
!  
! Net brineflow through marker beds (m**3)  
!  
!   Param 093: MB 138,           North --> BRM38NNC  
!   Param 094: Anhydrite A&B, North --> BRAABNNC  
!   Param 095: MB 139,           North --> BRM39NNC  
!   Param 096: MB 138,           South --> BRM38SNC  
!   Param 097: Anhydrite A&B, South --> BRAABSNC  
!   Param 098: MB 139,           South --> BRM39SNC  
!   Param 099: all marker beds -----> BRAALNC  
!  
!*****  
!  
! Net brineflow through MB 138, north (right) side  
!  
BRNM38NN = FLOWBRX[E:588]  
BRM38NNC = INTRIGHT(BRNM38NN)  
!  
!*****  
!  
! Net brineflow through Anhydrite A&B, north (right) side  
!  
BRNAABNN = FLOWBRX[E:556]  
BRAABNNC = INTRIGHT(BRNAABNN)  
!  
!*****  
!  
! Net brineflow through MB 139, north (right) side  
!  
BRNM39NN = FLOWBRX[E:540]  
BRM39NNC = INTRIGHT(BRNM39NN)  
!  
!*****  
!*****  
!  
! Net brineflow through MB 138, south (left) side  
!  
BRNM38SN = FLOWBRX[E:572]  
BRM38SNC = INTRIGHT(BRNM38SN)  
!  
!*****  
!  
! Net brineflow through Anhydrite A&B, south (left) side  
!  
BRNAABSN = FLOWBRX[E:482]  
BRAABSNC = INTRIGHT(BRNAABSN)  
!  
!*****  
!  
! Net brineflow through MB 139, south (left) side  
!  
BRNM39SN = FLOWBRX[E:436]
```



```
BRM39SNC = INTRIGHT(BRNM39SN)
!
!*****
!
! Net brineflow through all anhydrite layers
!
BRAALNC = BRM38NNC + BRAABNNC + BRM39NNC + BRM38SNC + BRAABSNC + BRM39SNC
!
!*****
!
! Clean up output--limit to requested quantities
!
DELETE BRNM38NN, BRNAABNN, BRNM39NN, BRNM38SN, BRNAABSN, BRNM39SN
!
!*****
!*****
! Cumulative gas flow (m**3)
!
! Param 100: up shaft (@element 661) -----> GASSHUPC
! Param 101: up borehole (@element 471) -----> GASBHUPC
! Param 102: up borehole (@element 575) -----> GASBHUDZ
! Param 103: into brine pocket (@element 985) -----> GASBPDNC
! Param 104: out of brine pocket (@element 985) -----> GASBPUPC
! Param 105: net into brine pocket (@element 985) --> GASBPNTC
!
!*****
!
! Cumulative gas flow up through shaft (past Salado/Rustler Interface)
GASSHUP = IFGT0(FLOWGASY[E:661],FLOWGASY[E:661],0.0)
GASSHUPC = INTRIGHT(GASSHUP)
!
!*****
!
! Cumulative gas flow up borehole (measured at repository top boundary)
GASBHUP = IFGT0(FLOWGASY[E:471],FLOWGASY[E:471],0.0)
GASBHUPC = INTRIGHT(GASBHUP)
!
!*****
!
! Cumulative gas flow up borehole (measured at top of DRZ)
GASBHUD = IFGT0(FLOWGASY[E:575],FLOWGASY[E:575],0.0)
GASBHUDZ = INTRIGHT(GASBHUD)
!
!*****
!
! Cumulative gas flow into brine pocket (at top of brine pocket)
GASBPDN = IFLT0(FLOWGASY[E:985],-1.0*FLOWGASY[E:985],0.0)
GASBPDNC = INTRIGHT(GASBPDN)
!
!*****
!
! Cumulative gas flow out of brine pocket (at top of brine pocket)
GASBPUP = IFGT0(FLOWGASY[E:985],FLOWGASY[E:985],0.0)
GASBPUPC = INTRIGHT(GASBPUP)
!
!*****
!
! Cumulative net gas flow into brine pocket (at top of brine pocket)
GASBPNT = -1.0*FLOWGASY[E:985]
```



```
GASBPNTC = INTRIGHT(GASBPNT)
!  
!*****  
!  
! Clean up output--limit to requested quantities  
!  
DELETE GASSHUP, GASBHUP, GASBHUD, GASBPDN, GASBPUP, GASBPNT  
!  
!*****  
!*****  
!  
! Total gas flow through marker beds away from repository (m**3)  
!  
!   Param 106: MB 138,      North --> GSM38NOC  
!   Param 107: Anhydrite A&B, North --> GSAABNOC  
!   Param 108: MB 139,      North --> GSM39NOC  
!   Param 109: MB 138,      South --> GSM38SOC  
!   Param 110: Anhydrite A&B, South --> GSAABSOC  
!   Param 111: MB 139,      South --> GSM39SOC  
!   Param 112: all marker beds -----> GSAALOC  
!  
!*****  
!  
! Total gas flow in MB 138 away from repository, north (right) side  
!  
GASM38NO = IFGT0(FLOWGASX[E:588],FLOWGASX[E:588],0.0)  
GSM38NOC = INTRIGHT(GASM38NO)  
!  
!*****  
!  
! Total gas flow in Anhydrite A&B away from repository, north side  
!  
GASAABNO = IFGT0(FLOWGASX[E:556],FLOWGASX[E:556],0.0)  
GSAABNOC = INTRIGHT(GASAABNO)  
!  
!*****  
!  
! Total gas flow in MB 139 away from repository, north (right) side  
!  
GASM39NO = IFGT0(FLOWGASX[E:540],FLOWGASX[E:540],0.0)  
GSM39NOC = INTRIGHT(GASM39NO)  
!  
!*****  
!*****  
!  
! Total gas flow in MB 138 away from repository, south (left) side  
!  
GASM38SO = IFLT0(FLOWGASX[E:572],-1.0*FLOWGASX[E:572],0.0)  
GSM38SOC = INTRIGHT(GASM38SO)  
!  
!*****  
!  
! Total gas flow in Anhydrite A&B away from repository, south side  
!  
GASAABSO = IFLT0(FLOWGASX[E:482],-1.0*FLOWGASX[E:482],0.0)  
GSAABSOC = INTRIGHT(GASAABSO)  
!  
!*****  
!  
! Total gas flow in MB 139 away from repository, south (left) side  
!  
GASM39SO = IFLT0(FLOWGASX[E:436],-1.0*FLOWGASX[E:436],0.0)  
GSM39SOC = INTRIGHT(GASM39SO)  
!  
!*****  
!
```



```
! Total gas flow into all anhydrite layers
!
GSAALOC = GSM38NOC + GSAABNOC + GSM39NOC + GSM38SOC + GSAABSOC + GSM39SOC
!
!*****
!
! Clean up output--limit to requested quantities
!
DELETE GASM38NO, GASAABNO, GASM39NO, GASM38SO, GASAABSO, GASM39SO
!
!*****
!
! Interbed fracturing: Length of fracturing zone (m)
!
!   Param 113: MB 138,           North --> FRACX38N
!   Param 114: Anhydrite A&B, North --> FRACXABN
!   Param 115: MB 139,           North --> FRACX39N
!   Param 116: MB 138,           South --> FRACX38S
!   Param 117: Anhydrite A&B, South --> FRACXABS
!   Param 118: MB 139,           South --> FRACX39S
!
!*****
!
! Fracturing in MB 138 away from repository, north (right) side
!
LIMIT ELEMENT 588 TO 595
!
!   Define meaningful fracturing as doubling of initial permeability
!
FR_TOL38 = 2.0*PERM_X[B:5]
!
!   Set reference point for fracturing length at the north repository border
!
XREF38N = X[N:1590]
!
!   Determine average x-coordinate of element centroid as element variable
!
XECENT = NOD2ELE(X)
!
!   Compare any change in permeability against fracture criterion
!   If criterion met (i.e., permeability of an element has at least doubled)
!   then calculate length of fracture as distance from reference point
!   to centroid of element, otherwise set fracture length to zero
!
XDIST = IFGT0(PERMBRX-FR_TOL38,XECENT-XREF38N,0.0)
!
!   Extract maximum value of fracture length at each time
!
FRACX38N = SMAX(XDIST)
!
!   Delete temporary variables (tolerance used repeated below, then deleted)
!
DELETE XREF38N, XECENT, XDIST
!
!*****
!
! Fracturing in Anhydrite A&B away from repository, north (right) side
!
LIMIT ELEMENT 556 TO 563
!
FR_TOLAB = 2.0*PERM_X[B:4]
XREFABN = X[N:1488]
XECENT = NOD2ELE(X)
XDIST = IFGT0(PERMBRX-FR_TOLAB,XECENT-XREFABN,0.0)
FRACXABN = SMAX(XDIST)
```

```
!
DELETE XREFABN, XECENT, XDIST
!
!*****
!
! Fracturing in MB 139 away from repository, north (right) side
!
LIMIT ELEMENT 540 TO 547
!
FR_TOL39 = 2.0*PERM_X[B:3]
XREF39N = X[N:1284]
XECENT = NOD2ELE(X)
XDIST = IFGT0(PERMBRX-FR_TOL39,XECENT-XREF39N,0.0)
FRACX39N = SMAX(XDIST)
!
DELETE XREF39N, XECENT, XDIST
!
!*****
!*****
!
! Fracturing in MB 138 away from repository, south (left) side
!
LIMIT ELEMENT 564 TO 571
!
XREF38S = X[N:1573]
XECENT = NOD2ELE(X)
XDIST = IFGT0(PERMBRX-FR_TOL38,XREF38S-XECENT,0.0)
FRACX38S = SMAX(XDIST)
!
DELETE XREF38S, XECENT, XDIST
!
!*****
!
! Fracturing in Anhydrite A&B away from repository, south (left) side
!
LIMIT ELEMENT 548 TO 555
!
XREFABS = X[N:1471]
XECENT = NOD2ELE(X)
XDIST = IFGT0(PERMBRX-FR_TOLAB,XREFABS-XECENT,0.0)
FRACXABS = SMAX(XDIST)
!
DELETE XREFABS, XECENT, XDIST
!
!*****
!
! Fracturing in MB 139 away from repository, south (left) side
!
LIMIT ELEMENT 532 to 539
!
XREF39S = X[N:1267]
XECENT = NOD2ELE(X)
XDIST = IFGT0(PERMBRX-FR_TOL39,XREF39S-XECENT,0.0)
FRACX39S = SMAX(XDIST)
!
DELETE XREF39S, XECENT, XDIST
!
!*****
!*****
!
! Interbed fracturing: Volume of fracturing zone (m**3)
!
! Param 119: MB 138, North -----> VFRAC38N
! Param 120: Anhydrite A&B, North -----> VFRACABN
```



```
! Param 121: MB 139, North -----> VFRAC39N
! Param 122: MB 138, South -----> VFRAC38S
! Param 123: Anhydrite A&B, South -----> VFRACABS
! Param 124: MB 139, South -----> VFRAC39S
! Param 125: Total marker bed fracture volume --> VFRACTMB
!
!*****
!
! Volume of fracture zone in MB 138 away from repository, north (right) side
!
LIMIT ELEMENT 588 TO 595
!
! Extract z-direction thickness of fractured elements, set result to zero
! for intact elements
!
EL_Z_38N = IFGT0(PERMBRX-FR_TOL38,THICK,0.0)
!
! Set flag for each fractured element to determine number of affected elements
!
FLAG_38N = IFGT0(EL_Z_38N,1.0,0.0)
TOTF_38N = SUM(FLAG_38N)
!
! Check whether any number of elements has fractured, if none then
! set to dummy number for division step to avoid divide by zero
!
TOTF_38N = IFGT0(TOTF_38N,TOTF_38N,999.0)
!
! Obtain average fractured y-z area--note that contributions to area sum
! from intact elements will be zero and that sum will be zero if no
! elements have fractured
!
A_AVG38N = SUM(EL_Z_38N*DEL_Y)/TOTF_38N
!
! Multiply average fractured element y-z area times the total fracture length
! to obtain fracture zone volume
!
VFRAC38N = FRACX38N * A_AVG38N
!
! Delete temporary variables except for tolerance and z-direction thickness
!
DELETE FLAG_38N, TOTF_38N, A_AVG38N
!
!*****
!
! Volume of fracture zone in Anhydrite A&B away from repository, north side
!
LIMIT ELEMENT 556 TO 563
!
EL_Z_ABN = IFGT0(PERMBRX-FR_TOLAB,THICK,0.0)
FLAG_ABN = IFGT0(EL_Z_ABN,1.0,0.0)
TOTF_ABN = SUM(FLAG_ABN)
TOTF_ABN = IFGT0(TOTF_ABN,TOTF_ABN,999.0)
A_AVGABN = SUM(EL_Z_ABN*DEL_Y)/TOTF_ABN
VFRACABN = FRACX39N * A_AVGABN
!
DELETE FLAG_ABN, TOTF_ABN, A_AVGABN
!
!*****
!
! Volume of fracture zone in MB 139 away from repository, north (right) side
!
LIMIT ELEMENT 540 TO 547
!
EL_Z_39N = IFGT0(PERMBRX-FR_TOL39,THICK,0.0)
FLAG_39N = IFGT0(EL_Z_39N,1.0,0.0)
TOTF_39N = SUM(FLAG_39N)
```



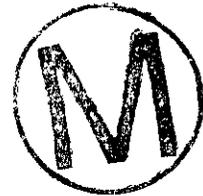
```
TOTF_39N = IFGT0(TOTF_39N,TOTF_39N,999.0)
A_AVG39N = SUM(EL_Z_39N*DEL_Y)/TOTF_39N
VFRAC39N = FRACX39N * A_AVG39N
!
DELETE FLAG_39N, TOTF_39N, A_AVG39N
!
!*****
!*****
!
! Volume of fracture zone in MB 138 away from repository, south (left) side
!
LIMIT ELEMENT 564 TO 571
!
EL_Z_38S = IFGT0(PERMBRX-FR_TOL38,THICK,0.0)
FLAG_38S = IFGT0(EL_Z_38S,1.0,0.0)
TOTF_38S = SUM(FLAG_38S)
TOTF_38S = IFGT0(TOTF_38S,TOTF_38S,999.0)
A_AVG38S = SUM(EL_Z_38S*DEL_Y)/TOTF_38S
VFRAC38S = FRACX38S * A_AVG38S
!
DELETE FLAG_38S, TOTF_38S, A_AVG38S, FR_TOL38
!
!*****
!
! Volume of fracture zone in Anhydrite A&B away from repository, south side
!
LIMIT ELEMENT 548 TO 555
!
EL_Z_ABS = IFGT0(PERMBRX-FR_TOLAB,THICK,0.0)
FLAG_ABS = IFGT0(EL_Z_ABS,1.0,0.0)
TOTF_ABS = SUM(FLAG_ABS)
TOTF_ABS = IFGT0(TOTF_ABS,TOTF_ABS,999.0)
A_AVGABS = SUM(EL_Z_ABS*DEL_Y)/TOTF_ABS
VFRACABS = FRACX39S * A_AVGABS
!
DELETE FLAG_ABS, TOTF_ABS, A_AVGABS, FR_TOLAB
!
!*****
!
! Volume of fracture zone in MB 139 away from repository, south (left) side
!
LIMIT ELEMENT 532 TO 539
!
EL_Z_39S = IFGT0(PERMBRX-FR_TOL39,THICK,0.0)
FLAG_39S = IFGT0(EL_Z_39S,1.0,0.0)
TOTF_39S = SUM(FLAG_39S)
TOTF_39S = IFGT0(TOTF_39S,TOTF_39S,999.0)
A_AVG39S = SUM(EL_Z_39S*DEL_Y)/TOTF_39S
VFRAC39S = FRACX39S * A_AVG39S
!
DELETE FLAG_39S, TOTF_39S, A_AVG39S, FR_TOL39
!
!*****
!
! Total volume of all fracture zones in marker beds away from repository
!
VFRAC38N = VFRAC38N + VFRAC38N + VFRAC39N + VFRAC38S + VFRACABS + VFRAC39S
!
!*****
!*****
!
! Interbed fracturing: Volume-averaged permeability in fracturing zone (m**2)
!
! Param 126: MB 138,          North --> APERM38N
```

```
! Param 127: Anhydrite A&B, North --> APERMABN
! Param 128: MB 139, North --> APERM39N
! Param 129: MB 138, South --> APERM38S
! Param 130: Anhydrite A&B, South --> APERMABS
! Param 131: MB 139, South --> APERM39S
!
!*****
!
! Volume-averaged permeability in MB 138 away from repository, north side
!
LIMIT ELEMENT 588 TO 595
!
! Calculate individual element volume using previously extracted z-direction
! thickness, with thickness set to zero for non-fractured elements
!
VOL_E38N = DEL_X * DEL_Y * EL_Z_38N
!
! Multiply individual element permeabilities times individual element volume,
! note that result will be zero for intact elements
!
VPERM38N = PERMBRX * VOL_E38N
!
! Add up total element volume of fractured elements, note that this could
! be zero if no element has fractured--if it is zero then set it to a
! dummy value to avoid divide by zero in next step
!
TVOLE38N = SUM(VOL_E38N)
TVOLE38N = IFGT0(TVOLE38N,TVOLE38N,-999.0)
!
! Calculate volume-averaged permeabilities for fractured elements only,
! for timesteps with no fracturing set average permeability to initial value
!
APERM38N = IFGT0(TVOLE38N,SUM(VPERM38N)/TVOLE38N,PERM_X[B:5])
!
! Delete temporary variables which aren't used later
!
DELETE EL_Z_38N, TVOLE38N, VPERM38N
!
!*****
!
! Volume-averaged permeability in Anhydrite A&B away from repository, north side
!
LIMIT ELEMENT 556 TO 563
!
VOL_EABN = DEL_X * DEL_Y * EL_Z_ABN
VPERMABN = PERMBRX * VOL_EABN
TVOLEABN = SUM(VOL_EABN)
TVOLEABN = IFGT0(TVOLEABN,TVOLEABN,-999.0)
APERMABN = IFGT0(TVOLEABN,SUM(VPERMABN)/TVOLEABN,PERM_X[B:4])
!
DELETE EL_Z_ABN, TVOLEABN, VPERMABN
!
!*****
!
! Volume-averaged permeability in MB 139 away from repository, north side
!
LIMIT ELEMENT 540 TO 547
!
VOL_E39N = DEL_X * DEL_Y * EL_Z_39N
VPERM39N = PERMBRX * VOL_E39N
TVOLE39N = SUM(VOL_E39N)
TVOLE39N = IFGT0(TVOLE39N,TVOLE39N,-999.0)
APERM39N = IFGT0(TVOLE39N,SUM(VPERM39N)/TVOLE39N,PERM_X[B:3])
!
DELETE EL_Z_39N, TVOLE39N, VPERM39N
!
```

```
!*****
!*****
!
! Volume-averaged permeability in MB 138 away from repository, south side
!
LIMIT ELEMENT 564 TO 571
!
VOL_E38S = DEL_X * DEL_Y * EL_Z_38S
VPERM38S = PERMBRX * VOL_E38S
TVOLE38S = SUM(VOL_E38S)
TVOLE38S = IFGT0(TVOLE38S, TVOLE38S, -999.0)
APERM38S = IFGT0(TVOLE38S, SUM(VPERM38S)/TVOLE38S, PERM_X[B:5])
!
DELETE EL_Z_38S, TVOLE38S, VPERM38S
!
!*****
!
! Volume-averaged permeability in Anhydrite A&B away from repository, south side
!
LIMIT ELEMENT 548 TO 555
!
VOL_EABS = DEL_X * DEL_Y * EL_Z_ABS
VPERMABS = PERMBRX * VOL_EABS
TVOLEABS = SUM(VOL_EABS)
TVOLEABS = IFGT0(TVOLEABS, TVOLEABS, -999.0)
APERMABS = IFGT0(TVOLEABS, SUM(VPERMABS)/TVOLEABS, PERM_X[B:4])
!
DELETE EL_Z_ABS, TVOLEABS, VPERMABS
!
!*****
!
! Volume-averaged permeability in MB 139 away from repository, south side
!
LIMIT ELEMENT 532 TO 539
!
VOL_E39S = DEL_X * DEL_Y * EL_Z_39S
VPERM39S = PERMBRX * VOL_E39S
TVOLE39S = SUM(VOL_E39S)
TVOLE39S = IFGT0(TVOLE39S, TVOLE39S, -999.0)
APERM39S = IFGT0(TVOLE39S, SUM(VPERM39S)/TVOLE39S, PERM_X[B:3])
!
DELETE EL_Z_39S, TVOLE39S, VPERM39S
!
!*****
!*****
!
! Interbed fracturing: Increase in pore volume in fracturing zone (m**3)
!
!   Param 132: MB 138,           North -----> PVOLI38N
!   Param 133: Anhydrite A&B,   North -----> PVOLIABN
!   Param 134: MB 139,           North -----> PVOLI39N
!   Param 135: MB 138,           South -----> PVOLI38S
!   Param 136: Anhydrite A&B,   South -----> PVOLIABS
!   Param 137: MB 139,           South -----> PVOLI39S
!   Param 138: Total frac zone pore volume increase --> PVOLI_T
!
!*****
!
! Increase in pore volume in MB 138, north side
!
LIMIT ELEMENT 588 TO 595
!
! Calculate total current pore volumes for fractured elements, note that
! contribution from intact elements will be zero since this measure of
```



```
!      their volume was set to zero
!  
PVC38N = SUM(POROS*VOL_E38N)
!  
!      Extract minimum porosity values (are these always initial values?)
!  
PORMIN = ENVMIN(POROS)
!  
!      Sum minimum pore volume in fractured zone
!  
PVM38N = SUM(PORMIN*VOL_E38N)
!  
!      Increase in pore volume is the current sum minus the minimum
!  
PVOLI38N = PVC38N - PVM38N
!  
!      Delete temporary variables
!  
DELETE VOL_E38N, PVC38N, PVM38N, PORMIN
!  
!*****
!  
!      Increase in pore volume in Anhydrite A&B, north side
!  
LIMIT ELEMENT 556 TO 563
!  
PVCABN = SUM(POROS*VOL_EABN)
PORMIN = ENVMIN(POROS)
PVMABN = SUM(PORMIN*VOL_EABN)
PVOLIABN = PVCABN - PVMABN
!  
DELETE VOL_EABN, PVCABN, PVMABN, PORMIN
!  
!*****
!  
!      Increase in pore volume in MB 139, north side
!  
LIMIT ELEMENT 540 TO 547
!  
PVC39N = SUM(POROS*VOL_E39N)
PORMIN = ENVMIN(POROS)
PVM39N = SUM(PORMIN*VOL_E39N)
PVOLI39N = PVC39N - PVM39N
!  
DELETE VOL_E39N, PVC39N, PVM39N, PORMIN
!  
!*****
!  
!      Increase in pore volume in MB 138, south side
!  
LIMIT ELEMENT 564 TO 571
!  
PVC38S = SUM(POROS*VOL_E38S)
PORMIN = ENVMIN(POROS)
PVM38S = SUM(PORMIN*VOL_E38S)
PVOLI38S = PVC38S - PVM38S
!  
DELETE VOL_E38S, PVC38S, PVM38S, PORMIN
!  
!*****
!  
!      Increase in pore volume in Anhydrite A&B, south side
!  
LIMIT ELEMENT 548 TO 555
!  
!
```



```
PVCABS = SUM(POROS*VOL_EABS)
PORMIN = ENVMIN(POROS)
PVMABS = SUM(PORMIN*VOL_EABS)
PVOLIABS = PVCABS - PVMABS
!
DELETE VOL_EABS, PVCABS, PVMABS, PORMIN
!
!*****
!
! Increase in pore volume in MB 139, south side
!
LIMIT ELEMENT 532 TO 539
!
PVC39S = SUM(POROS*VOL_E39S)
PORMIN = ENVMIN(POROS)
PVM39S = SUM(PORMIN*VOL_E39S)
PVOLI39S = PVC39S - PVM39S
!
DELETE VOL_E39S, PVC39S, PVM39S, PORMIN
!
!*****
!*****
!
! Total increase in pore volume in fractured zones
!
PVOLI_T = PVOLI38N + PVOLIABN + PVOLI39N + PVOLI38S + PVOLIABS + PVOLI39S
!
!*****
!*****
!
! Param 139: Brine volume in brine pocket -----> BRNVOL_B
! Param 140: Downward brine flow at E:223 -----> BNBHDNUZ
! Param 141: Downward brine flow at E:471 -----> BRNBHDNC
! Param 142: Steel mass remaining in waste panel -----> FEKG_W
! Param 143: Cellulose mass remaining in waste panel -----> CELLKG_W
! Param 144: Fraction steel remaining in waste panel -----> FEREM_W
! Param 145: Fraction cellulose remain in waste panel ----> CELREM_W
! Param 146: Total gas volume generated in waste panel --> GASVOL_W
! Param 147: Total pore volume in waste panel -----> PORVOL_W
!
!*****
!
! Brine volume (m**3) in brine pocket
!
LIMIT ELEMENT 1007 TO 1023
!
! Brine volume = porosity * volume * brine saturation
! Brine saturation = 1.0 - SATGAS
!
BRNVOL_B = SUM(POROS*GRIDVOL*(1.0-SATGAS))
!
!*****
!
! Cumulative brineflow down borehole at upper DRZ
!
BNBHDNU = IFLT0(FLOWBRY[E:223],-1.0*FLOWBRY[E:223],0.0)
BNBHDNUZ = INTRIGHT(BNBHDNU)
!
DELETE BNBHDNU
!
!*****
!
! Cumulative brineflow down borehole (measured at repository top boundary)
!
```

```
BRNBHDN = IFLT0(FLOWBRY[E:471],-1.0*FLOWBRY[E:471],0.0)
BRNBHDNC = INTRIGHT(BRNBHDN)
!
DELETE BRNBHDN
!
!*****
!
! Total gas volume (m**3) generated in waste panel
!
LIMIT ELEMENT 596 TO 616
!
! Define molecular weights of iron and cellulose (kg/mol)
!
MW_FE = 0.055847
MW_CELL = 0.03002628
!
! Calculate mass inventories (kg) remaining
!
FEKG_W = SUM(GRIDVOL*FECONC)
CELLKG_W = SUM(GRIDVOL*CELLCONC)
!
! Maximum Fe and bio is at time = 0.0
!
MXFE_W = ENVMAX(FEKG_W)
MXCELL_W = ENVMAX(CELLKG_W)
!
! Calculate masses consumed and divide by initial amount to get fractions gone
! Subtract fraction gone from one to get fractions remaining
!
FEREM_W = 1.0 - ((MXFE_W - FEKG_W)/MXFE_W)
CELREM_W = 1.0 - ((MXCELL_W - CELLKG_W)/MXCELL_W)
!
! Calculate total moles of gas (H2) generated from corrosion of Fe
!
FEMOL_W = (MXFE_W - FEKG_W)/MW_FE*(4.0-STOICOR[B:12])/3.0
!
! Calculate total moles of gas (H2) generated from biodegradation of cellulose
!
CELMOL_W = (MXCELL_W - CELLKG_W)/MW_CELL*STOIMIC[B:12]
!
! Total moles of gas generated
!
GASMOL_W = FEMOL_W + CELMOL_W
!
! Convert to volumetric units (m**3) using PV=nRT at reference P & T
!
! T = 300.15 K
! P = 101325.00 Pa = 101325 N/(m**2)
! R = 8.3145 J/(mol*K) = 8.3145 (N*m)/(mol*K)
! V = n*(R*T/P) m**3 = n moles * 0.024630 (m**3)/mole
!
GASVOL_W = 0.02463 * GASMOL_W
!
DELETE GASMOL_W
DELETE MW_FE, MXFE_W, FEMOL_W
DELETE MW_CELL, MXCELL_W, CELMOL_W
!
!*****
!
! Total pore volume (m**3) in waste panel
!
LIMIT ELEMENT 596 TO 616
!
! Pore volume = porosity (m**3 void/m**3 rock) * volume
!
PORVOL_W = SUM(POROS*GRIDVOL)
```

```
!
!*****
!
!*****
!*****
!
!   Param 148: Volume avgd "brine porosity" in waste panel -----> BRNPOR_W
!   Param 149: Volume avgd "brine porosity" in rest of repository --> BRNPOR_R
!   Param 150: Volume avgd "brine porosity" in waste regions -----> BRNPOR_T
!
!*****
!
! "Brine porosity" (dimensionless) averaged over Waste Panel
!
LIMIT ELEMENT 596 TO 616
!
! Brine saturation = 1.0 - SATGAS
!
WPVOL   = SUM(GRIDVOL)
BRNPORW = SUM(GRIDVOL*POROS*(1.0-SATGAS))
BRNPOR_W = BRNPORW/WPVOL
!
DELETE WPVOL, BRNPORW
!
!*****
!
! "Brine porosity" (dimensionless) averaged over Rest of Repository
!
LIMIT ELEMENT 617 TO 625
!
! Brine saturation = 1.0 - SATGAS
!
RRVOL   = SUM(GRIDVOL)
BRNPORR = SUM(GRIDVOL*POROS*(1.0-SATGAS))
BRNPOR_R = BRNPORR/RRVOL
!
DELETE RRVOL, BRNPORR
!
!*****
!
! "Brine porosity" (dimensionless) averaged over Waste Panel and Rest of
!                               Repository
!
LIMIT ELEMENT 596 TO 625
!
! Brine saturation = 1.0 - SATGAS
!
WRVOL   = SUM(GRIDVOL)
BRNPORT = SUM(GRIDVOL*POROS*(1.0-SATGAS))
BRNPOR_T = BRNPORT/WRVOL
!
DELETE WRVOL, BRNPORT
!
!*****
!*****
!*****
!
!   Param 151: Total brineflow out of MB 138 towards repository --> BRNM38I
!   Param 152: Total brineflow out of A. A&B towards repository --> BRNAABI
!   Param 153: Total brineflow out of MB 139 towards repository --> BRNM39I
!   Param 154: Total brineflow into MB 138 away from repository --> BRNM38O
!   Param 155: Total brineflow into A. A&B away from repository --> BRNAABO
!   Param 156: Total brineflow into MB 139 away from repository --> BRNM39O
!
!*****
```



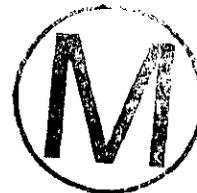
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!
! Total brineflow out of Marker Bed 138 toward repository (m**3)
!
BRNM38I = BRM38NIC + BRM38SIC
!
!*****
!
! Total brineflow out of Anhydrite A&B toward repository (m**3)
!
BRNAABI = BRAABNIC + BRAABSIC
!
!*****
!
! Total brineflow out of Anhydrite A&B toward repository (m**3)
!
BRNM39I = BRM39NIC + BRM39SIC
!
!*****
!
! Total brineflow into Marker Bed 138 away from repository (m**3)
!
BRNM38O = BRM38NOC + BRM38SOC
!
!*****
!
! Total brineflow into Anhydrite A&B away from repository (m**3)
!
BRNAABO = BRAABNOC + BRAABSOC
!
!*****
!
! Total brineflow into Marker Bed 139 away from repository (m**3)
!
BRNM39O = BRM39NOC + BRM39SOC
!
!*****
!
!*****
!*****
!
! Param 157: Brine consumed in Waste Panel (m**3) --> BRN_RMVW
!
LIMIT ELEMENT 596 TO 616
!
! Add up consumption rates (resulting units are kg/s)
!
BRN_CRW = SUM(BRINRATE*GRIDVOL)
!
! Integrate result to get kg of brine consumed
!
BRN_CONW = INTRIGHT(BRN_CRW)
!
! Convert to volumetric amount (m**3) by
! dividing by brine density (kg/m**3) at reference conditions
!
BRN_RMVW = -1.0*BRN_CONW/1220.0
!
! Delete temporary variables
!
DELETE BRN_CRW, BRN_CONW
!
!*****
!
! Param 158: Brine consumed in Rest of Repository (m**3) --> BRN_RMVR
!
LIMIT ELEMENT 617 TO 625
```



```
!
!   Add up consumption rates (resulting units are kg/s)
!
BRN_CRR = SUM(BRINRATE*GRIDVOL)
!
!   Integrate result to get kg of brine consumed
!
BRN_CONR = INTRIGHT(BRN_CRR)
!
!   Convert to volumetric amount (m**3) by
!   dividing by brine density (kg/m**3) at reference conditions
!
BRN_RMVR = -1.0*BRN_CONR/1220.0
!
!   Delete temporary variables
!
DELETE BRN_CRR, BRN_CONR
!
!*****
!
!   Param 159: Remaining fraction of steel in Rest of Repository --> FEREM_R
!   Param 160: Remaining fraction of cellulose in Rest of Repos. --> CELREM_R
!
!*****
LIMIT ELEMENT 617 TO 625
!
! Calculate mass inventories (kg) remaining
!
FE_KGR   = SUM(GRIDVOL*FECONC)
CELL_KGR = SUM(GRIDVOL*CELLCONC)
!
! Maximum Fe and bio is at time = 0.0
!
MXFER    = ENVMAX(FE_KGR)
MXCELLR  = ENVMAX(CELL_KGR)
!
! Calculate masses consumed and divide by initial amount to get fractions gone
! Subtract fraction gone from one to get fractions remaining
!
FEREM_R  = 1.0 - ((MXFER - FE_KGR)/MXFER)
CELREM_R = 1.0 - ((MXCELLR - CELL_KGR)/MXCELLR)
!
! Delete intermediate variables:
!
DELETE FE_KGR, CELL_KGR, MXFER, MXCELLR
!
!*****
!
!   Param 161: Cumulative Brineflow into Waste Panel excl. Borehole --> BRWI_XBH
!   Param 162: (Salado brine inflow)/(total brine inflow) at DRZ -----> SAL_BR_T
!   Param 163: (Salado br. inflow)/(unconsumed br. inflow) at DRZ -----> SAL_BR_U
!   Param 164: (Salado br. inflow)/(total br. in.) at Waste Panel -----> SB_TB_WP
!   Param 165: (Salado br. in.)/(unconsumed br. in.) at Waste Panel --> SB_UB_WP
!
!*****
!
! Cumulative brine inflow into Waste Panel, excluding Borehole
!
!   Bottom except for Borehole
!
BRWI_X  = IFGT0(FLOWBRY[E:596],FLOWBRY[E:596],0.0)
BRWI_X  = BRWI_X + IFGT0(FLOWBRY[E:597],FLOWBRY[E:597],0.0)
BRWI_X  = BRWI_X + IFGT0(FLOWBRY[E:598],FLOWBRY[E:598],0.0)
```



```
BRWI_X = BRWI_X + IFGT0(FLOWBRY[E:600],FLOWBRY[E:600],0.0)
BRWI_X = BRWI_X + IFGT0(FLOWBRY[E:601],FLOWBRY[E:601],0.0)
BRWI_X = BRWI_X + IFGT0(FLOWBRY[E:602],FLOWBRY[E:602],0.0)
!
!   Top except for Borehole
!
BRWI_X = BRWI_X + IFLT0(FLOWBRY[E:468],-1.0*FLOWBRY[E:468],0.0)
BRWI_X = BRWI_X + IFLT0(FLOWBRY[E:469],-1.0*FLOWBRY[E:469],0.0)
BRWI_X = BRWI_X + IFLT0(FLOWBRY[E:470],-1.0*FLOWBRY[E:470],0.0)
BRWI_X = BRWI_X + IFLT0(FLOWBRY[E:472],-1.0*FLOWBRY[E:472],0.0)
BRWI_X = BRWI_X + IFLT0(FLOWBRY[E:473],-1.0*FLOWBRY[E:473],0.0)
BRWI_X = BRWI_X + IFLT0(FLOWBRY[E:474],-1.0*FLOWBRY[E:474],0.0)
!
!   Left side
!
BRWI_X = BRWI_X + IFGT0(FLOWBRX[E:596],FLOWBRX[E:596],0.0)
BRWI_X = BRWI_X + IFGT0(FLOWBRX[E:603],FLOWBRX[E:603],0.0)
BRWI_X = BRWI_X + IFGT0(FLOWBRX[E:610],FLOWBRX[E:610],0.0)
!
!   Right side
!
BRWI_X = BRWI_X + IFLT0(FLOWBRX[E:602],-1.0*FLOWBRX[E:602],0.0)
BRWI_X = BRWI_X + IFLT0(FLOWBRX[E:609],-1.0*FLOWBRX[E:609],0.0)
BRWI_X = BRWI_X + IFLT0(FLOWBRX[E:616],-1.0*FLOWBRX[E:616],0.0)
!
!   Accumulate over time
!
BRWI_XBH = INTRIGHT(BRWI_X)
!
DELETE BRWI_X
!
!*****
!
! (Salado brine inflow)/(total brine inflow) at DRZ
!
!   Define a dummy denominator to avoid dividing by zero
!
DENDUM05 = BRAALIC + BNBHLDRZ + BNBHDNUZ
DENDUM06 = IFEQ0(DENDUM05,1.0,DENDUM05)
!
SAL_BR_T = BRAALIC/DENDUM06
!
DELETE DENDUM05, DENDUM06
!
!*****
!
! (Salado brine inflow)/(unconsumed brine inflow) at DRZ
!
!   Define a dummy denominator to avoid dividing by zero
!
DENDUM07 = BRAALIC + BNBHLDRZ + BNBHDNUZ - BRN_RMV
DENDUM08 = IFEQ0(DENDUM07,1.0,DENDUM07)
!
SAL_BR_U = BRAALIC/DENDUM08
!
DELETE DENDUM07, DENDUM08
!
!*****
!
! (Salado brine inflow)/(total brine inflow) at Waste Panel
!
!   Define a dummy denominator to avoid dividing by zero
!
DENDUM09 = BRWI_XBH + BRNBHDNC + BRNBHUPP
DENDUM10 = IFEQ0(DENDUM09,1.0,DENDUM09)
!
```

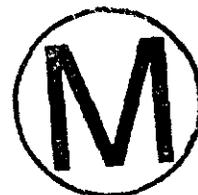


```
SB_TB_WP = BRWI_XBH/DENDUM10
!
DELETE DENDUM09, DENDUM10
!
!*****
!
! (Salado brine inflow)/(unconsumed brine inflow) at Waste Panel
!
! Define a dummy denominator to avoid dividing by zero
!
DENDUM11 = BRWI_XBH + BRNBHDNC + BRNBHUPP - BRN_RMVW
DENDUM12 = IFEQ0(DENDUM11,1.0,DENDUM11)
!
SB_UB_WP = BRWI_XBH/DENDUM12
!
DELETE DENDUM11, DENDUM12
!
!*****
!*****
!
! Cumulative brineflow (m**3) vertically at Magenta Dolomite Member
!
! Param 166: Brineflow up shaft (@element 664) -----> BRNSHUMC
! Param 167: Brineflow up borehole (@element 777) -----> BRNBHUMC
!
!*****
!
! Cumulative brineflow up through shaft (at Magenta Member)
!
BRNSHUM = IFGT0(FLOWBRY[E:664],FLOWBRY[E:664],0.0)
BRNSHUMC = INTRIGHT(BRNSHUM)
!
!*****
!
! Cumulative brineflow up borehole (at Magenta Member)
!
BRNBHUM = IFGT0(FLOWBRY[E:777],FLOWBRY[E:777],0.0)
BRNBHUMC = INTRIGHT(BRNBHUM)
!
!*****
!
! Clean up output--limit to requested quantities
!
DELETE BRNSHUM, BRNBHUM
!
!*****
!*****
!
! Total outward brineflow in marker beds across land-withdrawal boundary (m**3)
!
! Param 168: MB 138, North --> BRM38NLW
! Param 169: Anhydrite A&B, North --> BRAABNLW
! Param 170: MB 139, North --> BRM39NLW
! Param 171: MB 138, South --> BRM38SLW
! Param 172: Anhydrite A&B, South --> BRAABSLW
! Param 173: MB 139, South --> BRM39SLW
! Param 174: all marker beds -----> BRAALLWC
!
!*****
!
! Total outward brineflow in MB 138 across l-w boundary, north (right) side
!
BRNM38N0 = IFGT0(FLOWBRX[E:594],FLOWBRX[E:594],0.0)
BRM38NLW = INTRIGHT(BRNM38N0)
!
!*****
```

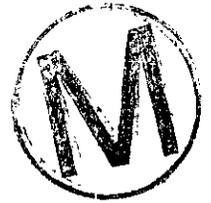


```
!  
! Total outward brineflow in Anhydrite A&B across l-w boundary, north side  
!  
BRNAABN0 = IFGT0(FLOWBRX[E:562],FLOWBRX[E:562],0.0)  
BRAABNLW = INTRIGHT(BRNAABN0)  
!  
!*****  
!  
! Total outward brineflow in MB 139 across l-w boundary, north (right) side  
!  
BRNM39N0 = IFGT0(FLOWBRX[E:546],FLOWBRX[E:546],0.0)  
BRM39NLW = INTRIGHT(BRNM39N0)  
!  
!*****  
!*****  
!  
! Total outward brineflow in MB 138 across l-w boundary, south (left) side  
!  
BRNM38S0 = IFLT0(FLOWBRX[E:566],-1.0*FLOWBRX[E:566],0.0)  
BRM38SLW = INTRIGHT(BRNM38S0)  
!  
!*****  
!  
! Total outward brineflow in Anhydrite A&B across l-w boundary, south side  
!  
BRNAABS0 = IFLT0(FLOWBRX[E:550],-1.0*FLOWBRX[E:550],0.0)  
BRAABSLW = INTRIGHT(BRNAABS0)  
!  
!*****  
!  
! Total outward brineflow in MB 139 across l-w boundary, south (left) side  
!  
BRNM39S0 = IFLT0(FLOWBRX[E:534],-1.0*FLOWBRX[E:534],0.0)  
BRM39SLW = INTRIGHT(BRNM39S0)  
!  
!*****  
!  
! Total outward brineflow in all anhydrite layers across l-w boundary  
!  
BRAALLWC = BRM38NLW + BRAABNLW + BRM39NLW + BRM38SLW + BRAABSLW + BRM39SLW  
!  
!*****  
!  
! Clean up output--limit to requested quantities  
!  
DELETE BRNM38N0, BRNAABN0, BRNM39N0, BRNM38S0, BRNAABS0, BRNM39S0  
!  
!*****  
!*****  
!  
! Contributions of gas generated from each source (%/100)  
!  
! Param 175: Fraction of total gas due to steel corrosion -----> FR_TG_C  
! Param 176: Fraction of total gas due to total microbial -----> FR_TG_M  
! Param 177: Fraction of total gas due to humid microbial -----> FR_TG_H  
! Param 178: Fraction of total gas due to inundated microbial -----> FR_TG_I  
! Param 179: Fraction of microbial gas from humid conditions -----> FR_MG_H  
! Param 180: Fraction of microbial gas from inundated conditions ---> FR_MG_I  
!  
!*****  
!  
! Fraction of total gas due to steel corrosion  
!  
! Check total amount of gas to avoid subsequent divide by zero (if total gas  
! is equal to zero, then divide by one since fraction will be zero)  
!  
!
```

```
GAS_SUM = IFEQ0(GAS_MOLE,1.0,GAS_MOLE)
!
! Check total amount of microbial-generated gas to avoid divide by zero
!
GM_SUM = IFEQ0(C_M_HI_T,1.0,C_M_HI_T)
!
FR_TG_C = FE_MOLE/GAS_SUM
!
!*****
!
! Fraction of total gas due to total microbial degradation
!
FR_TG_M = 1.0 - FR_TG_C
!
!*****
!
! Fraction of total gas due to humid microbial degradation
!
FR_TG_H = FR_TG_M*(CELL_M_H/GM_SUM)
!
!*****
!
! Fraction of total gas due to inundated microbial degradation
!
FR_TG_I = FR_TG_M*(1.0 - (CELL_M_H/GM_SUM))
!
!*****
!
! Fraction of microbial gas due to humid conditions
!
FR_MG_H = CELL_M_H/GM_SUM
!
!*****
!
! Fraction of microbial gas due to inundated conditions
!
FR_MG_I = 1.0 - (CELL_M_H/GM_SUM)
!
!*****
!
! Delete temporary variables
!
DELETE GAS_SUM, GM_SUM
!
!*****
!*****
!
! Cumulative brineflow (m**3) across panel seal
!
! Param 181: Total brineflow into waste panel -----> BRNPSIWC
! Param 182: Total brineflow into rest of repository --> BRNPSIRC
! Param 183: Net brineflow out of waste panel -----> BRNPSOWC
! Param 184: Net brineflow out of rest of repository --> BRNPSORC
! Param 185: Net brineflow into waste panel -----> BRNPSNWC
! Param 186: Net brineflow into rest of repository ----> BRNPSNRC
!
!*****
!
! Total cumulative brineflow across panel seal into waste panel
!
BRNPSIW = IFLT0(FLOWBRX[E:638],-1.0*FLOWBRX[E:638],0.0)
BRNPSIW = BRNPSIW + IFLT0(FLOWBRX[E:639],-1.0*FLOWBRX[E:639],0.0)
BRNPSIW = BRNPSIW + IFLT0(FLOWBRX[E:640],-1.0*FLOWBRX[E:640],0.0)
!
BRNPSIWC = INTRIGHT(BRNPSIW)
!
```



```
DELETE BRNPSIW
!
!*****
!
! Total cumulative brineflow across panel seal into rest of repository
!
BRNPSIR = IFGT0 (FLOWBRX[E:617],FLOWBRX[E:617],0.0)
BRNPSIR = BRNPSIR + IFGT0 (FLOWBRX[E:620],FLOWBRX[E:620],0.0)
BRNPSIR = BRNPSIR + IFGT0 (FLOWBRX[E:623],FLOWBRX[E:623],0.0)
!
BRNPSIRC = INTRIGHT (BRNPSIR)
!
DELETE BRNPSIR
!
!*****
!
! Total cumulative brineflow across panel seal out of waste panel
!
BRNPSOW = IFGT0 (FLOWBRX[E:638],FLOWBRX[E:638],0.0)
BRNPSOW = BRNPSOW + IFGT0 (FLOWBRX[E:639],FLOWBRX[E:639],0.0)
BRNPSOW = BRNPSOW + IFGT0 (FLOWBRX[E:640],FLOWBRX[E:640],0.0)
!
BRNPSOWC = INTRIGHT (BRNPSOW)
!
DELETE BRNPSOW
!
!*****
!
! Total cumulative brineflow across panel seal out of rest of repository
!
BRNPSOR = IFLT0 (FLOWBRX[E:617],-1.0*FLOWBRX[E:617],0.0)
BRNPSOR = BRNPSOR + IFLT0 (FLOWBRX[E:620],-1.0*FLOWBRX[E:620],0.0)
BRNPSOR = BRNPSOR + IFLT0 (FLOWBRX[E:623],-1.0*FLOWBRX[E:623],0.0)
!
BRNPSORC = INTRIGHT (BRNPSOR)
!
DELETE BRNPSOR
!
!*****
!
! Net inflow of brine across panel seal into waste panel
!
BRNPSNWC = BRNPSIWC - BRNPSOWC
!
!*****
!
! Net inflow of brine across panel seal into waste panel
!
BRNPSNRC = BRNPSIRC - BRNPSORC
!
!*****
!*****
!
LIMIT ELEMENT OFF
!
DELETE GRIDVOL
!
!*****
!*****
END
```



APPENDIX F: EXAMPLE OF PANEL'S OUTPUT DBG FILE

Explanatory comments, which do not ordinarily appear on PANEL's DBG files, are inserted on the DBG file that follows. The are intended to assist the reader and are printed in *italics* so as to set them off.

PANEL_PA96 3.60 PROD PA96 05/17/96 06/14/96 13:58:20

PPPPPP	AAAAA	N	NN	EEEEEEE	LL	PPPPPP	AAAAA	9999	6666					
PP	PP	AA	AA	NN	NN	EE	LL	PP	PP	AA	AA	9	9	6
PP	PP	AA	AA	NNN	NN	EE	LL	PP	PP	AA	AA	9	9	6
PPPPPP	AAAAAAA	NN	N	NN	EEEE	LL	PPPPPP	AAAAAAA	99999	66666				
PP	AA	AA	NN	NNN	EE	LL	PP	AA	AA	9	6	6		
PP	AA	AA	NN	NN	EE	LL	PP	AA	AA	9	6	6		
PP	AA	AA	NN	N	EEEEEE	LLLLLLL	PP	AA	AA	9999	6666			

PANEL_PA96 Version 3.60
PROD PA96 Built 05/17/96
Written by JIM GARNER
Sponsored by JIM GARNER

Run on 06/14/96 at 13:58:20
Run on ALPHA AXP BONNIE OpenVMS V6.1



Prepared for
Sandia National Laboratories
Albuquerque, New Mexico 87185-5800
for the United States Department of Energy
under Contract DE-AC04-76DP00789

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Explanatory Comment: The section that follows this comment echoes PANEL's input data and includes: (i) the values of arg1 through arg5 (see Chapter 6), namely: the run type plus four file specifications. It is arranged in twelve rows and includes file names, plus dates of origin of the two external files. (ii) The next row gives the number of seconds per year. (iii) The next six rows give the log to the base 10 of the solubilities (in moles/l), which are called LOGSOLM on the CAMDAT data base and are provided by ALGEBRA. (iv) In the next several dozen rows are given the initial inventories (in Curies) of contact-handled (INVCHD) and remote-handled (INVRHD) radioisotopes (note that unfound isotopes are set to zero inventory by default); (v) a three-column, 73-row listing of (1) time (in seconds) from zero to 10,000 years, (2) cumulative brine outflow from the repository (in m³) from BRAGFLO, and (3) volume of brine in the repository (in m³) from BRAGFLO (modified as required to conform to a 1000-m³ minimum); (vi) a one-row listing of (a) the panel index, which has no meaning or purpose in CCA runs and is set to unity, and (b) an initial time index, which is set to zero at the time of decommissioning; (vii) a 6-row, three-column listing of the elements PANEL will mobilize giving (1) the solubility for sorption onto large colloids (set to zero in CCA runs), (2) the solubility for sorption onto small colloids (set to zero in CCA runs), and (3) the solubilities by enhanced equivalent dissolution, in moles/l; (viii) a two-row listing of data that are unused in CCA runs, (ix) a 30-row (one row for each PANEL isotope), 7-column listing of (1) the numerical index from 1 to 30, (2) isotope identification, (3) half-life in years, (4) identification of daughter decay product, (5) the radioactivity of that isotope in Curies/mole, (6) the radioactivity of that isotope in Curies per kilogram, (7) the total WIPP inventory of that isotope in Curies, and (8) the total WIPP inventory of that isotope in kilograms; and (x) a final row stating the total initial inventory of the WIPP repository based on all transuranic alpha emitters having half lives greater than 20 years.

End of Comment.

FILE ASSIGNMENTS:

TYPE OF RUN, S=standard, R=radialysis, D=decay only:

S

CAMDAT data base:

BONNIESCCAL_WORKROOT: [PANEL.DATA.R1S6V23]ALG_ST_CCA_R1_S6_V023.CDB;1
Written on 06/02/96 19:59:16

output CAMDAT data base:

BONNIESCCAL_WORKROOT: [PANEL.DATA.R1S6V23]PANEL_CCA_R1_S6_V023.CDB

FLUX FILES FROM BRAGFLO:

BONNIESCCAL_WORKROOT: [PANEL.DATA.R1S6V23]BF_POSTALG_CCA_R1_S6_V023.CDB;1
Written on 06/10/96 20:21:36

diagnostics file:

BONNIESCCAL_WORKROOT: [PANEL.DATA.R1S6V23]PANEL_CCA_R1_S6_V023.DBG

FROM CDB, REFCON	YRSEC	3.1557E+07
FROM CDB, TH	LOGSOLM	-7.0535E+00
FROM CDB, U	LOGSOLM	-5.0733E+00
FROM CDB, NP	LOGSOLM	-4.5430E+00
FROM CDB, PU	LOGSOLM	-7.0651E+00
FROM CDB, AM	LOGSOLM	-6.4662E+00
FROM CDB, CM	LOGSOLM	-6.4662E+00
FROM CDB, SR90	INVCHD	6.8500E+03
FROM CDB, SR90	INVRHD	2.0900E+05
FROM CDB, CS137	INVCHD	8.0600E+03
FROM CDB, CS137	INVRHD	2.1600E+05
FROM CDB, PB210	INVCHD	2.5500E+00
FROM CDB, PB210	INVRHD	7.1600E-06
FROM CDB, RA226	INVCHD	1.1600E+01
FROM CDB, RA226	INVRHD	3.5800E-05
FROM CDB, RA228	INVCHD	7.4700E-01
FROM CDB, RA228	INVRHD	7.7700E-02
FROM CDB, TH229	INVCHD	2.8800E+00
FROM CDB, TH229	INVRHD	1.1700E-01
FROM CDB, TH230	INVCHD	8.0600E-02
FROM CDB, TH230	INVRHD	7.5600E-03
FROM CDB, TH232	INVCHD	9.1300E-01
FROM CDB, TH232	INVRHD	9.2500E-02
FROM CDB, PA231	INVCHD	4.5100E-01
FROM CDB, PA231	INVRHD	1.9100E-03



FROM CDB, U233	INVCHD	1.7900E+03		
FROM CDB, U233	INVRHD	1.5800E+02		
FROM CDB, U234	INVCHD	4.6500E+02		
FROM CDB, U234	INVRHD	4.2700E+01		
FROM CDB, U235	INVCHD	1.2800E+01		
FROM CDB, U235	INVRHD	4.6300E+00		
FROM CDB, U236	INVCHD	3.3300E-01		
FROM CDB, U236	INVRHD	9.6800E-02		
FROM CDB, U238	INVCHD	3.9600E+01		
FROM CDB, U238	INVRHD	1.0500E+01		
FROM CDB, NP237	INVCHD	5.6100E+01		
FROM CDB, NP237	INVRHD	2.8500E+00		
FROM CDB, PU238	INVCHD	2.6100E+06		
FROM CDB, PU238	INVRHD	1.4500E+03		
FROM CDB, PU239	INVCHD	7.8500E+05		
FROM CDB, PU239	INVRHD	1.0300E+04		
FROM CDB, PU240	INVCHD	2.1000E+05		
FROM CDB, PU240	INVRHD	5.0700E+03		
FROM CDB, PU241	INVCHD	2.3100E+06		
FROM CDB, PU241	INVRHD	1.4200E+05		
FROM CDB, PU242	INVCHD	1.1700E+03		
FROM CDB, PU242	INVRHD	1.5000E-01		
FROM CDB, PU244	INVCHD	1.5000E-06		
FROM CDB, PU244	INVRHD	2.2100E-11		
FROM CDB, AM241	INVCHD	4.4200E+05		
FROM CDB, AM241	INVRHD	5.9600E+03		
FROM CDB, CM244	INVCHD	3.1500E+04		
FROM CDB, CM244	INVRHD	3.1500E+02		
FROM CDB, CM248	INVCHD	8.9500E-02		
FROM CDB, CM248	INVRHD	2.0500E-04		
FROM CDB, CF252	INVCHD	2.3900E+02		
FROM CDB, CF252	INVRHD	1.2900E+00		
FROM CDB, PM147	INVCHD	7.8700E+00		
FROM CDB, PM147	INVRHD	1.0700E+01		
ELBNAM SMI47	AND PROPNAM INVCHD	NOT FOUND!!	SET TO	0.000E+00
ELBNAM SMI47	AND PROPNAM INVRHD	NOT FOUND!!	SET TO	0.000E+00
FROM CDB, AM243	INVCHD	3.2600E+01		
FROM CDB, AM243	INVRHD	2.2800E-04		
FROM CDB, CM243	INVCHD	2.7200E+00		
FROM CDB, CM243	INVRHD	4.9500E+01		
FROM CDB, CM245	INVCHD	1.1500E+02		
FROM CDB, CM245	INVRHD	1.4600E-06		
1	0.0000E+00	0.0000E+00	1.0000E+03	
2	7.0909E+03	1.3455E-10	1.0000E+03	
3	6.9351E+05	1.1810E-08	1.0000E+03	
4	3.0444E+07	2.3075E-07	1.0000E+03	
5	2.2386E+08	9.2151E-07	1.1838E+03	
6	3.1569E+08	1.1035E-06	1.2347E+03	
7	3.2622E+08	1.1226E-06	1.2401E+03	
8	7.8892E+08	1.7046E-06	1.4220E+03	
9	7.8938E+08	1.7051E-06	1.4222E+03	
10	8.2954E+08	1.7438E-06	1.4357E+03	
11	1.5778E+09	2.2735E-06	1.6603E+03	
12	1.5789E+09	2.2741E-06	1.6606E+03	
13	1.6770E+09	2.3283E-06	1.6881E+03	
14	3.1557E+09	2.8999E-06	2.0817E+03	
15	3.1571E+09	2.9003E-06	2.0820E+03	
16	3.2797E+09	2.9364E-06	2.1138E+03	
17	4.4737E+09	3.2248E-06	2.4182E+03	
18	4.5101E+09	3.2325E-06	2.4274E+03	
19	6.3114E+09	3.5390E-06	2.8754E+03	
20	6.3119E+09	3.5390E-06	2.8755E+03	
21	6.3520E+09	3.5449E-06	2.8854E+03	
22	6.7391E+09	3.5987E-06	2.9805E+03	
23	7.2882E+09	3.6694E-06	3.1148E+03	
24	8.5446E+09	3.8106E-06	3.4172E+03	



25	1.0732E+10	4.0056E-06	3.9304E+03						
26	1.1244E+10	4.0457E-06	4.0395E+03						
27	1.2486E+10	4.1342E-06	4.2385E+03						
28	1.2623E+10	4.1434E-06	4.2147E+03						
29	1.2632E+10	4.1439E-06	4.2139E+03						
30	1.2680E+10	4.1472E-06	4.2190E+03						
31	1.3110E+10	4.1743E-06	4.1700E+03						
32	1.3574E+10	4.2030E-06	4.1125E+03						
33	1.4459E+10	5.1364E-06	4.0265E+03						
34	1.7279E+10	6.1555E-06	3.8144E+03						
35	2.8169E+10	1.2136E-05	3.3158E+03						
36	3.1557E+10	1.2136E-05	3.2414E+03						
37	3.1557E+10	1.2136E-05	3.2414E+03						
38	3.1557E+10	1.2136E-05	3.2414E+03						
39	3.1557E+10	1.2136E-05	3.2414E+03						
40	3.1557E+10	1.2136E-05	3.2420E+03						
41	3.1596E+10	1.2136E-05	3.2927E+03						
42	3.2488E+10	1.2136E-05	3.6356E+03						
43	3.4302E+10	1.2136E-05	3.6149E+03						
44	3.7428E+10	1.2136E-05	3.6104E+03						
45	3.9652E+10	1.2136E-05	3.6314E+03						
46	4.3479E+10	1.2136E-05	3.7210E+03						
47	4.3933E+10	1.2136E-05	3.7426E+03						
48	4.6069E+10	1.2136E-05	3.8196E+03						
49	4.9520E+10	1.2136E-05	3.9900E+03						
50	5.3592E+10	1.2136E-05	4.1723E+03						
51	5.6446E+10	1.2136E-05	4.2664E+03						
52	6.3114E+10	1.2136E-05	4.4583E+03						
53	6.3114E+10	1.2136E-05	4.4713E+03						
54	6.3118E+10	1.2136E-05	5.1120E+03						
55	6.3372E+10	1.2136E-05	5.2406E+03						
56	6.9425E+10	1.2136E-05	4.7056E+03						
57	6.9426E+10	1.2136E-05	4.7056E+03						
58	6.9476E+10	1.2136E-05	4.7080E+03						
59	7.3830E+10	1.2136E-05	4.8012E+03						
60	8.8820E+10	1.2136E-05	5.0775E+03						
61	1.0098E+11	1.3066E+02	5.2020E+03						
62	1.0098E+11	1.3083E+02	5.2021E+03						
63	1.0128E+11	1.4678E+02	5.2072E+03						
64	1.0979E+11	8.6931E+02	5.2682E+03						
65	1.2583E+11	3.1457E+03	5.3303E+03						
66	1.4125E+11	5.9569E+03	5.3494E+03						
67	1.6228E+11	9.9205E+03	5.3267E+03						
68	1.9684E+11	1.6271E+04	5.2509E+03						
69	2.3140E+11	2.2559E+04	5.1746E+03						
70	2.6596E+11	2.8795E+04	5.0981E+03						
71	3.0052E+11	3.4789E+04	5.0619E+03						
72	3.1557E+11	3.7294E+04	5.0531E+03						
73	3.2557E+11	3.7294E+04	5.0531E+03						
IPANEL, TZERO= 1 0.0									
SOLS	TH	0.0000E+00	0.0000E+00	8.8400E-08					
SOLS	U	0.0000E+00	0.0000E+00	8.4470E-06					
SOLS	NP	0.0000E+00	0.0000E+00	2.8642E-05					
SOLS	PU	0.0000E+00	0.0000E+00	8.6083E-08					
SOLS	AM	0.0000E+00	0.0000E+00	3.4184E-07					
SOLS	CM	0.0000E+00	0.0000E+00	3.4184E-07					
SOL3, SOL4, SOL5, SOL6 = 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00									
RAN1, RAN2, RAN3, RAN4 = 1.000E-01 5.000E-01 5.000E-01 5.000E-01									
1	IDION	RHL	IDAUG	CUPMO	CUPKG	WIPP	CURIES	WIPP	KG
1	SR-90	2.9120E+01		1.2277E+04	1.3641E+05	0	2.1585E+05	1.5824E+00	
2	CS-137	3.0000E+01		1.1917E+04	8.6982E+04	0	2.2406E+05	2.5759E+00	
3	PB-210	2.2300E+01		1.6031E+04	7.6339E+04	0	2.5500E+00	3.3404E-05	
4	RA-226	1.6000E+03	PB-210	2.2344E+02	9.8865E+02	1	1.1600E+01	1.1733E-02	
5	RA-228	5.7500E+00		6.2173E+04	2.7269E+05	0	8.2470E-01	3.0243E-06	
6	TH-229	7.3400E+03		4.8705E+01	2.1269E+02	1	2.9970E+00	1.4091E-02	
7	TH-230	7.7000E+04	RA-226	4.6428E+00	2.0186E+01	1	8.8160E-02	4.3673E-03	

8	TH-232	1.4050E+10	RA-228	2.5445E-05	1.0968E-04	1	1.0055E+00	9.1680E+03
9	PA-231	3.2760E+04		1.0913E+01	4.7241E+01	1	4.5291E-01	9.5873E-03
10	U -233	1.5850E+05	TH-229	2.2555E+00	9.6803E+00	1	1.9480E+03	2.0123E+02
11	U -234	2.4450E+05	TH-230	1.4622E+00	6.2485E+00	1	5.0770E+02	8.1251E+01
12	U -235	7.0380E+08	PA-231	5.0795E-04	2.1615E-03	1	1.7430E+01	8.0638E+03
13	U -236	2.3420E+07	TH-232	1.5265E-02	6.4681E-02	1	4.2980E-01	6.6450E+00
14	U -238	4.4680E+09	U -234	8.0013E-05	3.3619E-04	1	5.0100E+01	1.4902E+05
15	NP-237	2.1400E+06	U -233	1.6705E-01	7.0487E-01	1	5.8950E+01	8.3632E+01
16	PU-238	8.7740E+01	U -234	4.0745E+03	1.7120E+04	1	2.6115E+06	1.5254E+02
17	PU-239	2.4070E+04	U -235	1.4852E+01	6.2144E+01	1	7.9530E+05	1.2798E+04
18	PU-240	6.5370E+03	U -236	5.4688E+01	2.2787E+02	1	2.1507E+05	9.4384E+02
19	PU-241	1.4400E+01	AM-241	2.4826E+04	1.0301E+05	0	2.4520E+06	2.3803E+01
20	PU-242	3.7630E+05	U -238	9.5003E-01	3.9258E+00	1	1.1702E+03	2.9807E+02
21	PU-244	8.2600E+07	PU-240	4.3281E-03	1.7738E-02	1	1.5000E-06	8.4566E-05
22	AM-241	4.3220E+02	NP-237	8.2716E+02	3.4322E+03	1	4.4796E+05	1.3052E+02
23	CM-244	1.8110E+01	PU-240	1.9740E+04	8.0903E+04	0	3.1815E+04	3.9325E-01
24	CM-248	3.3900E+05	PU-244	1.0546E+00	4.2523E+00	1	8.9705E-02	2.1096E-02
25	CF-252	2.6380E+00	CM-248	1.3552E+05	5.3777E+05	0	2.4029E+02	4.4683E-04
26	PM-147	2.6234E+00	SM-147	1.3627E+05	9.2702E+05	0	1.8570E+01	2.0032E-05
27	SM-147	1.0600E+11		3.3726E-06	2.2943E-05	1	0.0000E+00	0.0000E+00
28	AM-243	7.3700E+03	PU-239	4.8507E+01	1.9962E+02	1	3.2600E+01	1.6331E-01
29	CM-243	2.9100E+01	PU-239	1.2285E+04	5.0556E+04	1	5.2220E+01	1.0329E-03
30	CM-245	8.5300E+03	PU-241	4.1911E+01	1.7106E+02	1	1.1500E+02	6.7226E-01

0 TOTAL CURIES OF ALPHA EMITTERS WITH HALF-LIFE > 20 YEARS = 4.0737E+06



Explanatory Comment: The data that follow are the scenario-revised initial inventory for PANEL. This step is designed to reduce PANEL's working inventory to accommodate scenarios in which only a fraction of the repository's contents are wetted. Only one standard panel is wetted by brine. Consequently, the scale of the run is set at 0.1044, which represents the area of one standard panel divided by the area of the entire repository. The initial inventory is a one-for-one echo of the entire inventory reported above, with the exception that PANEL has deleted SM-147 from the list. That is because its net individual inventory on the given inventory list is zero and it is not generated as a result of decay. The initial-inventory data are listed as a 6-column, 29-row matrix. The first column identifies the isotope. The 2nd column states its half-life. The third column gives the total initial inventory in Curies and matches identically the 6th column in the preceding data matrix. The fourth column lists the same data in kilograms and matches identically the 7th column in the matrix above. The fifth and sixth columns match the third and fourth columns, but are smaller by a factor of 0.1044, which is the scaling factor listed on the second line below and represents the fact that the contents of only one panel of the repository are accessible. *End of comment.*

1
 0 INITIAL CONDITIONS FOR PANEL # 1
 SCALE OF THIS RUN= 0.1044

ISOTOPE	HL	WIPP INVENTORY		SCALED INVENTORY	
		CURIES	KG	CURIES	KG
SR-90	2.912E+01	2.159E+05	1.582E+00	2.253E+04	1.652E-01
CS-137	3.000E+01	2.241E+05	2.576E+00	2.339E+04	2.689E-01
PB-210	2.230E+01	2.550E+00	3.340E-05	2.662E-01	3.487E-06
RA-226	1.600E+03	1.160E+01	1.173E-02	1.211E+00	1.225E-03
RA-228	5.750E+00	8.247E-01	3.024E-06	8.609E-02	3.157E-07
TH-229	7.340E+03	2.997E+00	1.409E-02	3.129E-01	1.471E-03
TH-230	7.700E+04	8.816E-02	4.367E-03	9.203E-03	4.559E-04
TH-232	1.405E+10	1.005E+00	9.168E+03	1.050E-01	9.571E+02
PA-231	3.276E+04	4.529E-01	9.587E-03	4.728E-02	1.001E-03
U -233	1.585E+05	1.948E+03	2.012E+02	2.034E+02	2.101E+01
U -234	2.445E+05	5.077E+02	8.125E+01	5.300E+01	8.482E+00
U -235	7.038E+08	1.743E+01	8.064E+03	1.820E+00	8.418E+02
U -236	2.342E+07	4.298E-01	6.645E+00	4.487E-02	6.937E-01
U -238	4.468E+09	5.010E+01	1.490E+05	5.230E+00	1.556E+04
NP-237	2.140E+06	5.895E+01	8.363E+01	6.154E+00	8.730E+00
PU-238	8.774E+01	2.611E+06	1.525E+02	2.726E+05	1.592E+01
PU-239	2.407E+04	7.953E+05	1.280E+04	8.302E+04	1.336E+03
PU-240	6.537E+03	2.151E+05	9.438E+02	2.245E+04	9.853E+01
PU-241	1.440E+01	2.452E+06	2.380E+01	2.560E+05	2.485E+00
PU-242	3.763E+05	1.170E+03	2.981E+02	1.222E+02	3.112E+01
PU-244	8.260E+07	1.500E-06	8.457E-05	1.566E-07	8.828E-06
AM-241	4.322E+02	4.480E+05	1.305E+02	4.676E+04	1.362E+01
CM-244	1.811E+01	3.181E+04	3.932E-01	3.321E+03	4.105E-02
CM-248	3.390E+05	8.971E-02	2.110E-02	9.364E-03	2.202E-03
CF-252	2.638E+00	2.403E+02	4.468E-04	2.508E+01	4.664E-05
PM-147	2.623E+00	1.857E+01	2.003E-05	1.939E+00	2.091E-06
AM-243	7.370E+03	3.260E+01	1.633E-01	3.403E+00	1.705E-02
CM-243	2.910E+01	5.222E+01	1.033E-03	5.451E+00	1.078E-04
CM-245	8.530E+03	1.150E+02	6.723E-01	1.200E+01	7.018E-02



Explanatory Comment: The remaining data represent a summary overview synopsis of the results of PANEL's calculations. The data are presented in eleven similarly-structured clusters herein printed as three-clusters-per-two-pages after this first page. Each cluster conforms to the following format: The first row identifies the timestep in years and the volume (in m³) of brine in the repository. The next six rows are a five-column summary of the mobilization. The first column represents an effective dissolution solubility (in moles/l) for all isotopes of the element combined in that it, multiplied by the brine volume (converted from m³ to l, and assuming mobilization is NOT inventory limited) gives the amount in the third column, which is the overall amount (in moles) of all isotopes of that element in solution during that timestep. If mobilization is inventory limited, the limit will appear in the third column. The second column represents the inventory available for mobilization (in moles). The next column is the amounts of that element dissolved on the basis of the enhanced equivalent solubility during that time step. The last two columns are not used in CCA runs and list zeros. The final column is a flag that signals (if it is one) that the entire available inventory of that element has been mobilized during that timestep (as is the case for NP and CM during the second timestep [i.e., time = 100years]), or (if it is zero) that stocks of unmobilized inventory remain at the end of that timestep. The next grouping is a 30-row, eight-column matrix that lists the symbol for the isotope followed by the results of the release during that timestep. The 2nd and 3rd columns are not used in CCA runs. The fourth column gives the amount of that isotope released via enhanced equivalent dissolution (in Kg) during that timestep. The next two columns give the remaining inventory in Curies and kilograms. The last two columns give the sum of the first three columns first in Curies and then in kilograms. The final row of the data cluster gives the integrated (from t = 0) brine outflow from the repository in m³. End of Comment.

1 TIME= 0. YEARS, BRINE VOLUME= 1000. M**3							
0 ELEMENT	SOLUBILITY	LOADING	DISOLVED	LARGE COL	SMALL COL		
TH	8.840E-08	4.125E+03	8.840E-02	0.000E+00	0.000E+00	0	0
U	8.447E-06	6.909E+04	8.447E+00	0.000E+00	0.000E+00	0	0
NP	2.864E-05	3.926E+01	2.864E+01	0.000E+00	0.000E+00	0	0
PU	8.608E-08	6.185E+03	8.608E-02	0.000E+00	0.000E+00	0	0
AM	3.418E-07	5.887E+01	3.418E-01	0.000E+00	0.000E+00	0	0
CM	3.418E-07	3.917E-01	3.418E-01	0.000E+00	0.000E+00	0	0
0 ISOTOPE	AMOUNT RELEASED (KG)			INVENTORY REMAINING		TOTAL RELEASED	
	LARGE COL	SMALL COL	DISOLVED	CURIES	KG	CURIES	KG
SR-90	0.000E+00	0.000E+00	0.000E+00	2.253E+04	1.652E-01	0.000E+00	0.000E+00
CS-137	0.000E+00	0.000E+00	0.000E+00	2.339E+04	2.689E-01	0.000E+00	0.000E+00
PB-210	0.000E+00	0.000E+00	0.000E+00	2.562E-01	3.487E-06	0.000E+00	0.000E+00
RA-226	0.000E+00	0.000E+00	0.000E+00	1.211E+00	1.225E-03	0.000E+00	0.000E+00
RA-228	0.000E+00	0.000E+00	0.000E+00	8.609E-02	3.157E-07	0.000E+00	0.000E+00
TH-229	0.000E+00	0.000E+00	0.000E+00	3.129E-01	1.471E-03	0.000E+00	0.000E+00
TH-230	0.000E+00	0.000E+00	0.000E+00	9.203E-03	4.559E-04	0.000E+00	0.000E+00
TH-232	0.000E+00	0.000E+00	0.000E+00	1.050E-01	9.571E+02	0.000E+00	0.000E+00
PA-231	0.000E+00	0.000E+00	0.000E+00	4.728E-02	1.001E-03	0.000E+00	0.000E+00
U -233	0.000E+00	0.000E+00	0.000E+00	2.034E+02	2.101E+01	0.000E+00	0.000E+00
U -234	0.000E+00	0.000E+00	0.000E+00	5.300E+01	8.482E+00	0.000E+00	0.000E+00
U -235	0.000E+00	0.000E+00	0.000E+00	1.820E+00	8.418E+02	0.000E+00	0.000E+00
U -236	0.000E+00	0.000E+00	0.000E+00	4.487E-02	6.937E-01	0.000E+00	0.000E+00
U -238	0.000E+00	0.000E+00	0.000E+00	5.230E+00	1.556E+04	0.000E+00	0.000E+00
NP-237	0.000E+00	0.000E+00	0.000E+00	6.154E+00	8.730E+00	0.000E+00	0.000E+00
PU-238	0.000E+00	0.000E+00	0.000E+00	2.726E+05	1.592E+01	0.000E+00	0.000E+00
PU-239	0.000E+00	0.000E+00	0.000E+00	8.302E+04	1.336E+03	0.000E+00	0.000E+00
PU-240	0.000E+00	0.000E+00	0.000E+00	2.245E+04	9.853E+01	0.000E+00	0.000E+00
PU-241	0.000E+00	0.000E+00	0.000E+00	2.560E+05	2.485E+00	0.000E+00	0.000E+00
PU-242	0.000E+00	0.000E+00	0.000E+00	1.222E+02	3.112E+01	0.000E+00	0.000E+00
PU-244	0.000E+00	0.000E+00	0.000E+00	1.566E-07	8.828E-06	0.000E+00	0.000E+00
AM-241	0.000E+00	0.000E+00	0.000E+00	4.676E+04	1.362E+01	0.000E+00	0.000E+00
CM-244	0.000E+00	0.000E+00	0.000E+00	3.321E+03	4.105E-02	0.000E+00	0.000E+00
CM-248	0.000E+00	0.000E+00	0.000E+00	9.364E-03	2.202E-03	0.000E+00	0.000E+00
CF-252	0.000E+00	0.000E+00	0.000E+00	2.508E+01	4.664E-05	0.000E+00	0.000E+00
PM-147	0.000E+00	0.000E+00	0.000E+00	1.939E+00	2.091E-06	0.000E+00	0.000E+00
SM-147	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
AM-243	0.000E+00	0.000E+00	0.000E+00	3.403E+00	1.705E-02	0.000E+00	0.000E+00
CM-243	0.000E+00	0.000E+00	0.000E+00	5.451E+00	1.078E-04	0.000E+00	0.000E+00
CM-245	0.000E+00	0.000E+00	0.000E+00	1.200E+01	7.018E-02	0.000E+00	0.000E+00

SMFLOW0 0.000E+00
 1 TIME= 100. YEARS, BRINE VOLUME= 2082. M**3

0 ELEMENT	SOLUBILITY	LOADING	DISOLVED	LARGE COL	SMALL COL		
TH	8.840E-08	4.125E+03	1.840E-01	0.000E+00	0.000E+00	0	
U	8.447E-06	6.914E+04	1.758E+01	0.000E+00	0.000E+00	0	
NP	2.864E-05	4.864E+01	4.864E+01	0.000E+00	0.000E+00	1	
PU	8.608E-08	6.129E+03	1.792E-01	0.000E+00	0.000E+00	0	
AM	3.418E-07	5.506E+01	7.116E-01	0.000E+00	0.000E+00	0	
CM	3.418E-07	2.947E-01	2.947E-01	0.000E+00	0.000E+00	1	

0 ISOTOPE	AMOUNT RELEASED (KG)			INVENTORY REMAINING		TOTAL RELEASED	
	LARGE COL	SMALL COL	DISOLVED	CURIES	KG	CURIES	KG
SR-90	0.000E+00	0.000E+00	0.000E+00	2.085E+03	1.528E-02	0.000E+00	0.000E+00
CS-137	0.000E+00	0.000E+00	0.000E+00	2.321E+03	2.668E-02	0.000E+00	0.000E+00
PB-210	0.000E+00	0.000E+00	0.000E+00	1.134E+00	1.486E-05	0.000E+00	0.000E+00
RA-226	0.000E+00	0.000E+00	0.000E+00	1.161E+00	1.175E-03	0.000E+00	0.000E+00
RA-228	0.000E+00	0.000E+00	0.000E+00	1.050E-01	3.849E-07	0.000E+00	0.000E+00
TH-229	0.000E+00	0.000E+00	2.913E-16	2.221E+00	1.044E-02	6.196E-14	2.913E-16
TH-230	0.000E+00	0.000E+00	1.017E-16	8.405E-02	4.164E-03	2.053E-15	1.017E-16
TH-232	0.000E+00	0.000E+00	5.947E-11	1.050E-01	9.571E+02	6.523E-15	5.947E-11
PA-231	0.000E+00	0.000E+00	0.000E+00	5.103E-02	1.080E-03	0.000E+00	0.000E+00
U -233	0.000E+00	0.000E+00	7.446E-12	2.033E+02	2.100E+01	7.208E-11	7.446E-12
U -234	0.000E+00	0.000E+00	4.239E-12	1.064E+02	1.703E+01	2.649E-11	4.239E-12
U -235	0.000E+00	0.000E+00	2.989E-10	1.828E+00	8.456E+02	6.461E-13	2.989E-10
U -236	0.000E+00	0.000E+00	3.759E-13	1.110E-01	1.716E+00	2.431E-14	3.759E-13
U -238	0.000E+00	0.000E+00	5.515E-09	5.230E+00	1.556E+04	1.854E-12	5.515E-09
NP-237	0.000E+00	0.000E+00	1.937E-08	7.758E+00	1.101E+01	1.366E-08	1.937E-08
PU-238	0.000E+00	0.000E+00	5.003E-13	1.237E+05	7.227E+00	8.565E-09	5.003E-13
PU-239	0.000E+00	0.000E+00	5.392E-11	8.278E+04	1.332E+03	3.351E-09	5.392E-11
PU-240	0.000E+00	0.000E+00	3.967E-12	2.222E+04	9.753E+01	9.039E-10	3.967E-12
Pu-241	0.000E+00	0.000E+00	4.392E-14	2.090E+03	2.029E-02	4.525E-09	4.392E-14
PU-242	0.000E+00	0.000E+00	1.257E-12	1.221E+02	3.111E+01	4.935E-12	1.257E-12
PU-244	0.000E+00	0.000E+00	3.632E-19	1.646E-07	9.280E-06	6.443E-21	3.632E-19
AM-241	0.000E+00	0.000E+00	2.386E-10	4.728E+04	1.378E+01	8.190E-07	2.386E-10
CM-244	0.000E+00	0.000E+00	4.805E-11	7.229E+01	8.935E-04	3.887E-06	4.805E-11
CM-248	0.000E+00	0.000E+00	5.263E-12	9.558E-03	2.248E-03	2.238E-11	5.263E-12
CF-252	0.000E+00	0.000E+00	0.000E+00	9.730E-11	1.809E-16	0.000E+00	0.000E+00
PM-147	0.000E+00	0.000E+00	0.000E+00	6.496E-12	7.008E-18	0.000E+00	0.000E+00
SM-147	0.000E+00	0.000E+00	0.000E+00	4.798E-11	2.091E-06	0.000E+00	0.000E+00
AM-243	0.000E+00	0.000E+00	2.858E-13	3.371E+00	1.689E-02	5.705E-11	2.858E-13
CM-243	0.000E+00	0.000E+00	1.476E-13	5.035E-01	9.960E-06	7.460E-09	1.476E-13
CM-245	0.000E+00	0.000E+00	1.653E-10	1.191E+01	6.961E-02	2.828E-08	1.653E-10

SMFLOW0 2.900E-06

1 TIME= 200. YEARS, BRINE VOLUME= 2875. M**3

0 ELEMENT	SOLUBILITY	LOADING	DISOLVED	LARGE COL	SMALL COL		
TH	8.840E-08	4.125E+03	2.542E-01	0.000E+00	0.000E+00	0	
U	8.447E-06	6.918E+04	2.429E+01	0.000E+00	0.000E+00	0	
NP	2.864E-05	5.680E+01	5.680E+01	0.000E+00	0.000E+00	1	
PU	8.608E-08	6.095E+03	2.475E-01	0.000E+00	0.000E+00	0	
AM	3.418E-07	4.695E+01	9.829E-01	0.000E+00	0.000E+00	0	
CM	3.418E-07	2.904E-01	2.904E-01	0.000E+00	0.000E+00	1	

0 ISOTOPE	AMOUNT RELEASED (KG)			INVENTORY REMAINING		TOTAL RELEASED	
	LARGE COL	SMALL COL	DISOLVED	CURIES	KG	CURIES	KG
SR-90	0.000E+00	0.000E+00	0.000E+00	1.929E+02	1.414E-03	0.000E+00	0.000E+00
CS-137	0.000E+00	0.000E+00	0.000E+00	2.302E+02	2.647E-03	0.000E+00	0.000E+00
PB-210	0.000E+00	0.000E+00	0.000E+00	1.130E+00	1.480E-05	0.000E+00	0.000E+00
RA-226	0.000E+00	0.000E+00	0.000E+00	1.118E+00	1.131E-03	0.000E+00	0.000E+00
RA-228	0.000E+00	0.000E+00	0.000E+00	1.050E-01	3.849E-07	0.000E+00	0.000E+00
TH-229	0.000E+00	0.000E+00	4.904E-16	4.110E+00	1.932E-02	1.043E-13	4.904E-16
TH-230	0.000E+00	0.000E+00	1.915E-16	1.920E-01	9.513E-03	3.866E-15	1.915E-16
TH-232	0.000E+00	0.000E+00	7.258E-11	1.050E-01	9.571E+02	7.960E-15	7.258E-11
PA-231	0.000E+00	0.000E+00	0.000E+00	5.480E-02	1.160E-03	0.000E+00	0.000E+00
U -233	0.000E+00	0.000E+00	9.085E-12	2.032E+02	2.099E+01	8.794E-11	9.085E-12
U -234	0.000E+00	0.000E+00	5.723E-12	1.306E+02	2.090E+01	3.576E-11	5.723E-12
U -235	0.000E+00	0.000E+00	3.650E-10	1.836E+00	8.493E+02	7.890E-13	3.650E-10

U -236	0.000E+00	0.000E+00	5.462E-13	1.764E-01	2.727E+00	3.533E-14	5.462E-13
U -238	0.000E+00	0.000E+00	6.729E-09	5.230E+00	1.556E+04	2.262E-12	6.729E-09
NP-237	0.000E+00	0.000E+00	2.278E-08	9.174E+00	1.302E+01	1.606E-08	2.278E-08
PU-238	0.000E+00	0.000E+00	5.472E-13	5.615E+04	3.280E+00	9.368E-09	5.472E-13
PU-239	0.000E+00	0.000E+00	6.588E-11	8.255E+04	1.328E+03	4.094E-09	6.588E-11
PU-240	0.000E+00	0.000E+00	4.839E-12	2.199E+04	9.650E+01	1.103E-09	4.839E-12
PU-241	0.000E+00	0.000E+00	4.399E-14	2.870E+01	2.786E-04	4.531E-09	4.399E-14
PU-242	0.000E+00	0.000E+00	1.537E-12	1.221E+02	3.110E+01	6.033E-12	1.537E-12
PU-244	0.000E+00	0.000E+00	4.485E-19	1.726E-07	9.732E-06	7.956E-21	4.485E-19
AM-241	0.000E+00	0.000E+00	2.912E-10	4.034E+04	1.175E+01	9.995E-07	2.912E-10
CM-244	0.000E+00	0.000E+00	4.815E-11	1.573E+00	1.945E-05	3.895E-06	4.815E-11
CM-248	0.000E+00	0.000E+00	5.906E-12	9.556E-03	2.247E-03	2.512E-11	5.906E-12
CF-252	0.000E+00	0.000E+00	0.000E+00	3.774E-22	7.018E-28	0.000E+00	0.000E+00
PM-147	0.000E+00	0.000E+00	0.000E+00	2.177E-23	2.348E-29	0.000E+00	0.000E+00
SM-147	0.000E+00	0.000E+00	0.000E+00	4.798E-11	2.091E-06	0.000E+00	0.000E+00
AM-243	0.000E+00	0.000E+00	3.548E-13	3.340E+00	1.673E-02	7.083E-11	3.548E-13
CM-243	0.000E+00	0.000E+00	1.489E-13	4.651E-02	9.200E-07	7.529E-09	1.489E-13
CM-245	0.000E+00	0.000E+00	1.851E-10	1.181E+01	6.905E-02	3.167E-08	1.851E-10
SMFLOW0	3.539E-06						

1 TIME= 300. YEARS, BRINE VOLUME= 3634. M**3

0 ELEMENT	SOLUBILITY	LOADING	DISOLVED	LARGE COL	SMALL COL	
TH	8.840E-08	4.125E+03	3.212E-01	0.000E+00	0.000E+00	0
U	8.447E-06	6.920E+04	3.069E+01	0.000E+00	0.000E+00	0
NP	2.864E-05	6.374E+01	6.374E+01	0.000E+00	0.000E+00	1
PU	8.608E-08	6.068E+03	3.128E-01	0.000E+00	0.000E+00	0
AM	3.418E-07	4.001E+01	1.242E+00	0.000E+00	0.000E+00	0
CM	3.418E-07	2.880E-01	2.880E-01	0.000E+00	0.000E+00	1

0 ISOTOPE	AMOUNT RELEASED (KG)			INVENTORY REMAINING		TOTAL RELEASED	
	LARGE COL	SMALL COL	DISOLVED	CURIES	KG	CURIES	KG
SR-90	0.000E+00	0.000E+00	0.000E+00	1.785E+01	1.308E-04	0.000E+00	0.000E+00
CS-137	0.000E+00	0.000E+00	0.000E+00	2.284E+01	2.626E-04	0.000E+00	0.000E+00
PB-210	0.000E+00	0.000E+00	0.000E+00	1.093E+00	1.431E-05	0.000E+00	0.000E+00
RA-226	0.000E+00	0.000E+00	0.000E+00	1.081E+00	1.094E-03	0.000E+00	0.000E+00
RA-228	0.000E+00	0.000E+00	0.000E+00	1.050E-01	3.849E-07	0.000E+00	0.000E+00
TH-229	0.000E+00	0.000E+00	6.683E-16	5.981E+00	2.812E-02	1.421E-13	6.683E-16
TH-230	0.000E+00	0.000E+00	2.851E-16	3.150E-01	1.560E-02	5.756E-15	2.851E-16
TH-232	0.000E+00	0.000E+00	7.984E-11	1.050E-01	9.571E+02	8.756E-15	7.984E-11
PA-231	0.000E+00	0.000E+00	0.000E+00	5.857E-02	1.240E-03	0.000E+00	0.000E+00
U -233	0.000E+00	0.000E+00	9.991E-12	2.031E+02	2.098E+01	9.672E-11	9.991E-12
U -234	0.000E+00	0.000E+00	6.665E-12	1.416E+02	2.266E+01	4.165E-11	6.665E-12
U -235	0.000E+00	0.000E+00	4.018E-10	1.844E+00	8.531E+02	8.685E-13	4.018E-10
U -236	0.000E+00	0.000E+00	6.844E-13	2.411E-01	3.728E+00	4.427E-14	6.844E-13
U -238	0.000E+00	0.000E+00	7.401E-09	5.230E+00	1.556E+04	2.488E-12	7.401E-09
NP-237	0.000E+00	0.000E+00	2.439E-08	1.038E+01	1.473E+01	1.719E-08	2.439E-08
PU-238	0.000E+00	0.000E+00	5.590E-13	2.548E+04	1.489E+00	9.569E-09	5.590E-13
PU-239	0.000E+00	0.000E+00	7.252E-11	8.231E+04	1.324E+03	4.507E-09	7.252E-11
PU-240	0.000E+00	0.000E+00	5.319E-12	2.176E+04	9.548E+01	1.212E-09	5.319E-12
PU-241	0.000E+00	0.000E+00	4.399E-14	1.187E+01	1.153E-04	4.531E-09	4.399E-14
PU-242	0.000E+00	0.000E+00	1.692E-12	1.221E+02	3.110E+01	6.644E-12	1.692E-12
PU-244	0.000E+00	0.000E+00	4.983E-19	1.806E-07	1.018E-05	8.838E-21	4.983E-19
AM-241	0.000E+00	0.000E+00	3.203E-10	3.436E+04	1.001E+01	1.099E-06	3.203E-10
CM-244	0.000E+00	0.000E+00	4.815E-11	3.425E-02	4.233E-07	3.896E-06	4.815E-11
CM-248	0.000E+00	0.000E+00	6.169E-12	9.554E-03	2.247E-03	2.623E-11	6.169E-12
CF-252	0.000E+00	0.000E+00	0.000E+00	1.464E-33	0.000E+00	0.000E+00	0.000E+00
PM-147	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
SM-147	0.000E+00	0.000E+00	0.000E+00	4.798E-11	2.091E-06	0.000E+00	0.000E+00
AM-243	0.000E+00	0.000E+00	3.993E-13	3.308E+00	1.657E-02	7.971E-11	3.993E-13
CM-243	0.000E+00	0.000E+00	1.490E-13	4.296E-03	8.498E-08	7.532E-09	1.490E-13
CM-245	0.000E+00	0.000E+00	1.932E-10	1.172E+01	6.849E-02	3.304E-08	1.932E-10
SMFLOW0	3.893E-05						



1 TIME= 400. YEARS, BRINE VOLUME= 4215. M**3

0 ELEMENT	SOLUBILITY	LOADING	DISOLVED	LARGE COL	SMALL COL	
TH	8.840E-08	4.126E+03	3.726E-01	0.000E+00	0.000E+00	0
U	8.447E-06	6.923E+04	3.560E+01	0.000E+00	0.000E+00	0
NP	2.864E-05	6.966E+01	6.966E+01	0.000E+00	0.000E+00	1
PU	8.608E-08	6.045E+03	3.628E-01	0.000E+00	0.000E+00	0
AM	3.418E-07	3.409E+01	1.441E+00	0.000E+00	0.000E+00	0
CM	3.418E-07	2.858E-01	2.858E-01	0.000E+00	0.000E+00	1

ISOTOPE	AMOUNT RELEASED (KG)			INVENTORY REMAINING		TOTAL RELEASED	
	LARGE COL	SMALL COL	DISOLVED	CURIES	KG	CURIES	KG
SR-90	0.000E+00	0.000E+00	0.000E+00	1.651E+00	1.210E-05	0.000E+00	0.000E+00
CS-137	0.000E+00	0.000E+00	0.000E+00	2.266E+00	2.605E-05	0.000E+00	0.000E+00
PB-210	0.000E+00	0.000E+00	0.000E+00	1.061E+00	1.389E-05	0.000E+00	0.000E+00
RA-226	0.000E+00	0.000E+00	0.000E+00	1.052E+00	1.064E-03	0.000E+00	0.000E+00
RA-228	0.000E+00	0.000E+00	0.000E+00	1.050E-01	3.849E-07	0.000E+00	0.000E+00
TH-229	0.000E+00	0.000E+00	8.415E-16	7.833E+00	3.683E-02	1.790E-13	8.415E-16
TH-230	0.000E+00	0.000E+00	3.852E-16	4.446E-01	2.203E-02	7.777E-15	3.852E-16
TH-232	0.000E+00	0.000E+00	8.497E-11	1.050E-01	9.571E+02	9.320E-15	8.497E-11
PA-231	0.000E+00	0.000E+00	0.000E+00	6.235E-02	1.320E-03	0.000E+00	0.000E+00
U -233	0.000E+00	0.000E+00	1.063E-11	2.030E+02	2.097E+01	1.029E-10	1.063E-11
U -234	0.000E+00	0.000E+00	7.371E-12	1.465E+02	2.345E+01	4.606E-11	7.371E-12
U -235	0.000E+00	0.000E+00	4.280E-10	1.852E+00	8.568E+02	9.250E-13	4.280E-10
U -236	0.000E+00	0.000E+00	8.128E-13	3.052E-01	4.719E+00	5.257E-14	8.128E-13
U -238	0.000E+00	0.000E+00	7.877E-09	5.230E+00	1.556E+04	2.648E-12	7.877E-09
NP-237	0.000E+00	0.000E+00	2.541E-08	1.141E+01	1.619E+01	1.791E-08	2.541E-08
PU-238	0.000E+00	0.000E+00	5.627E-13	1.157E+04	6.756E-01	9.634E-09	5.627E-13
PU-239	0.000E+00	0.000E+00	7.722E-11	8.207E+04	1.321E+03	4.799E-09	7.722E-11
PU-240	0.000E+00	0.000E+00	5.657E-12	2.153E+04	9.448E+01	1.289E-09	5.657E-12
PU-241	0.000E+00	0.000E+00	4.399E-14	1.164E+01	1.130E-04	4.531E-09	4.399E-14
PU-242	0.000E+00	0.000E+00	1.803E-12	1.221E+02	3.109E+01	7.078E-12	1.803E-12
PU-244	0.000E+00	0.000E+00	5.352E-19	1.887E-07	1.064E-05	9.494E-21	5.352E-19
AM-241	0.000E+00	0.000E+00	3.409E-10	2.927E+04	8.528E+00	1.170E-06	3.409E-10
CM-244	0.000E+00	0.000E+00	4.815E-11	7.454E-04	9.213E-09	3.896E-06	4.815E-11
CM-248	0.000E+00	0.000E+00	6.317E-12	9.552E-03	2.246E-03	2.686E-11	6.317E-12
CF-252	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
FM-147	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
SM-147	0.000E+00	0.000E+00	0.000E+00	4.798E-11	2.091E-06	0.000E+00	0.000E+00
AM-243	0.000E+00	0.000E+00	4.360E-13	3.278E+00	1.642E-02	8.702E-11	4.360E-13
CM-243	0.000E+00	0.000E+00	1.490E-13	3.969E-04	7.850E-09	7.532E-09	1.490E-13
CM-245	0.000E+00	0.000E+00	1.977E-10	1.162E+01	6.793E-02	3.382E-08	1.977E-10
SMFLOW0	4.143E-06						

1 TIME= 500. YEARS, BRINE VOLUME= 3927. M**3

0 ELEMENT	SOLUBILITY	LOADING	DISOLVED	LARGE COL	SMALL COL	
TH	8.840E-08	4.126E+03	3.472E-01	0.000E+00	0.000E+00	0
U	8.447E-06	6.925E+04	3.317E+01	0.000E+00	0.000E+00	0
NP	2.864E-05	7.470E+01	7.470E+01	0.000E+00	0.000E+00	1
PU	8.608E-08	6.024E+03	3.381E-01	0.000E+00	0.000E+00	0
AM	3.418E-07	2.905E+01	1.343E+00	0.000E+00	0.000E+00	0
CM	3.418E-07	2.835E-01	2.835E-01	0.000E+00	0.000E+00	1

ISOTOPE	AMOUNT RELEASED (KG)			INVENTORY REMAINING		TOTAL RELEASED	
	LARGE COL	SMALL COL	DISOLVED	CURIES	KG	CURIES	KG
SR-90	0.000E+00	0.000E+00	0.000E+00	1.528E-01	1.120E-06	0.000E+00	0.000E+00
CS-137	0.000E+00	0.000E+00	0.000E+00	2.248E-01	2.585E-06	0.000E+00	0.000E+00
PB-210	0.000E+00	0.000E+00	0.000E+00	1.036E+00	1.357E-05	0.000E+00	0.000E+00
RA-226	0.000E+00	0.000E+00	0.000E+00	1.029E+00	1.040E-03	0.000E+00	0.000E+00
RA-228	0.000E+00	0.000E+00	0.000E+00	1.050E-01	3.849E-07	0.000E+00	0.000E+00
TH-229	0.000E+00	0.000E+00	2.139E-15	9.667E+00	4.545E-02	4.549E-13	2.139E-15
TH-230	0.000E+00	0.000E+00	1.183E-15	5.772E-01	2.859E-02	2.388E-14	1.183E-15
TH-232	0.000E+00	0.000E+00	1.151E-10	1.050E-01	9.571E+02	1.263E-14	1.151E-10
PA-231	0.000E+00	0.000E+00	0.000E+00	6.614E-02	1.400E-03	0.000E+00	0.000E+00
U -233	0.000E+00	0.000E+00	1.439E-11	2.029E+02	2.096E+01	1.393E-10	1.439E-11
U -234	0.000E+00	0.000E+00	1.161E-11	1.488E+02	2.381E+01	7.256E-11	1.161E-11
U -235	0.000E+00	0.000E+00	5.820E-10	1.860E+00	8.606E+02	1.258E-12	5.820E-10
U -236	0.000E+00	0.000E+00	1.748E-12	3.686E-01	5.698E+00	1.131E-13	1.748E-12



U -238	0.000E+00	0.000E+00	1.067E-08	5.230E+00	1.556E+04	3.586E-12	1.067E-08
NP-237	0.000E+00	0.000E+00	3.140E-08	1.228E+01	1.743E+01	2.213E-08	3.140E-08
PU-238	0.000E+00	0.000E+00	5.726E-13	5.249E+03	3.066E-01	9.803E-09	5.726E-13
PU-239	0.000E+00	0.000E+00	1.048E-10	8.184E+04	1.317E+03	6.516E-09	1.048E-10
PU-240	0.000E+00	0.000E+00	7.626E-12	2.130E+04	9.348E+01	1.738E-09	7.626E-12
PU-241	0.000E+00	0.000E+00	4.399E-14	1.155E+01	1.121E-04	4.532E-09	4.399E-14
PU-242	0.000E+00	0.000E+00	2.454E-12	1.220E+02	3.109E+01	9.635E-12	2.454E-12
PU-244	0.000E+00	0.000E+00	7.628E-19	1.967E-07	1.109E-05	1.353E-20	7.628E-19
AM-241	0.000E+00	0.000E+00	4.618E-10	2.494E+04	7.265E+00	1.585E-06	4.618E-10
CM-244	0.000E+00	0.000E+00	4.815E-11	1.622E-05	2.005E-10	3.896E-06	4.815E-11
CM-248	0.000E+00	0.000E+00	7.116E-12	9.550E-03	2.246E-03	3.026E-11	7.116E-12
CF-252	0.000E+00						
PM-147	0.000E+00						
SM-147	0.000E+00	0.000E+00	0.000E+00	4.798E-11	2.091E-06	0.000E+00	0.000E+00
AM-243	0.000E+00	0.000E+00	6.870E-13	3.247E+00	1.627E-02	1.371E-10	6.870E-13
CM-243	0.000E+00	0.000E+00	1.490E-13	3.666E-05	7.251E-10	7.532E-09	1.490E-13
CM-245	0.000E+00	0.000E+00	2.218E-10	1.153E+01	6.738E-02	3.793E-08	2.218E-10
SMFLOW0	5.613E-06						

1 TIME= 1000. YEARS, BRINE VOLUME= 3241. M**3

0 ELEMENT	SOLUBILITY	LOADING	DISOLVED	LARGE COL	SMALL COL		
TH	8.840E-08	4.126E+03	2.865E-01	0.000E+00	0.000E+00	0	
U	8.447E-06	6.935E+04	2.738E+01	0.000E+00	0.000E+00	0	
NP	2.864E-05	9.067E+01	9.067E+01	0.000E+00	0.000E+00	1	
PU	8.608E-08	5.924E+03	2.790E-01	0.000E+00	0.000E+00	0	
AM	3.418E-07	1.307E+01	1.108E+00	0.000E+00	0.000E+00	0	
CM	3.418E-07	2.726E-01	2.726E-01	0.000E+00	0.000E+00	1	
OISOTOPE	AMOUNT RELEASED (KG)		INVENTORY	REMAINING	TOTAL RELEASED		
	LARGE COL	SMALL COL	DISOLVED	CURIES	KG	CURIES	KG
SR-90	0.000E+00	0.000E+00	0.000E+00	1.036E-06	7.593E-12	0.000E+00	0.000E+00
CS-137	0.000E+00	0.000E+00	0.000E+00	2.161E-06	2.485E-11	0.000E+00	0.000E+00
PB-210	0.000E+00	0.000E+00	0.000E+00	1.006E+00	1.317E-05	0.000E+00	0.000E+00
RA-226	0.000E+00	0.000E+00	0.000E+00	1.008E+00	1.020E-03	0.000E+00	0.000E+00
RA-228	0.000E+00	0.000E+00	0.000E+00	1.050E-01	3.849E-07	0.000E+00	0.000E+00
TH-229	0.000E+00	0.000E+00	1.091E-14	1.857E+01	8.731E-02	2.320E-12	1.091E-14
TH-230	0.000E+00	0.000E+00	7.075E-15	1.249E+00	6.186E-02	1.428E-13	7.075E-15
TH-232	0.000E+00	0.000E+00	2.489E-10	1.050E-01	9.571E+02	2.730E-14	2.489E-10
PA-231	0.000E+00	0.000E+00	0.000E+00	8.523E-02	1.804E-03	0.000E+00	0.000E+00
U -233	0.000E+00	0.000E+00	3.105E-11	2.025E+02	2.092E+01	3.006E-10	3.105E-11
U -234	0.000E+00	0.000E+00	3.071E-11	1.504E+02	2.407E+01	1.919E-10	3.071E-11
U -235	0.000E+00	0.000E+00	1.272E-09	1.900E+00	8.791E+02	2.750E-12	1.272E-09
U -236	0.000E+00	0.000E+00	7.839E-12	6.756E-01	1.044E+01	5.070E-13	7.839E-12
U -238	0.000E+00	0.000E+00	2.304E-08	5.230E+00	1.556E+04	7.745E-12	2.304E-08
NP-237	0.000E+00	0.000E+00	6.631E-08	1.506E+01	2.137E+01	4.674E-08	6.631E-08
PU-238	0.000E+00	0.000E+00	5.809E-13	1.011E+02	5.904E-03	9.945E-09	5.809E-13
PU-239	0.000E+00	0.000E+00	2.276E-10	8.067E+04	1.298E+03	1.414E-08	2.276E-10
PU-240	0.000E+00	0.000E+00	1.620E-11	2.020E+04	8.865E+01	3.693E-09	1.620E-11
PU-241	0.000E+00	0.000E+00	4.400E-14	1.109E+01	1.076E-04	4.533E-09	4.400E-14
PU-242	0.000E+00	0.000E+00	5.368E-12	1.219E+02	3.106E+01	2.107E-11	5.368E-12
PU-244	0.000E+00	0.000E+00	1.889E-18	2.367E-07	1.335E-05	3.351E-20	1.889E-18
AM-241	0.000E+00	0.000E+00	9.975E-10	1.119E+04	3.260E+00	3.423E-06	9.975E-10
CM-244	0.000E+00	0.000E+00	4.815E-11	7.925E-14	9.795E-19	3.896E-06	4.815E-11
CM-248	0.000E+00	0.000E+00	1.116E-11	9.540E-03	2.244E-03	4.746E-11	1.116E-11
CF-252	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
PM-147	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
SM-147	0.000E+00	0.000E+00	0.000E+00	4.798E-11	2.091E-06	0.000E+00	0.000E+00
AM-243	0.000E+00	0.000E+00	2.340E-12	3.098E+00	1.552E-02	4.671E-10	2.340E-12
CM-243	0.000E+00	0.000E+00	1.490E-13	2.465E-10	4.876E-15	7.532E-09	1.490E-13
CM-245	0.000E+00	0.000E+00	3.411E-10	1.107E+01	6.470E-02	5.835E-08	3.411E-10
SMFLOW0	1.214E-05						

1 TIME= 1500. YEARS, BRINE VOLUME= 3882. M**3

0 ELEMENT	SOLUBILITY	LOADING	DISOLVED	LARGE COL	SMALL COL	
TH	8.840E-08	4.126E+03	3.432E-01	0.000E+00	0.000E+00	0
U	8.447E-06	6.944E+04	3.279E+01	0.000E+00	0.000E+00	0
NP	2.864E-05	9.784E+01	9.784E+01	0.000E+00	0.000E+00	1
PU	8.608E-08	5.827E+03	3.342E-01	0.000E+00	0.000E+00	0
AM	3.418E-07	5.901E+00	1.327E+00	0.000E+00	0.000E+00	0
CM	3.418E-07	2.621E-01	2.621E-01	0.000E+00	0.000E+00	1

0 ISOTOPE	AMOUNT RELEASED (KG)			INVENTORY REMAINING		TOTAL RELEASED	
	LARGE COL	SMALL COL	DISOLVED	CURIES	KG	CURIES	KG
SR-90	0.000E+00	0.000E+00	0.000E+00	7.022E-12	5.148E-17	0.000E+00	0.000E+00
CS-137	0.000E+00	0.000E+00	0.000E+00	2.077E-11	2.388E-16	0.000E+00	0.000E+00
PB-210	0.000E+00	0.000E+00	0.000E+00	1.112E+00	1.457E-05	0.000E+00	0.000E+00
RA-226	0.000E+00	0.000E+00	0.000E+00	1.123E+00	1.136E-03	0.000E+00	0.000E+00
RA-228	0.000E+00	0.000E+00	0.000E+00	1.050E-01	3.849E-07	0.000E+00	0.000E+00
TH-229	0.000E+00	0.000E+00	1.091E-14	2.704E+01	1.272E-01	2.320E-12	1.091E-14
TH-230	0.000E+00	0.000E+00	7.075E-15	1.918E+00	9.502E-02	1.428E-13	7.075E-15
TH-232	0.000E+00	0.000E+00	2.489E-10	1.050E-01	9.571E+02	2.730E-14	2.489E-10
PA-231	0.000E+00	0.000E+00	0.000E+00	1.045E-01	2.213E-03	0.000E+00	0.000E+00
U -233	0.000E+00	0.000E+00	3.105E-11	2.021E+02	2.088E+01	3.006E-10	3.105E-11
U -234	0.000E+00	0.000E+00	3.071E-11	1.502E+02	2.404E+01	1.919E-10	3.071E-11
U -235	0.000E+00	0.000E+00	1.272E-09	1.940E+00	8.973E+02	2.750E-12	1.272E-09
U -236	0.000E+00	0.000E+00	7.839E-12	9.667E-01	1.495E+01	5.070E-13	7.839E-12
U -238	0.000E+00	0.000E+00	2.304E-08	5.230E+00	1.556E+04	7.745E-12	2.304E-08
NP-237	0.000E+00	0.000E+00	6.631E-08	1.630E+01	2.313E+01	4.674E-08	6.631E-08
PU-238	0.000E+00	0.000E+00	5.809E-13	1.946E+00	1.137E-04	9.945E-09	5.809E-13
PU-239	0.000E+00	0.000E+00	2.276E-10	7.951E+04	1.279E+03	1.414E-08	2.276E-10
PU-240	0.000E+00	0.000E+00	1.620E-11	1.916E+04	8.407E+01	3.693E-09	1.620E-11
PU-241	0.000E+00	0.000E+00	4.400E-14	1.065E+01	1.033E-04	4.533E-09	4.400E-14
PU-242	0.000E+00	0.000E+00	5.368E-12	1.218E+02	3.103E+01	2.107E-11	5.368E-12
PU-244	0.000E+00	0.000E+00	1.889E-18	2.767E-07	1.560E-05	3.351E-20	1.889E-18
AM-241	0.000E+00	0.000E+00	9.975E-10	5.024E+03	1.464E+00	3.423E-06	9.975E-10
CM-244	0.000E+00	0.000E+00	4.815E-11	3.871E-22	4.785E-27	3.896E-06	4.815E-11
CM-248	0.000E+00	0.000E+00	1.116E-11	9.530E-03	2.241E-03	4.746E-11	1.116E-11
CF-252	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
PM-147	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
SM-147	0.000E+00	0.000E+00	0.000E+00	4.798E-11	2.091E-06	0.000E+00	0.000E+00
AM-243	0.000E+00	0.000E+00	2.340E-12	2.955E+00	1.481E-02	4.671E-10	2.340E-12
CM-243	0.000E+00	0.000E+00	1.490E-13	1.658E-15	3.279E-20	7.532E-09	1.490E-13
CM-245	0.000E+00	0.000E+00	3.411E-10	1.063E+01	6.213E-02	5.835E-08	3.411E-10
SMFLOW0	1.214E-05						

1 TIME= 2000. YEARS, BRINE VOLUME= 4458. M**3

0 ELEMENT	SOLUBILITY	LOADING	DISOLVED	LARGE COL	SMALL COL	
TH	8.840E-08	4.127E+03	3.941E-01	0.000E+00	0.000E+00	0
U	8.447E-06	6.954E+04	3.766E+01	0.000E+00	0.000E+00	0
NP	2.864E-05	1.010E+02	1.010E+02	0.000E+00	0.000E+00	1
PU	8.608E-08	5.733E+03	3.838E-01	0.000E+00	0.000E+00	0
AM	3.418E-07	2.684E+00	1.524E+00	0.000E+00	0.000E+00	0
CM	3.418E-07	2.520E-01	2.520E-01	0.000E+00	0.000E+00	1

0 ISOTOPE	AMOUNT RELEASED (KG)			INVENTORY REMAINING		TOTAL RELEASED	
	LARGE COL	SMALL COL	DISOLVED	CURIES	KG	CURIES	KG
SR-90	0.000E+00	0.000E+00	0.000E+00	4.761E-17	3.490E-22	0.000E+00	0.000E+00
CS-137	0.000E+00	0.000E+00	0.000E+00	1.997E-16	2.296E-21	0.000E+00	0.000E+00
PB-210	0.000E+00	0.000E+00	0.000E+00	1.328E+00	1.740E-05	0.000E+00	0.000E+00
RA-226	0.000E+00	0.000E+00	0.000E+00	1.345E+00	1.360E-03	0.000E+00	0.000E+00
RA-228	0.000E+00	0.000E+00	0.000E+00	1.050E-01	3.849E-07	0.000E+00	0.000E+00
TH-229	0.000E+00	0.000E+00	1.091E-14	3.511E+01	1.651E-01	2.320E-12	1.091E-14
TH-230	0.000E+00	0.000E+00	7.075E-15	2.584E+00	1.280E-01	1.428E-13	7.075E-15
TH-232	0.000E+00	0.000E+00	2.489E-10	1.050E-01	9.571E+02	2.730E-14	2.489E-10
PA-231	0.000E+00	0.000E+00	0.000E+00	1.241E-01	2.626E-03	0.000E+00	0.000E+00
U -233	0.000E+00	0.000E+00	3.105E-11	2.017E+02	2.084E+01	3.006E-10	3.105E-11
U -234	0.000E+00	0.000E+00	3.071E-11	1.500E+02	2.401E+01	1.919E-10	3.071E-11
U -235	0.000E+00	0.000E+00	1.272E-09	1.978E+00	9.153E+02	2.750E-12	1.272E-09
U -236	0.000E+00	0.000E+00	7.839E-12	1.243E+00	1.921E+01	5.070E-13	7.839E-12

U -238	0.000E+00	0.000E+00	2.304E-08	5.230E+00	1.556E+04	7.745E-12	2.304E-08
NP-237	0.000E+00	0.000E+00	6.631E-08	1.686E+01	2.392E+01	4.674E-08	6.631E-08
PU-238	0.000E+00	0.000E+00	5.809E-13	3.747E-02	2.189E-06	9.945E-09	5.809E-13
PU-239	0.000E+00	0.000E+00	2.276E-10	7.838E+04	1.261E+03	1.414E-08	2.276E-10
PU-240	0.000E+00	0.000E+00	1.620E-11	1.817E+04	7.973E+01	3.693E-09	1.620E-11
PU-241	0.000E+00	0.000E+00	4.400E-14	1.022E+01	9.922E-05	4.533E-09	4.400E-14
PU-242	0.000E+00	0.000E+00	5.368E-12	1.217E+02	3.100E+01	2.107E-11	5.368E-12
PU-244	0.000E+00	0.000E+00	1.889E-18	3.167E-07	1.785E-05	3.351E-20	1.889E-18
AM-241	0.000E+00	0.000E+00	9.975E-10	2.259E+03	6.582E-01	3.423E-06	9.975E-10
CM-244	0.000E+00	0.000E+00	4.815E-11	1.891E-30	2.337E-35	3.896E-06	4.815E-11
CM-248	0.000E+00	0.000E+00	1.116E-11	9.521E-03	2.239E-03	4.746E-11	1.116E-11
CF-252	0.000E+00						
PM-147	0.000E+00						
SM-147	0.000E+00	0.000E+00	0.000E+00	4.798E-11	2.091E-06	0.000E+00	0.000E+00
AM-243	0.000E+00	0.000E+00	2.340E-12	2.820E+00	1.413E-02	4.671E-10	2.340E-12
CM-243	0.000E+00	0.000E+00	1.490E-13	1.115E-20	2.205E-25	7.532E-09	1.490E-13
CM-245	0.000E+00	0.000E+00	3.411E-10	1.020E+01	5.965E-02	5.835E-08	3.411E-10
SMFLOW0	1.214E-05						

1 TIME= 5000. YEARS, BRINE VOLUME= 5332. M**3

0 ELEMENT	SOLUBILITY	LOADING	DISOLVED	LARGE COL	SMALL COL	
TH	8.840E-08	4.127E+03	4.713E-01	0.000E+00	0.000E+00	0
U	8.447E-06	6.999E+04	4.504E+01	0.000E+00	0.000E+00	0
NP	2.864E-05	1.801E+01	1.801E+01	0.000E+00	0.000E+00	1
PU	8.608E-08	5.204E+03	4.590E-01	0.000E+00	0.000E+00	0
AM	3.418E-07	1.280E-02	1.280E-02	0.000E+00	0.000E+00	1
CM	3.418E-07	3.455E-02	3.455E-02	0.000E+00	0.000E+00	1



0 ISOTOPE	AMOUNT RELEASED (KG)			INVENTORY REMAINING		TOTAL RELEASED	
	LARGE COL	SMALL COL	DISOLVED	CURIES	KG	CURIES	KG
SR-90	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
CS-137	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
PB-210	0.000E+00	0.000E+00	0.000E+00	3.941E+00	5.163E-05	0.000E+00	0.000E+00
RA-226	0.000E+00	0.000E+00	0.000E+00	3.976E+00	4.022E-03	0.000E+00	0.000E+00
RA-228	0.000E+00	0.000E+00	0.000E+00	1.049E-01	3.849E-07	0.000E+00	0.000E+00
TH-229	0.000E+00	0.000E+00	6.021E-05	7.587E+01	3.567E-01	1.281E-02	6.021E-05
TH-230	0.000E+00	0.000E+00	5.248E-05	6.494E+00	3.217E-01	1.059E-03	5.248E-05
TH-232	0.000E+00	0.000E+00	1.860E-01	1.049E-01	9.569E+02	2.040E-05	1.860E-01
PA-231	0.000E+00	0.000E+00	0.000E+00	2.451E-01	5.187E-03	0.000E+00	0.000E+00
U -233	0.000E+00	0.000E+00	2.264E-02	1.990E+02	2.056E+01	2.191E-01	2.264E-02
U -234	0.000E+00	0.000E+00	2.616E-02	1.486E+02	2.379E+01	1.635E-01	2.616E-02
U -235	0.000E+00	0.000E+00	1.086E+00	2.198E+00	1.017E+03	2.348E-03	1.086E+00
U -236	0.000E+00	0.000E+00	3.877E-02	2.622E+00	4.054E+01	2.508E-03	3.877E-02
U -238	0.000E+00	0.000E+00	1.705E+01	5.224E+00	1.554E+04	5.733E-03	1.705E+01
NP-237	0.000E+00	0.000E+00	2.026E+01	3.009E+00	4.269E+00	1.428E+01	2.026E+01
PU-238	0.000E+00	0.000E+00	5.841E-13	1.909E-12	1.115E-16	1.000E-08	5.841E-13
PU-239	0.000E+00	0.000E+00	1.730E-01	7.188E+04	1.157E+03	1.075E+01	1.730E-01
PU-240	0.000E+00	0.000E+00	9.243E-03	1.322E+04	5.800E+01	2.106E+00	9.243E-03
PU-241	0.000E+00	0.000E+00	6.077E-09	1.479E+00	1.435E-05	6.260E-04	6.077E-09
PU-242	0.000E+00	0.000E+00	4.512E-03	1.210E+02	3.083E+01	1.771E-02	4.512E-03
PU-244	0.000E+00	0.000E+00	3.826E-09	4.877E-07	2.750E-05	6.786E-11	3.826E-09
AM-241	0.000E+00	0.000E+00	3.381E-02	4.444E+00	1.295E-03	1.161E+02	3.381E-02
CM-244	0.000E+00	0.000E+00	4.815E-11	0.000E+00	0.000E+00	3.896E-06	4.815E-11
CM-248	0.000E+00	0.000E+00	1.842E-03	1.645E-03	3.869E-04	7.834E-03	1.842E-03
CF-252	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
PM-147	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
SM-147	0.000E+00	0.000E+00	0.000E+00	4.798E-11	2.091E-06	0.000E+00	0.000E+00
AM-243	0.000E+00	0.000E+00	9.717E-03	3.682E-01	1.844E-03	1.940E+00	9.717E-03
CM-243	0.000E+00	0.000E+00	1.490E-13	0.000E+00	0.000E+00	7.532E-09	1.490E-13
CM-245	0.000E+00	0.000E+00	4.207E-02	1.385E+00	8.099E-03	7.196E+00	4.207E-02
SMFLOW0	9.074E+03						

1 TIME= 10000. YEARS, BRINE VOLUME= 5053. M**3

0 ELEMENT	SOLUBILITY	LOADING	DISOLVED	LARGE COL	SMALL COL		
TH	8.840E-08	4.127E+03	4.467E-01	0.000E+00	0.000E+00	0	
U	8.447E-06	7.049E+04	4.268E+01	0.000E+00	0.000E+00	0	
NP	2.864E-05	6.601E-02	6.601E-02	0.000E+00	0.000E+00	1	
PU	8.608E-08	4.453E+03	4.350E-01	0.000E+00	0.000E+00	0	
AM	3.418E-07	2.148E-05	2.148E-05	0.000E+00	0.000E+00	1	
CM	3.418E-07	8.532E-05	8.532E-05	0.000E+00	0.000E+00	1	

0 ISOTOPE	AMOUNT RELEASED (KG)			INVENTORY REMAINING		TOTAL RELEASED	
	LARGE COL	SMALL COL	DISOLVED	CURIES	KG	CURIES	KG
SR-90	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
CS-137	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
PB-210	0.000E+00	0.000E+00	0.000E+00	9.856E+00	1.291E-04	0.000E+00	0.000E+00
RA-226	0.000E+00	0.000E+00	0.000E+00	9.895E+00	1.001E-02	0.000E+00	0.000E+00
RA-228	0.000E+00	0.000E+00	0.000E+00	1.049E-01	3.846E-07	0.000E+00	0.000E+00
TH-229	0.000E+00	0.000E+00	3.447E-04	1.212E+02	5.697E-01	7.332E-02	3.447E-04
TH-230	0.000E+00	0.000E+00	3.391E-04	1.269E+01	6.286E-01	6.846E-03	3.391E-04
TH-232	0.000E+00	0.000E+00	7.642E-01	1.049E-01	9.563E+02	8.381E-05	7.642E-01
PA-231	0.000E+00	0.000E+00	0.000E+00	4.579E-01	9.694E-03	0.000E+00	0.000E+00
U -233	0.000E+00	0.000E+00	9.155E-02	1.941E+02	2.005E+01	8.862E-01	9.155E-02
U -234	0.000E+00	0.000E+00	1.062E-01	1.461E+02	2.339E+01	6.637E-01	1.062E-01
U -235	0.000E+00	0.000E+00	4.791E+00	2.519E+00	1.166E+03	1.036E-02	4.791E+00
U -236	0.000E+00	0.000E+00	2.187E-01	4.127E+00	6.381E+01	1.414E-02	2.187E-01
U -238	0.000E+00	0.000E+00	6.970E+01	5.207E+00	1.549E+04	2.343E-02	6.970E+01
NP-237	0.000E+00	0.000E+00	2.451E+01	1.103E-02	1.565E-02	1.728E+01	2.451E+01
PU-238	0.000E+00	0.000E+00	5.841E-13	1.336E-29	7.806E-34	1.000E-08	5.841E-13
PU-239	0.000E+00	0.000E+00	7.158E-01	6.221E+04	1.001E+03	4.448E+01	7.158E-01
PU-240	0.000E+00	0.000E+00	3.188E-02	7.774E+03	3.412E+01	7.265E+00	3.188E-02
PU-241	0.000E+00	0.000E+00	7.237E-09	3.554E-03	3.450E-08	7.455E-04	7.237E-09
PU-242	0.000E+00	0.000E+00	1.998E-02	1.198E+02	3.053E+01	7.845E-02	1.998E-02
PU-244	0.000E+00	0.000E+00	1.798E-08	5.000E-07	2.819E-05	3.190E-10	1.798E-08
AM-241	0.000E+00	0.000E+00	3.457E-02	3.614E-03	1.053E-06	1.186E+02	3.457E-02
CM-244	0.000E+00	0.000E+00	4.815E-11	0.000E+00	0.000E+00	3.896E-06	4.815E-11
CM-248	0.000E+00	0.000E+00	2.227E-03	5.971E-06	1.404E-06	9.470E-03	2.227E-03
CF-252	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
PM-147	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
SM-147	0.000E+00	0.000E+00	0.000E+00	4.798E-11	2.091E-06	0.000E+00	0.000E+00
AM-243	0.000E+00	0.000E+00	1.141E-02	8.324E-04	4.170E-06	2.278E+00	1.141E-02
CM-243	0.000E+00	0.000E+00	1.490E-13	0.000E+00	0.000E+00	7.532E-09	1.490E-13
CM-245	0.000E+00	0.000E+00	4.959E-02	3.345E-03	1.955E-05	8.483E+00	4.959E-02
SMFLOW0	3.729E+04						

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APPENDIX G: PANEL'S COLLOIDAL-SUSPENSION MODEL (NOT AVAILABLE FOR THE CCA PA)



This section describes, as a matter of record, a colloidal suspension model that is included within PANEL, but is hard-wired in the off position for CCA calculations. It is included for information and completeness, and is *not* part of PANEL's QAed software documentation.

PANEL's sorption model is based on the assumption that all isotopes present in the repository sorb rapidly onto colloidal particulates, and all rapidly reach the same maximum capacity C_{\max}^l or C_{\max}^s in moles/l of brine for large and small colloids, respectively. Clearly, this application of sorption mechanics is both primitive and inconsistent. Sorption is normally a time-dependent process. Moreover, different elements have different affinities for sorption onto colloids, and sorptive concentration of an element onto colloidal materials depends (i) on the concentration of that element in solution, (ii) the concentration of mobile colloids, and (iii) the reversible or irreversible exchange characteristics between dissolved and sorbed materials. These more advanced issues are being addressed. The inconsistency arises from the fact that repository wastes are permitted to sorb onto mobile colloids and thereby readily exit the repository in its brine outflows, however, they are not permitted to sorb onto immobile repository materials, where they would be help captive and thereby prevented from exiting the repository. That approach to sorption is clearly conservative, but it is also inconsistent.

F.1 LARGE COLLOIDS

At each timestep, PANEL combines, by element, the amounts (in moles) of all the isotopes of each element present in the repository. Then, to each $V(t_n)$ liters of brine in the repository, PANEL assigns exactly $V(t_n) C_{\max,i}^l$ moles of each inventoried element to be sorbed onto large colloidal particles, assuming that amount is available in the repository. The parameters $C_{\max,i}^l$ are assumed to be given for each of the i elements. If the required amount of the i th inventoried element is not available at that timestep, PANEL assigns whatever amount remains in the inventory, namely, $I_i(t_n)$. Thus, at the n th timestep, the amount (in moles) of i th element in the repository sorbed onto large colloids is

$$m_{i,j}^l(t_n) = \begin{cases} C_{\max,i}^l V(t_n) & , \text{ if } C_{\max,i}^l V(t_n) \leq I_i(t_n) \\ I_i(t_n) & , \text{ if } C_{\max,i}^l V(t_n) \geq I_i(t_n) \end{cases}$$

where $V(t_n)$ is the total volume of brine in the repository at the n th timestep. PANEL assumes the j th isotope of the i th element sorbs onto large colloids in the same proportion that the j th isotope occurs in the inventory itself. Thus, the resultant concentration of the j th isotope of the i th element due to sorption onto large colloids is

$$C_{i,j}^l(t_n) = [I_{i,j}(t_n) / I_i(t_n)] m_{i,j}^l(t_n) / V(t_n) ,$$

where $I_{i,j}(t_n)$ is the number of moles of the j th isotope of the i th element in the repository.

PANEL then corrects the inventory to account for sorption onto large colloids during that timestep. The corrected inventory is given by $I'(t_n)$, where

$$I'_i(t_n) = I_i(t_n) - m^l_i(t_n)$$

At present, numerical values of $C_{\max,i}^l$ are not available in the controlled WIPP database. Consequently, its values are specified within PANEL and are presently set at 10^{-7} moles/l for all inventoried elements within the repository that are to be mobilized for removal.

F.2 SMALL COLLOIDS

At each timestep, PANEL combines the masses (in moles) of all the isotopes of every element present in the repository. Then, to each $V(t_n)$ liters of brine in the repository, PANEL assigns exactly $V(t_n) C_{\max,i}^s$ moles of each radioactive element to be sorbed onto small colloidal particles, assuming that amount is available in the repository. If that amount is not available, PANEL assigns whatever amount remains in the inventory, namely, $I'_i(t_n)$. Thus, at the n th timestep, the amount (in moles) of i th element in the repository sorbed onto small colloids is

$$m^s_i(t_n) = \begin{cases} C_{\max,i}^s V(t_n) & , \text{ if } C_{\max,i}^s V(t_n) \leq I'_i(t_n) \\ I'_i(t_n) & , \text{ if } C_{\max,i}^s V(t_n) \geq I'_i(t_n) \end{cases}$$

where $V(t_n)$ is the volume of brine in the repository at the n th timestep, and I'_i is the inventory of the i th element adjusted for sorption onto large colloids. PANEL assumes the j th isotope of the i th element sorbs onto small colloids in the same proportion that it occurs in the inventory itself. Thus, the resultant concentration of the j th isotope of the i th element due to sorption onto small colloids is

$$C_{i,j}^s(t_n) = [I_{i,j}(t_n) / I_i(t_n)] m^s_i(t_n) / V(t_n)$$

In the above equation, note that although the inventory $I_i(t_n)$ changes due to sorption onto large colloids, the ratio $I_{i,j}(t_n) / I_i(t_n)$ does not change.

PANEL then recorrects the inventory to account, in addition, for sorption onto small colloids. The recorrected inventory becomes $I''(t_n)$, where

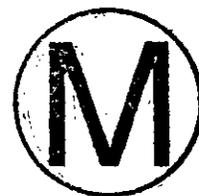
$$I''_i(t_n) = I'_i(t_n) - m^s_i(t_n)$$

At present, numerical values of $C_{max,i}^s$ are not available in the controlled WIPP database. Consequently, its values are specified within PANEL and are presently set at 2×10^{-6} moles/l for all inventoried elements in the repository that are to be mobilized for removal.

Overiewing the behavior of colloidal sorption from $t = 0$, the colloidal load for a given isotope will quickly rise from its initial value to a maximum (saturation) and remain there until the stores of that isotope can no longer maintain maximum saturation. If that event occurs before 10,000 years, it will affect the PA release response for that isotope. Specifically, uncontaminated brine will continue to enter the repository, but, because excess inventory stores have been depleted, except for production of that element as a daughter, the incoming nuclide-free brine will mix as is with the near-maximally loaded contents of the wetted repository. As a result, the concentration of that element will slowly decrease in the repository.

In the actual sorption calculation as it is written in the code, a multiplicative factor of 1000 appears in the colloidal mobilization equation. It represents the number of liters in a cubic meter and accounts for the fact that brine volume (from BRAGFLO via NUTS) is reported in cubic meters, but is required in liters for PANEL's adsorption calculation.

PANEL calculates the mobilized mass of each isotope in moles. However, the next code in the sequence (SECOFL2D) prefers to receive the mobilized mass to date in kilograms. That conversion involves multiplication by a constant, namely $W_i/1000$, where W_i is the atomic weight of the i th isotope (in grams per mole) and 1000 is the number of grams in a kilogram. The conversion is performed by PANEL.



END OF APPENDIX G

APPENDIX H: PANEL'S OXIDATION-STATE SAMPLING SCHEME (NOT AVAILABLE FOR THE CCA PA)

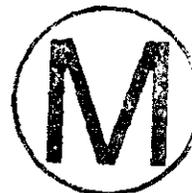
PANEL includes a random sampling scheme that apportions each element into its possible oxidation states. The scheme is unavailable for CCA calculations and so is *not* to be regarded as part of PANEL's QAed software documentation. However, for information and completeness, the scheme is described in this appendix.

Chemical solubility depends on the oxidation state of the compound to be dissolved. Because the oxidation states of the radioisotopes in the repository inventory are not known, nor are they readily knowable, a sampling method was devised to estimate the breadth of possibilities. It subdivides the amount of a radioactive element present in the repository into its various possible valence states using four randomly-generated numbers whose values vary between zero and unity. They are called RAN1, RAN2, RAN3, and RAN4, and are related to the 6th, 3rd, 4th, and 5th valence states, respectively. Once the four random numbers have been generated for a given realization, the sampling method is as follows:

- The mass of valence-state-6 uranium is taken to be the entire inventory mass of uranium corrected for suspended uranium times $0.2 \times \text{RAN1}$. The remainder is taken to be the mass of valence-state-4 uranium.
- The mass of valence-state-6 plutonium is taken to be the entire inventory mass corrected for suspended plutonium times $0.2 \times \text{RAN1}$. The remaining plutonium is taken to be distributed over the three remaining valence states 3, 4, and 5 in the following proportions: $\text{RAN2}/\text{SUM1}$, $\text{RAN3}/\text{SUM1}$, and $\text{RAN4}/\text{SUM1}$, respectively, where $\text{SUM1} = \text{RAN2} + \text{RAN3} + \text{RAN4}$.
- Thorium is assumed to exist entirely in valence state 4.
- The inventory mass of neptunium corrected for the amount sorbed onto colloidal particles is apportioned between valence states 4 and 5 in the proportions $\text{RAN3}/\text{SUM2}$ and $\text{RAN4}/\text{SUM2}$, respectively, where SUM2 is $\text{RAN3} + \text{RAN4}$.
- The entire inventory mass of americium, corrected for sorption, is assumed to occur in valence state 3.

For example: Suppose the four randomly-generated numbers for the present realization are $\text{RAN1} = 0.5$, $\text{RAN2} = 0.4$, $\text{RAN3} = 0.6$, and $\text{RAN4} = 0.2$. Suppose further, the amount of plutonium available for dissolution at the n th timestep is $I'_n(\text{Pu})$. Then the amounts of plutonium assigned to the four possible valence states are as follows:

Valence State	Amount
6	$[I'_n(\text{Pu})][0.2][0.5] = 0.1 I'_n(\text{Pu})$
3	$[I'_n(\text{Pu})][1-0.1][0.4/(0.4 + 0.6 + 0.2)] = 0.30 I'_n(\text{Pu})$



$$\begin{aligned} 4 & \quad [\Gamma'_n(\text{Pu})][1-0.1][0.6/(0.4 + 0.6 + 0.2)] = 0.45 \Gamma'_n(\text{Pu}) \\ 5 & \quad [\Gamma'_n(\text{Pu})][1-0.1][0.2/(0.4 + 0.6 + 0.2)] = 0.15 \Gamma'_n(\text{Pu}) \end{aligned}$$

Thus, the entire available mass of plutonium is apportioned 10% to valence state 6, 30% to valence state 3, 45% to valence state 4, and 15% to valence state 5. In the same realization (i.e., using the same numerical values for the four random numbers), the entire available mass of neptunium would be apportioned 75% in valence state 4 and 25% in valence state 5, that is, $0.6/(0.6+0.2)$ and $0.2/(0.6+0.2)$. The random numbers would, of course, change for each realization.

Each valence state has a different solubility. Using these different solubilities and the amounts of each element apportioned into the various possible valence states, the dissolved concentration of each valence state of each element is calculated using the formulation given above. The fractional concentrations (in moles/l) for all the possible valence states of an element are then added. The sum, multiplied by the volume of repository brine removed during that timestep, represents the mass transport (in moles) of that element due to dissolution during that timestep. As was the case for transport due to sorption, the final results are apportioned to the various isotopes of each element present in the repository according to the present fractional distribution of isotopes in the repository. These amounts are added timestep for timestep to form a running total release. Finally, the final results are converted to kilograms (i.e., multiplied by molecular weight [in grams per mole] divided by 1000) in preparation for input to the next code in the PA sequence.

It remains (i) to discuss PANEL's decay model, (ii) to review, in summary form, the calculation by which radioisotopes are removed from the repository, and (iii) to discuss adjustments of the inventory to account for removal from the repository. Those topics are discussed sequentially in the sections that follow. However, we state here that once all of those things have taken place, that is, once a timestep's worth of radionuclides have been removed from the repository and the inventory has been decayed, PANEL allows the fractional distribution of elements to the various valence states to readjust themselves to their initial (i.e., prior to dissolution) ratios as determined by the random sampling scheme. That readjustment takes place before the $n+1$ st timestep's calculation is begun. Thus, if, say, the 6th valence state suffers a large removal in one timestep, compared to other valence states, PANEL will assume chemical reactions take place that resupply valence state 6 at the expense of the other valence states, until the overall ratio of valence states is returned to its original distribution in time for the next 50-year timestep.

END OF APPENDIX H

APPENDIX I: QA REVIEW FORMS

As a convenience to users, this section contains a complete history of all the Quality-Assurance Review Forms issued during the review of this User's Manual. Review forms are issued after the User's Manual has been completed and reviewed. Thus, they will be appended to the manual after it has been paginated and therefore they may not, themselves, be paginated.

END OF APPENDIX I

END OF THE USER'S MANUAL

NOTE: Copies of the User's Manual Reviewer's Forms are available in the Sandia WIPP Central Files.

