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1. Purpose

The Monitored Geologic Repository (MGR) Waste Package Operations of the Civilian Radioactive Waste Management System Management & Operating (CRWMS M&O) contractor performed calculations to provide input to the design of a waste package (WP). This document analyzes the degradation processes of two types of pressurized water reactor (PWR) spent nuclear fuel (SNF):

- Fuel fabricated from low enriched uranium oxide, which has been used, or will be used, in commercial nuclear power plants. This SNF is referred to as LEU (low enriched uranium) SNF.
- Fuel fabricated from plutonium oxide and uranium oxide, which may be used in commercial nuclear power plants in the future. This fuel has not yet been fabricated. It is referred to as MOX (mixed oxide) SNF.

The specific objectives were to determine the geochemical conditions under which:

1) The criticality control material suggested for this design will remain in the degraded waste package after the corrosion/dissolution of its initial form (such that it can be effective in preventing criticality), and

2) The fissile plutonium and uranium will be carried out of the degraded waste package by infiltrating water (such that internal criticality is no longer possible, but the possibility of external criticality may be enhanced).

The results will be used to determine the nominal chemical composition for the criticality evaluations of the waste package design, and to suggest the range of parametric variations for additional evaluations. These chemical compositions (and consequent criticality evaluations) are determined for time periods up to 100,000 years because it is considered likely that the US Nuclear Regulatory Commission will require demonstration of criticality control for longer than 10,000 years. This longer time frame extends the calculations closer to the 1 million years time horizon recently recommended by the National Academy of Sciences to the Environmental Protection Agency for performance assessment related to a nuclear repository (National Research Council, 1995, Ref. 1).

Boron (B) in the form of borated stainless steel was included in the calculations, as were various neutron absorbing fission products, notably Gd and Nd. These elements are important for inclusion in calculations of WP internal criticality. The results of this analysis will be used to ensure that the type and amount of criticality control material used in the waste package design will prevent criticality.

2. Method

The method used for this analysis involves the following steps:

Use of basic EQ3/6 (software package, see Section 4.1) capability for tracing the progress of reactions with evolution of the chemistry, including the estimation of the concentrations remaining in solution and the composition of the precipitated solids. (EQ3 is used to set up EQ6 calculations; it does not simulate reaction progress.)

Evaluation of available data on the range of dissolution rates for the materials involved, to be used as material/species input for each time step.

Use of "pseudo flow-through" mode in which:

1) Water is added continuously to the waste package and builds up in the waste package over a sequence of time steps (typically 15 to 18 steps per sequence, except for the initial sequence). The first sequence typically ranges from 200 to 600 steps. The duration of a time step modeled for the individual EQ6 time steps range from 0.01 seconds to 1000 days as determined automatically by the

first sequence typically ranges from 200 to 600 steps. The duration of a time step modeled for the individual EQ6 time steps range from 0.01 seconds to 1000 days as determined automatically by the program. The modeled duration of a sequence, including the initial sequence, stays constant within the limits imposed internally by the program. This time is determined from the selected drip rate, e.g., 0.15 m^3/yr entering the WP, and the percentage of added water selected. This percentage is set at 10% at the beginning of a set of runs, and typically increased to 100% to enable modeling of very long times after initial relatively rapid chemical changes have settled down to a quasi-steady state.

2) Flushing action (removal of water added during one EQ6 sequence) is simulated by specifying smaller amounts of water and solutes for input to the next EQ6 sequence than were present at the end of the preceding sequence. The mass of water simulated as removed equals the mass of water added, adjusted for water calculated to enter, or released from, solids. Solutes are removed in proportion to their concentrations in that mass of water.

Determination of fissile concentrations in solution as a function of time (from the output of EQ6 sequences over times up to or somewhat greater than 100,000 years).

Calculation of the amount of fissile material released from the waste package as a function of time (which thereby reduces the chance of criticality within the waste package).

Determination of concentrations of neutron absorbers, such as B and Gd, in solution as a function of time (from the output of EQ6 sequences over times up to or somewhat greater than 100,000 years).

Calculation of the amount of neutron absorbers retained within the waste package as a function of time.

Further detail on the specific methods employed for each step is available in Section 5 of this set of calculations.

3. Assumptions

All assumptions are for preliminary design; these assumptions will require verification before this analysis can be used to support procurement, fabrication, or construction activities. All assumptions are used throughout Section 5.

3.1 It is assumed that J-13 well water fills all voids within waste packages. It is further assumed that the composition of this water will remain as given in Harrer et al., 1990 (Ref. 2) for up to 100,000 years. The basis for the first part of this assumption is that it provides the maximum degradation rate with the potential for the fastest flushing of the neutron absorber from the DOE SNF canister and from the waste package, and is, thereby conservative. The basis for the second part of the assumption is that there is no basis for predicting any change in this composition over a 100,000-year time period, although for a few thousand years after waste emplacement the composition may differ because of perturbations resulting from reactions with engineered materials and from the thermal pulse. These are not taken into account in this calculation because the corrosion allowance and corrosion resistant barriers are not expected to breach until after that perturbed period. Therefore, the early perturbation is not relevant to the calculations reported in this document. See Assumption 3.3.

3.2 It is assumed that the density of J-13 well water is 1.0 g/cm^3. The basis is that for dilute solutions, the density differs extremely little from that for pure water and that any differences are insignificant in respect to other uncertainties in the data and calculations. Moreover, this number is used only initially in EQ3/6 to convert concentrations of dissolved substances from parts per million to molalities.

3.3 The assumption that the water entering the waste package can be approximated by the J-13 water implicitly assumes: (1) that the infiltrating water will have only a minimal contact, if any at all, with undegraded metal in the corrosion allowance barrier, and (2) that any effects of contact with the drift liner will be minimal after a few thousand years. The basis for the first part of this assumption is that the water should move rapidly enough through openings in the waste package barriers that its residence time in the corroded barrier will be too small for significant reaction to occur. Furthermore, the water flowing through the barriers will be in contact with the corrosion products left from the barrier corrosion that created the holes in the first place, but these corrosion products will closely resemble iron oxides and hydroxides in the overlying rock. Consequently, the water should already be close to equilibrium with these compounds and would be unaffected by further contact with them, even if it flowed slowly enough to permit significant reaction. The second part of this assumption is justified by the following: (1) The drift liner at the top of the drift is expected to collapse with the roof support well before 1000 years. (2) The water flowing through the concrete liner, dominantly along fractures, will be in contact with the degradation products of the liner which will have come close to equilibrium with the water moving through the rock above the repository. Interaction of water in the fractures with any undegraded concrete between fractures would be minimal owing to the slow rate of diffusion through the matrix compared to rate of flow through fractures.

3.4 It is assumed water may circulate freely enough in the partially degraded WP that all degraded solid products may react with each other through the aqueous solution medium. The basis is that this provides one bound for the extent of chemical interactions within the WP and conservatively simulates potential preferential loss of neutron absorbers from the waste package by facilitating contact of any acid, which may result from corrosion of steel, with neutron absorbers in spent fuel.

3.5 It has been assumed that the database supplied with the EQ3/6 computer package is sufficiently accurate for the purposes of this report. The basis is that the data have been carefully scrutinized by many experts over the course of several decades and carefully selected by Lawrence Livermore National Laboratory (LLNL) for incorporation into the data base (Wolery, 1992a, Ref. 3; Daveler and Wolery, 1992, Ref. 4; Wolery, 1992b, Ref. 5; Wolery and Daveler, 1992, Ref. 6). These databases are periodically updated and/or new databases added, such as one including extensive data on the lanthanides (Spahiu and Bruno, 1995, Ref. 7). Every run of either EQ3 or EQ6 documents automatically which database is used. The databases include references internally for the sources of the data. The reader is referred to this documentation, included in electronic files labeled data0 that accompany this report, for details. Nevertheless, this review and documentation do not absolutely guarantee that all the data are adequate.

3.6 In general it is assumed that chromium and molybdenum will oxidize fully to chromate (or dichromate) and molybdate, respectively. This is based on the available thermodynamic data, which indicate that in the presence of air the chromium and molybdenum would both oxidize to the +6 valence state. Laboratory observation of the corrosion of Cr and Mo containing steels and alloys, however, indicates that any such oxidation would be extremely slow. It in fact may not occur at a significant rate in respect to the time frame of interest. For the present analyses, the assumption is made that over the times of concern the oxidation will occur. This is conservative for times of several thousand years after waste package breach, when the high pH solution from any drift liner effects, has been flushed out of the waste package. Acidification of the water will enhance solubility and transport of neutron absorbers out of the WP thereby separating it preferentially from fissile material.

3.7 It is assumed that the inner corrosion resistant barrier will react so slowly with the infiltrating water as to have negligible effect on the chemistry. The bases consist of the facts that this metal corrodes very slowly compared: (1) to other reactions in the waste package, and (2) to the rate at which soluble corrosion products will likely be flushed from the package.

3.8 It is assumed that gases in the solution in the waste package will remain in equilibrium with the ambient atmosphere outside the waste package. In other words, it is assumed that there is sufficient contact with the gas phase in the repository to maintain equilibrium with the CO_2 and O_2 present, whether or not this be the hence on the solubility of uranium, gadolinium, and other elements. As discussed in CRWMS M&O, 1997a (Ref. 8), the measured composition of J-13 water is not in equilibrium with the partial pressure of CO_2 in the atmosphere. By adjusting the average measured composition of the water slightly, well within the standard deviation of the measurements, it is possible to determine a partial pressure of CO_2 nearly ten times atmospheric (Yang, et al., 1996, Ref. 9, Table 8, and Weast, 1977, Ref. 10, p. F-210), with which this water was apparently in equilibrium at depth in the well. Computer runs j13avg1.3o, j13avg19.3o, j13avg20.6o, and j13avg21.6o (provided on tape, CRWMS M&O, 1998a, Ref. 11) show the details of these adjustments. This high partial pressure is close to the maximum found by measurement of the rock gas composition (Yang, et al., 1996, Ref. 9, Table 8). Therefore this high partial pressure was conservatively chosen for the computer runs used in this analysis. The basis for this assumption is that it minimizes the pH and thereby conservatively maximizes the solubility of Gd and the likelihood that this neutron absorber can be separated from the U. The high CO_2 tends to increase the concentration of free carbonate ion and its complexation with the dissolved U (uranyl ion), thereby tending to increase the solubility of U, but this is moderated by the reduction of the pH. There is little overall net effect for otherwise comparable conditions.

3.9 It is assumed that all solids that are deposited remain in place; no solids are entrained or otherwise re-mobilized, except possibly by dissolving at a later time. The basis for this assumption is that it conservatively maximizes the size of potential deposits of fissile material inside the WP.

3.10 It is assumed that the corrosion rates will not be significantly enhanced by biologically mediated corrosion. The bases for this assumption are that even at the time that the repository is closed there will be little organic material present to serve as nutrients for biological activity and that by the time the corrosion barriers are breached essentially all of such material will most likely have decayed to carbon dioxide and dissipated. Whereas a few organisms can use CO_2 directly as a nutrient and two other essential factors necessary for biological activity are present (water and an energy source, in this case chemical disequilibrium between the metal and atmospheric oxygen), the impact on corrosion is likely to be low and the effect on the chemistry of fissile isotopes and neutron absorbers is expected to be negligible.

3.11 It is assumed that sufficient decay heat is retained within the waste package over times of interest to cause convective circulation and mixing of the water inside the package. The basis for this assumption is discussed in CRWMS M&O, 1996 (Ref. 12, p. 5-7).

3.12 It is assumed that the alkalinity reported in analyses of J-13 water correspond to bicarbonate (HCO_3^-) alkalinity. Contributors to alkalinity in J-13 water, in addition to bicarbonate, potentially include borate, phosphate, and silicate. However, at pH less than 9 the contribution of silicate will be small, and in any case the concentrations of all three of these components in J-13 water is small. Fluoride ion will not contribute to a typical measured alkalinity because the titration will not be carried out to a sufficiently low pH for its influence to be detectable. Nitrate will likewise not contribute. The validity of this assumption is justified by the observation that the calculated electrical neutrality, using the assumption, is zero within the analytical uncertainty, as it should be. The same assumption is implicitly made by Harrar et al., 1990 (Ref. 2, Table 4.1, p. 4.2).

3.13 It is assumed that the rate of entry of water into, as well as the rate of egress from, a waste package is equal to the rate at which water drips onto the package. For most of the time frame of interest, i.e., long after the corrosion barriers become largely degraded, it is more reasonable to assume that all or most of the drip will enter the degraded package than to assume that a significant portion will instead be diverted around the remains. Diversion of the water with a consequent lower entry rate has not been incorporated into the present calculations.

3.14 It is assumed that the most insoluble solids for a fissile radionuclide will form, i.e., that equilibrium will be

3.14 It is assumed that the most insoluble solids for a fissile radionuclide will form, i.e., that equilibrium will be reached. This is conservative for internal criticality because the assumption will lead to simulation for maximal retention of fissile material within the waste package.

3.15 It was assumed that the degradation rate for alloy SB-209 A96061 T4 (hereafter referred to as Al alloy) is such that the alloy will last for 200 years. The corrosion rate under conditions applicable to Yucca Mountain appears not to be well known. However, common experience derived from observations of the durability of aluminum window frames and other widely used aluminum items indicates that it will persist for several decades. On the other hand corrosion of the aluminum does occur, as evidenced by the buildup of white solid products over such time frames. This suggests that the alloy will corrode entirely in a few centuries. The exact lifetime of the alloy is of only minor importance to the chemical simulation so long as it is modeled as corroding much faster than the stainless steels.

4. Use of Computer Software

This section describes the computer software used to carry out the analysis.

4.1 EQ3/6 Software Package

The EQ3/6 software package originated in the mid-1970's at Northwestern University (Wolery, 1992a, Ref. 3). Since 1978 Lawrence Livermore National Laboratory has been responsible for its maintenance. It has most recently been maintained under the sponsorship of the Civilian Radioactive Waste Management Program of the U.S. Department of Energy. The major components of the EQ3/6 package include: EQ3NR, a speciation-solubility code; EQ6, a reaction path code which models water/rock interaction or fluid mixing in either a pure reaction progress mode or a time mode; EQPT, a data file preprocessor; EQLIB, a supporting software library; and several (>5) supporting thermodynamic data files. The software deals with the concepts of the thermodynamic equilibrium, thermodynamic disequilibrium, and reaction kinetics. The supporting data files contain both standard state and activity coefficient-related data. Most of the data files support the use of the Davies or B-dot equations for the activity coefficients; two others support the use of Pitzer's equations. The temperature range of the thermodynamic data on the data files varies from 25 °C only for some species to a full range of 0-300 °C for others. EQPT takes a formatted data file (a data0 file) and writes an unformatted near-equivalent called a data1 file, which is actually the form read by EQ3NR and EQ6. EQ3NR is useful for analyzing groundwater chemistry data, calculating solubility limits and determining whether certain reactions are in states of partial equilibrium or disequilibrium. EQ3NR is also required to initialize an EQ6 calculation.

EQ6 models the consequences of reacting an aqueous solution with a set of reactants which react irreversibly. It can also model fluid mixing and the consequences of changes in temperature. This code operates both in a pure reaction progress frame and in a time frame. In a time frame calculation, the user specifies rate laws for the progress of the irreversible reactions. Otherwise, only relative rates are specified. EQ3NR and EQ6 use a hybrid Newton-Raphson technique to make thermodynamic calculations. This is supported by a set of algorithms which create and optimize starting values. EQ6 uses an ordinary differential equation integration algorithm to solve rate equations in time mode. The codes in the EQ3/6 package are written in FORTRAN 77 and have been developed to run under the UNIX operating system on computers ranging from workstations to supercomputers. Further information on the codes of the EQ3/6 package is provided in Wolery (1992a and 1992b, Refs. 3 and 5), Daveler and Wolery (1992, Ref. 4), and Wolery and Daveler (1992, Ref. 6).

In this study EQ3/6 was used to provide:

1) a general overview of the nature of chemical reactions to be expected,
2) the degradation products likely to result from corrosion of the waste forms and canisters, and
3) an indication of the minerals, and their amounts, likely to precipitate within the WP.

The programs have not been used outside the range of parameters for which they have been verified. The EQ3/6 calculations reported in this document used version 7.2b of the code, which is appropriate for the application, and were executed on the Hewlett-Packard (HP) 9000 Series 735 workstation and on Pentium personal computers (PCs). The source codes were obtained from Software Configuration Management in accordance with M&O QAP-SI-3.

The EQ3/6 package has been verified by its present custodian, Lawrence Livermore National Laboratory, and has been installed under the Management and Operating Contractor Quality Administrative Procedure (M&O QAP-SI-3) prior to performing the calculations reported in Section 5. However, the documentation (the Installation and Test Report) for this installation has not yet received all required signatures. Therefore all the results are considered "to be verified" (TBV) with respect to any design or procurement decisions or specifications.

4.2 Software Routines for Chaining Successive EQ6 Cases

The following software routines were developed specifically for this study for the purpose of facilitating the setup and execution of successive cases of EQ6, by transforming the output of one case to the input of the following case. An individual EQ6 run diluted the solution constituents to reflect the inflow of fresh water and the routines periodically remove water and solutes corresponding to the inflow. The routines also read the output of one run and reformat it as input for the next run. The data reformatting aspect of these routines was verified by visual inspection in accordance with QAP-SI-0, 5.3.2C by an individual independent of the person doing the original development. The mathematical algorithms for these routines are given in Attachment I. An individual independent of the person doing the original development verified the calculations by hand in accordance with QAP-SI-0, 5.3.2C. Both the program and the hand calculation are documented in Attachment II, in accordance with QAP-SI-0, 5.3.2D. The routines were originally developed for a Hewlett-Packard HP 6000 computer (UNIX operating system), and were subsequently modified slightly for use on PCs. Both versions have been checked. The CSCI numbers apply to both the HP and the corresponding PC versions. Both file names are provided in Section 4.2 subsections below.

4.2.1 Files bldinput.bat (for HP), CSCI# 30044 V1.0

This is a routine which does the following:

1) runs the program bldinput.c which builds the initial input (bldinput.out) for the sequence of EQ6 runs,
2) executes the initial iteration of EQ6,
3) runs the program (nxtinput.c) to transfer the output from one iteration to the input of the next iteration,
4) runs the next iteration of EQ6, and

condition occurs (which causes nxtinput.c to write an error message to a file which is read and interpreted by this script file).

(This HP routine is actually not needed, inasmuch as others can accomplish the same result. A corresponding routine was not implemented for PCs.)

4.2.2 File bldinput.c, CSCI# 30045 V1.0

This C program builds the EQ3/6 input from a template and an input file containing filename (internally, it's called "root" in the supplementary input file, "bldinput.in"), date, and maximum simulation time. (This HP routine is actually not needed, inasmuch as nxtinput.c can accomplish the same result. A corresponding routine was not implemented for PCs.)

4.2.3 Files nxtinput.bat (for HP), CSCI# 30046 V1.0, and nxti_bat.c (for PC), CSCI# 30046 V1.1

This shell script runs the same iteration loop as bldinput.bat, but starts from the output of a previous iteration.

4.2.4 File nxtinput.c (for both HP and PC), CSCI# 30047 V1.0

This C program reads the output and pickup (program file names) files of an EQ3/6 iteration and generates the input file for the next iteration. In this process it makes two basic data changes:

1) the amounts of all the species in solution are reduced to simulate the flushing out of an amount of solution corresponding to an infusion of fresh J-13 water into the waste package as calculated by EQ6, and

2) some alternative species are switched into, or out of, the basis set for the chemical reactions, according to which member of the alternative set has achieved the largest concentration.

4.2.5 Files Allpost.bat (for HP), CSCI# 30050 V1.0 and Allp_bat.c (for PC), CSCI# 30050 V1.1

This shell script operates in essentially the same was as do bldinput.bat and nxtinput.bat, but in addition runs the C program postproc.c and deletes the allout files produced by these programs after the desired data have been extracted. This deletion avoids complete filling of available file space.

4.2.6 Files PostprocP.c (for HP), CSCI# 30049 V1.1, and postprocP.c (for PC), CSCI# 30049 V1.2

This C program was originally written for a different problem, and was modified to expand its capabilities for the present application. The expanded "P" version was verified in the same manner as was the original. This C program locates specific data outputs in the concatenated EQ6 output files generated by running the programs, bldinput.c and nxtinput.c, and copies the selected data to a separate file to facilitate analysis and entry into spreadsheets.

4.2.7 Files Lastpost.c (for both HP and PC), CSCI# 30051 V1.0

This C program processes the output of allpost.bat and reduces the still extensive output to a form more amenable to plotting by selecting only every tenth output line.

4.3 Pro/Engineer version 17.0

Pro/Engineer is drafting software that is used to produce WP drawings and is not required to be qualified under the M&O QAP SI series procedures. Based on the component dimensions used to create the drawings, Pro/Engineer provides the option of determining the volume, surface area, and other parameters for the component. This Pro/Engineer volume information for the 21 PWR LEU WP components is included as Attachment III, and is summarized in Table 5.1.1.1-3.

4.4 Spreadsheets

Spreadsheet analyses were performed with Microsoft Excel version 97, loaded on a PC. The specific spreadsheets used for results reported in this document are included for reference on electronic tape (Ref. 11).

4.5 Software Approved for QA Work

The software package, EQ3/6, Version 7.2b, was approved for quality assurance (QA) work by LLNL (Memorandum to File from Royce E. Monks, dated March 28, 1997, QA designator 97/026). Before computer runs were performed, the codes were installed and tested on the computers used in accordance with the requirements of CRWMS M&O, 1997b (Ref. 13). However, the documentation for this installation and testing has not yet been completed. The input files used are echoed in the output files. The output files are listed in Ref. 11.

5. Calculations

The general scheme of the calculations starts with obtaining data for compositions, amounts, surface areas, and reaction rates of the various components of the PWR LEU and PWR MOX waste packages. These quantities are recalculated to the form required for entry into EQ6; mostly this consists of making such conversions as weight percentages of elements or component oxides to mole fractions of elements, degradation rates in micrometers/year into moles per square centimeter per second, etc. Attached spreadsheets (Ref. 11) provide details of these calculations. The final part of the input to EQ6 consists of the composition of J-13 well water together with a rate of influx into the waste package that corresponds to suitably chosen percolation rates into a drift and drip rate into a waste package (see Section 5.1.1.3). From time to time the water added to the waste package from this simulated influx is removed, together with its solutes, to approximate reactive flow and transport through the waste package via routines described in Section 4.2.1. The EQ6 output provides the results of modeling of the chemical degradation of the waste package, or components thereof. Sometimes the degradation of the waste package is divided into phases, e.g., degradation of basket materials before breach of the Zircaloy cladding and exposure of the spent fuel to the water. The results include the compositions and amounts of solid products and of substances in solution. Details of the results are presented below and in Ref. 11.

The number of digits cited for values converted from English to metric units does not indicate the accuracy; it is an artifact of the conversion process.

5.1 Calculation Inputs

5.1.1 WP Materials and Performance Parameters

This section provides a brief overview of the chemical characteristics of PWR LEU and PWR MOX waste packages. The emphasis is on the chemical composition and reactivity, rather than on the physical configurations within different waste packages, although the configurations were used for volume calculations to determine the overall chemistries and surface areas. Material nomenclature used throughout this document is: SA-516 K02700 (hereafter referred to as A516), SB-575 N06022 (hereafter referred to as Alloy 22), SB-209 A96061 T4 (hereafter referred to as Al alloy), and SS316B6A less 20% boron (hereafter referred to as borated SS).

5.1.1.1 Chemical Characteristics of Representative Spent Nuclear Fuel (SNF) Waste Packages

A commercial spent fuel waste package will consist of 21 PWR LEU or 21 PWR MOX assemblies of spent fuel held in a basket and placed inside a corrosion barrier. The design for the corrosion barrier itself specifies an outer corrosion allowance and an inner corrosion resistant metal. For modeling the chemical behavior of this system, the chemical compositions of each of these materials, their masses, their surface areas, and their corrosion or degradation rates are required. As explained in Assumptions 3.1, 3.3, and 3.7, an exception is made for the materials of the corrosion barrier and for Zircaloy cladding, which are not included in the modeling. Tables 5.1.1.1-1 shows data for commercial SNF. Tables 5.1.1.1-3 through 5.1.1.1-7 show the data used that are specific to SNF, both LEU and MOX.

Table 5.1.1.1-1. Elemental Composition in Gram-atoms/Assembly for 4.9%, 34 GWd/MTU B&W 15x15 PWR LEU Fuel Assembly

	Age of Fuel				Age of Fuel	
Element	10000.0 yr	25000.0 yr		Element	10000.0 yr	25000.0 yr
He	9.21E+00	1.40E+01		Y	2.71E+00	2.71E+00
Tl	1.03E-13	2.37E-13		Zr	2.10E+01	2.09E+01
Pb	7.67E-04	5.80E-03		Nb	1.16E-02	2.88E-02
Bi	5.41E-05	6.87E-04		Mo	1.65E+01	1.65E+01
Po	9.32E-08	2.53E-07		Tc	3.73E+00	3.55E+00
At	2.33E-17	1.06E-16		Ru	9.90E+00	1.01E+01
Rn	2.58E-09	6.98E-09		Rh	2.16E+00	2.16E+00
Fr	2.19E-13	9.81E-13		Pd	5.03E+00	5.02E+00
Ra	3.94E-04	1.07E-03		Ag	3.09E-01	3.10E-01
Ac	2.43E-07	5.52E-07		Cd	2.85E-01	2.85E-01
Th	2.77E-02	6.56E-02		In	5.45E-03	5.45E-03
Pa	3.65E-04	8.25E-04		Sn	1.73E-01	1.67E-01
U	1.86E+03	1.87E+03		Sb	3.02E-02	3.02E-02
Np	3.67E+00	3.65E+00		Te	1.68E+00	1.68E+00
Pu	1.21E+01	7.44E+00		I	7.83E-01	7.82E-01
Am	4.72E-02	1.15E-02		Xe	1.74E+01	1.74E+01
Cm	4.83E-04	1.39E-04		Cs	6.91E+00	6.89E+00
Bk	4.26E-25	2.35E-25		Ba	9.58E+00	9.59E+00
Cf	4.86E-14	4.64E-19		La	4.25E+00	4.25E+00
H	0.00E+00	0.00E+00		Ce	8.32E+00	8.32E+00
Li	2.02E-05	2.02E-05		Pr	3.87E+00	3.87E+00
Be	7.30E-06	7.26E-06		Nd	1.36E+01	1.36E+01
C	2.71E-07	4.41E-08		Pm	0.00E+00	0.00E+00
Zn	5.09E-08	5.09E-08		Sm	2.74E+00	2.74E+00
Ga	4.53E-07	4.53E-07		Eu	3.94E-01	3.94E-01

Ge	2.51E-03	2.51E-03		Gd	2.93E-01	2.93E-01
As	7.46E-04	7.46E-04		Tb	5.21E-03	5.21E-03
Se	3.34E-01	3.33E-01		Dy	2.49E-03	2.49E-03
Br	1.23E-01	1.23E-01		Ho	1.21E-04	1.21E-04
Kr	2.07E+00	2.07E+00		Er	2.50E-05	2.50E-05
Rb	2.14E+00	2.14E+00		Tm	6.86E-09	6.86E-09
Sr	2.04E+00	2.04E+00		Yb	1.59E-08	1.59E-08
Ref. CRWMS M&O, 1997c (Ref. 14)						

The data in Table 5.1.1.1-1 provided input to EQ6 runs. The actual input to EQ6 was reduced from the data in this table by deleting noble gases and constituents comprising less than 0.1 atom percent of the total and modified by adding oxygen equivalent to the initial U inventory (two gram-atoms of oxygen for every gram-atom of uranium). Table 5.2.1-1 shows the calculation for oxygen and the reduced data set. The weight of the SNF in one assembly is taken as 526.38 kg (CRWMS M&O, 1997c, Ref. 14).

A waste package for spent PWR MOX fuel closely resembles that for PWR LEU spent fuel. It will consist of 21 MOX assemblies of spent fuel held in a basket and placed inside a corrosion barrier. The design for the corrosion barrier itself specifies an outer corrosion allowance and an inner corrosion resistant metal. For modeling of the chemical behavior of this system, the chemical compositions of each of these materials, their masses, their surface areas, and their corrosion or degradation rates are required. An exception is made, however, for the materials of the corrosion barrier, as explained in Assumptions 3.1, 3.3, and 3.7. Table 5.1.1.1-2 shows the data used that are specific to PWR MOX SNF.

Table 5.1.1.1-2. Elemental Composition in Gram-atoms/Assembly for 4.0%, 35.6 GWd/MTU 15x15 Westinghouse PWR MOX Fuel Assembly

	Age of Fuel				Age of Fuel	
Element	10000.0 yr	25000.0 yr		Element	10000.0 yr	25000.0 yr
H	1.28E-02	1.28E-02		Te	1.91E+00	1.93E+00
He	3.59E+01	4.81E+01		I	1.11E+00	1.11E+00
Li	9.44E+00	9.44E+00		Xe	1.76E+01	1.76E+01
Be	3.65E-04	3.64E-04		Cs	6.15E+00	6.14E+00
B	9.27E-07	2.31E-06		Ba	8.80E+00	8.81E+00
C	3.53E-05	3.51E-05		La	3.62E+00	3.62E+00
N	3.28E-11	4.45E-11		Ce	7.05E+00	7.05E+00
O	8.39E-12	8.39E-12		Pr	3.33E+00	3.33E+00
F	2.11E-18	2.11E-18		Nd	1.09E+01	1.09E+01
Ne	2.22E-08	2.22E-08		Pm	0.00E+00	0.00E+00
Na	9.72E-10	9.72E-10		Sm	2.79E+00	2.79E+00
Mg	2.31E-03	2.31E-03		Eu	5.45E-01	5.45E-01
Al	7.37E-10	7.37E-10		Gd	5.14E-01	5.14E-01
Si	8.73E-02	8.73E-02		Tb	1.40E-02	1.40E-02
P	3.13E-14	3.13E-14		Dy	7.48E-03	7.48E-03
S	2.05E-18	2.05E-18		Ho	4.09E-04	4.09E-04
Zn	1.28E-07	1.28E-07		Er	9.06E-05	9.07E-05
Ga	1.05E-06	1.05E-06		Tm	2.10E-08	2.10E-08

Ge	1.83E-03	1.83E-03		Yb	5.34E-08	5.34E-08
As	6.60E-04	6.60E-04		T	1.84E-14	7.80E-14
Se	2.40E-01	2.39E-01		Pb	2.23E-04	1.75E-03
Br	9.81E-02	9.89E-02		Bi	1.21E-04	1.59E-03
Kr	1.06E+00	1.06E+00		Po	2.84E-08	7.78E-08
Rb	1.03E+00	1.03E+00		At	5.31E-17	2.47E-16
Sr	9.24E-01	9.24E-01		Rn	7.84E-10	2.15E-09
Y	1.16E+00	1.16E+00		Fr	4.85E-13	2.25E-12
Zr	1.29E+01	1.29E+01		Ra	1.20E-04	3.28E-04
Nb	7.50E-03	1.87E-02		Ac	3.48E-08	1.43E-07
Mo	1.45E+01	1.45E+01		Th	9.49E-03	2.62E-02
Tc	3.47E+00	3.30E+00		Pa	5.04E-05	2.06E-04
Ru	1.20E+01	1.21E+01		U	1.67E+03	1.69E+03
Rh	3.26E+00	3.26E+00		Np	8.62E+00	8.58E+00
Pd	1.10E+01	1.10E+01		Pu	2.93E+01	1.75E+01
Ag	8.09E-01	8.12E-01		Am	1.79E-01	4.36E-02
Cd	8.40E-01	8.40E-01		Cm	3.39E-03	9.83E-04
In	9.11E-03	9.11E-03		Bk	9.35E-25	5.15E-25
Sn	4.09E+01	4.09E+01		Cf	1.29E-13	1.22E-18
Sb	7.24E-02	7.24E-02				
Ref. CRWMS M&O, 1998b (Ref. 15)						

The data in Table 5.1.1.1-2 provided input to EQ6 runs. The actual input to EQ6 was reduced from the data in this table by deleting noble gases and constituents comprising less than 0.1 atom percent of the total and modified by adding oxygen equivalent to the initial U inventory. Table 5.2.1-2 shows the calculation for oxygen and the reduced data set. The weight of the PWR MOX SNF is taken as the sum of the light elements, 4.89 kg, actinides, 407 kg, fission products, 15.2 kg (all from CRWMS M&O, 1998b, Ref. 15), and the weight of the oxygen (calculated in Table 5.2.1-2).

Tables 5.1.1.1-3 and 5.1.1.1-4 show the basic dimensional data from which the volumes of the various components and the void space in the waste packages were calculated. Table 5.1.1.1-5 includes data on metal compositions, Table 5.1.1.1-6 tabulates the metal corrosion rates, Table 5.1.1.1-7 shows metal densities, and Table 5.1.1.1-8 includes overall waste package dimensions.

Table 5.1.1.1-3. Dimensions for Basket Components

Basket Component	Material	Volume, mm^3	Surf. Area, mm^2	Number per WP
A-Guide	CS	8.10E+06	1.68E+06	16
B-Guide	CS	9.20E+05	2.08E+05	32
Corner Guide	CS	5.34E+06	1.10E+06	16
Corner Stiffener	CS	2.95E+05	6.74E+04	32
Side Cover	CS	5.01E+05	1.16E+05	4
A-Plate	BSS	9.47E+06	2.77E+06	8
B-Plate	BSS	9.47E+06	2.77E+06	8
C-Plate	BSS	5.69E+06	1.67E+06	16
D-Plate	Al	6.74E+06	2.74E+06	8
E-Plate	Al	6.74E+06	2.74E+06	8
Tube	CS	2.09E+07	8.36E+06	21

CS = A516
BSS = Borated SS
Al = Al alloy
Data from calculations using Pro/Engineer (Attachment III)

Table 5.1.1.1-4. Basket Dimensions for Westinghouse Vantage 5 17x17 Assembly

Item	Size, inches	Page in Ref. 16
Pellet OD	0.3088	2.1.2.2-3
Rod OD	0.36	2.1.2.2-3
Assy Length	160.1	2.1.2.2-3
Guide Tube OD	0.474	2.1.2.2-3
Active Fuel Length	144	2.1.2.2-3
Clad ID	0.315	2.1.2.2-3
End Fitting Mass	12.5 kg	2.1.2.1-10

Ref. Stout and Leider, 1997 (Ref. 16)

Table 5.1.1.1-5. Metal Compositions, Weight Percent

Element	A516	Borated SS	Al Alloy
Fe	98.535%	60.639%	0.700%
B10	-	0.231%	-
B11	-	1.053%	-
B10 + B11	-	1.284%	-
Cr	-	19.061%	0.195%
Ni	-	13.543%	-
Mn	0.900%	2.006%	0.150%
Mg	-	-	1.000%
Mo	-	2.508%	-
Zn	-	-	0.250%
N	-	0.100%	-
S	0.035%	0.030%	-
Si	0.275%	0.752%	0.600%
P	0.035%	0.045%	-
C	0.220%	0.030%	-
O	-	-	-
Cu	-	-	0.275%
Ti	-	-	0.150%
Al	-	-	96.680%
Co			-
50% Nb + 50% Ta	-	-	-
Zr	-	-	-
Sn	-	-	-
V	-	-	-
W	-	-	-
Density (g/cm^3)	7.832	7.745	2.713
Reference	12	12	12, 17

Table 5.1.1.1-6. Metal Corrosion Rates

	Corrosion Rate, mm/yr			
	High (5%)	Mean	Low (95%)	
A516	0.1	0.035	0.01	CRWMS M&O, 1995 (Ref. 18)
Borated SS	0.0025	0.00025	0.00005	CRWMS M&O, 1997c (Ref. 14, pp. 11-13)

Table 5.1.1.1-7. Metal Densities

Material	Density, kg/m^3	Reference
A516	7832	CRWMS M&O, 1996b (Ref. 28)
Borated SS	7745	CRWMS M&O, 1996b (Ref. 28)
Al alloy	2713	ASME Code Table NF-2 (Ref. 17)
C 22	8691	CRWMS M&O, 1996b (Ref. 28)

Table 5.1.1.1-8. 21 PWR LEU or PWR MOX Waste Package Dimensions

Parameter	Value	Units
WP Inner Diameter	1.4234	M
WP Inner Length	4.585	M
Fuel Assembly Volume	0.081	m^3
Data from CRWMS M&O, 1997c (Ref. 14) and CRWMS M&O, 1997d (Ref. 19)		

The surface area for both LEU SNF and MOX SNF is taken to be 39.6 cm^2/g (CRWMS M&O, 1995, Ref.14, p. 6-3). The degradation rate for both LEU SNF and MOX SNF is taken to be 1.24 $g/m^2/yr$ (CRWMS M&O, 1997e, Ref. 20). This is the rate reported for the mid range of both carbonate concentration and pH.

5.1.1.2 Chemical Composition of J-13 Well Water

It was assumed that the water composition entering the waste package would be the same as for water from well J-13 (Assumptions 3.1 and 3.3). This water has been analyzed repeatedly over a span of at least two decades (Harrer, et al., 1990, Ref. 2). This composition is reproduced in Table 5.1.1.2-1.

Table 5.1.1.2-1. Composition of J-13 Well Water

Component	Units**
Na^+	45.8
K^+	5.04
Ca^{++}	13.0
Mg^{++}	2.01
NO_3^-	8.78
Cl^-	7.14
F^-	2.18
SO_4^{--}	18.4
Si	28.5
PO_4^{---}	0.12
Alkalinity*	128.9
pH	7.41

* Assumed to be HCO_3^-
** mg/L, except for pH
Ref. Harrer, et al., 1990, Ref. 2

5.1.1.3 Drip Rate of J-13 Water into a Waste Package

It is assumed (Assumption 3.13) that the drip rate onto a waste package is the same as the rate at which water flows through the waste package. The drip rate is taken from a correlation between percolation rate and drip rate. Specifically percolation rates of 40 mm/yr and 8 mm/yr correlate with drip rates onto the waste package of 0.15 m^3/yr and 0.015 m^3/yr, respectively.

Data for the rate of influx of J-13 water into a waste package were taken from Ho and Wilson, 1998 (Ref. 21). Table 5.1.1.3-1 provides the data from this preliminary report, and Figure 5.1.1.3-1 shows the information graphically. Statements on p. 2.3-105 of Ref. 21 indicate that the drip rates correspond to an area considerably larger than the horizontal (as emplaced) cross-sectional area of waste packages. The rationale is that, in some poorly defined manner, such as movement through rubble that will fall on top of a WP, water from this larger area may drip onto the WP. A minimum rate of 0.015 m^3/yr and an approximate median value of 0.15 m^3/yr were chosen from these data for use in the present calculations. The maximum drip rate in Ref. 21 (p. 2.3-106) was set to a large value, at 10 standard deviations above the mean. The reader is referred to that document for the rationale.

Table 5.1.1.3-1. Correlation between Percolation Rate and Drip Rate onto a Waste Package (Data Taken from Tables 2.3-49 and 2.3-50 of Ref. 21)

Percolation rate, mm/yr	Mean drip rate, m^3/yr	Standard Deviation (SD)	Mean + 10 SD
3.9	0.0123	0.0159	0.1713
9.2	0.0125	0.0866	0.8785
14.6	0.0366	0.283	2.8666
73.2	0.323	0.408	4.403
213	1.2	0.4	5.2

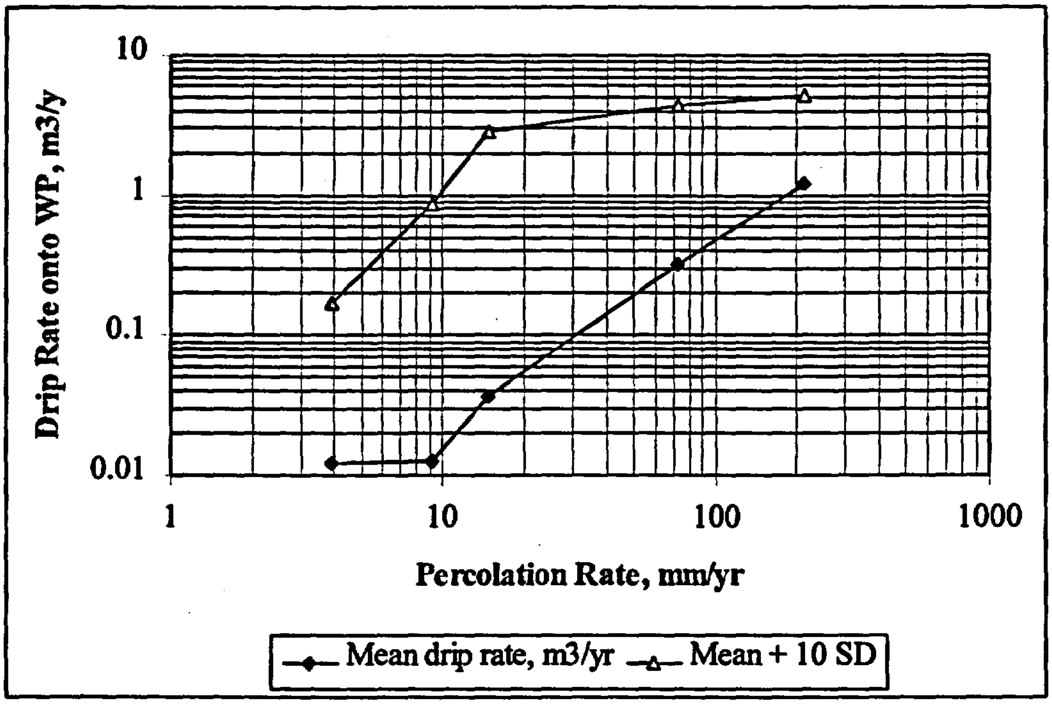

Figure 5.1.1.3-1. Percolation to drip rate correlation.

5.1.1.4 Densities and Molecular Weights of Solids

For input to criticality calculations conversions one must convert moles of solids, simulated to form, to solid volumes. Table 5.1.1.4-1 provides some of these data.

Table 5.1.1.4-1. Densities and Molecular Weights of Precipitated Solids

Solid	Density, kg/m^3	Molecular Weight[c]	Mol. Vol., cm^3/mol [c]	Calc. Dens., g/cm^3
Diaspore (AlOOH)	3400[a]	59.988	17.760	3.378
Hematite (Fe2O3)	5240[b]	159.692	30.274	5.275
Pyrolusite (MnO2)	5060[a]	86.937	17.181	5.060a
Goethite (FeOOH)		88.854	20.820	4.268
Ni2SiO4		209.463	42.610	4.916
Nontronite-Ca		424.293	131.100	3.236
Nontronite-K		430.583	135.270	3.183
Nontronite-Mg		421.691	129.760	3.250
Nontronite-Na		425.267	132.110	3.219

References:

[a] Roberts, et al., 1974 (Ref. 22)

[b] Weast, 1977 (Ref. 10)

[c] Ref. 11 (EQ3/6 Data base, data0.nuc.R8), g/mole, except for pyrolusite, which is calculated from the density and molecular weight.

Table 5.1.1.4-2 provides constants required for these conversions, and Table 5.1.1.4-3 provides thermodynamic data required for calculation of equilibrium constants for Rh.

Table 5.1.1.4-2. Miscellaneous Constants

Constant	Value	Reference
Ideal Gas Constant	83143200 erg/K/mole	10, p. F-241
Conversion, erg to cal	41840000 erg/cal	10, p F-305
Conversion, °C to K	273.15 (to be added to °C)	10, p. F-128

Table 5.1.1.4-3. Thermodynamic Data

Substance	Delta H°, kcal/mole	Delta G°, kcal/mole	S°, cal/°K/mole	Reference	Page
Rh	0	0	7.53	23	93
Rh^{+++}		55.3		24	215
RhO		-16		24	215
Rh_2O		-19.1		24	215
Rh_2O_3	-82		26.5	23 & 24, resp.	93 & 215, resp.
RhCl		-12.4		24	215
$RhCl_2$		-26.4		24	215
$RhCl_3$	-71.5		33	23 & 24, resp.	93 & 215, resp.
$RhCl_6^{---}$	-202.8		50	23 & 24, resp.	93 & 215, resp.
H_2O		-56.687		25	13
Cl^-		-31.371		25	24
$H_2(g)$		0		25	12
$O_2(g)$		0		25	11
$Cl_2(g)$		0		25	24

5.1.1.5 Atomic Weights

Atomic weights were taken from CRWMS M&O, 1996b (Ref. 28) and Walker, et al., 1989 (Ref. 26). These are listed in Ref. 11 (spreadsheet volmas21c, sheet VOLMASS).

5.2 Data Conversion

The data presented in Section 5.1 are largely not in a form suitable for entry into EQ3/6. This section presents the conversions and combinations required for input to the computer codes. Ref. 11 includes the spreadsheets for the calculations. This section includes only the results and related discussion.

5.2.1 Mole Fractions of Elements in SNF

These calculations started with the numbers of gram-atoms for the spent fuels presented in Tables 5.1.1.1-1 and 5.1.1.1-2 and the weights of the SNF. The noble gases, He, Ne, Ar, Kr, and Xe and H were deleted because they are volatile and will not be retained within the waste package following breach, except possibly for a small amount of the hydrogen, which, however, will be insignificant compared to the amount of hydrogen in the water. In addition an amount of oxygen equivalent to the uranium originally present in UO_2 in LEU SNF, or, in the case of MOX SNF,

UO_2 NpO_2, PuO_2, and AmO_2. In other words two gram-atoms of O were added for every gram-atom of U, Np, Pu, and Am. The list of elements included in the calculation was also reduced by deleting those that constitute less than 0.1 atom percent of the total. This markedly reduces the number of elements to be considered and results in significantly improved efficiency for the running of EQ6. Tables 5.2.1-1 and 5.2.1-2 show the atom fractions for the elements used for the calculations. These values were entered directly into the EQ6 input files.

Table 5.2.1-1. Elemental Composition in Atom Fraction for 21 B&W 15x15 PWR LEU Assemblies with 4.9%, 34 GWd/MTU

	Atom fraction	
Element	10000 yrs	25000 yrs
U	3.15799E-01	3.17218E-01
Np	6.23109E-04	6.19168E-04
Pu	2.05439E-03	1.26209E-03
Am	8.01383E-06	1.95080E-06
Mo	2.80144E-03	2.79898E-03
Tc	6.33296E-04	6.02205E-04
Ru	1.68087E-03	1.71332E-03
Rh	3.66735E-04	3.66412E-04
Ag	5.24634E-05	5.25869E-05
Nd	2.30907E-03	2.30704E-03
Sm	4.65210E-04	4.64800E-04
Eu	6.68951E-05	6.68363E-05
Gd	4.97469E-05	4.97031E-05
Rb	3.63339E-04	3.63019E-04
Sr	3.46360E-04	3.46056E-04
Y	4.60116E-04	4.59711E-04
Zr	3.56548E-03	3.54538E-03
Pd	8.54016E-04	8.51569E-04
Cs	1.17321E-03	1.16879E-03
Ba	1.62654E-03	1.62680E-03
La	7.21584E-04	7.20950E-04
Ce	1.41261E-03	1.41136E-03
Pr	6.57066E-04	6.56488E-04
O	6.61909E-01	6.61327E-01
Total	1.00E+00	1.00E+00

Table 5.2.1-2. Elemental Composition in Atom Fraction for 4.0%, 35.6 GWd/MTU 17x17 Westinghouse MOX SNF Fuel Assembly

	Atom fraction	
Element	10000 yrs	25000 yrs
Li	1.78390E-03	0.00000E+00
O	6.47906E-01	6.48089E-01
Rb	1.94641E-04	1.94696E-04
Sr	1.74610E-04	1.74659E-04
Y	2.19208E-04	2.19269E-04
Zr	2.43774E-03	2.43843E-03
Mo	2.74009E-03	2.74087E-03
Tc	6.55733E-04	6.23784E-04
Ru	2.26766E-03	2.28721E-03
Rh	6.16049E-04	6.16223E-04
Pd	2.07869E-03	2.07928E-03
Ag	1.52878E-04	1.53489E-04
Sn	7.73217E-03	7.73209E-03
Cs	1.16218E-03	1.16062E-03
Ba	1.66295E-03	1.66531E-03
La	6.84079E-04	6.84272E-04
Ce	1.33225E-03	1.33263E-03
Pr	6.29277E-04	6.29455E-04
Nd	2.05980E-03	2.06038E-03
Sm	5.27232E-04	5.27381E-04
Eu	1.02990E-04	1.03019E-04
Gd	9.71316E-05	9.71591E-05
U	3.15583E-01	3.19453E-01
Np	1.62894E-03	1.62184E-03
Pu	5.53688E-03	3.30794E-03
Am	3.38260E-05	8.24151E-06
Total	1.00E+00	1.00E+00

5.2.2 Atom Fractions of Elements in Basket Metals

These calculations are straight forward conversions from weight percentages of elements in the metals to atom fractions. Details are in Ref. 11. The results in Tables 5.2.2-1 through 5.2.2-3 are entered directly into EQ6 input files.

Table 5.2.2-1. Atom Fractions for A516

Element		Atom fr.
Fe		0.9742064
Mn		0.0090454
S		0.0006044
P		0.0006239
Si		0.0054063
C		0.0101134
Total		1

Table 5.2.2-2. Atom Fractions for Borated SS

Element		Atom fr.
B		0.0623405
C		0.0013154
N		0.0037597
Si		0.0140616
P		0.0016906
S		0.0004942
Cr		0.1924212
Mn		0.01917
Fe		0.5699404
Ni		0.1210848
Mo		0.0137216
Total		1

Table 5.2.2-3. Atom Fractions for Al Alloy

Element		Atom fr.
Fe		0.0034132
Mn		0.0007435
Mg		0.0112008
Zn		0.0010414
Si		0.0058174
Cu		0.0011786
Ti		0.0008528
Al		0.9757523
Total		1

5.2.3 Degradation Rates

The degradation rates, as well as the rate of influx of water, must be converted to moles/cm^2/sec for entry into EQ6. The data presented in Section 5.1.1.1 (e.g., Table 5.1.1.1-5), however, are for millimeters/yr for metals, g/m^2/yr for SNF, and m^3/yr for rate of addition of water. These conversions are all relatively simple. The conversion to moles is accomplished by determining the number of gram-atoms in some known weight of the material. For example, for the metals a weight of 100 g was taken and the number of gram-atoms of each element determined and summed. Then the weight, 100 g, divided by the number of gram-atoms yields the "molecular weight". Parallel calculations were made for the SNF and the water, even though different total weights were used for the SNF. The "molecular weights" determined in this way are listed in Table 5.2.3-1. (See Ref. 11 for details of the calculations.) (The "molecular weights" for the SNF are not actually needed because the "molecular weight" is determined by dividing the weight of SNF in an assembly by the number of gram-atoms in the assembly, as reported above in Section 5.2. The number of moles of SNF in an assembly is then calculated by dividing the weight of SNF in an assembly by the "molecular weight", which, of course, simply returns the number of gram-atoms per assembly.)

Table 5.2.3-1. Molecular Weights of Reactants

Reactant		Mol. Wt.
A516		55.215412
Borated SS		52.490083
Al alloy		27.231379
LEU SNF		90.00
MOX SNF		91.16
Water		18.00

The values of molecular weight enable the conversion of grams to moles. For metals the weight corroded is obtained from taking arbitrarily a 1 cm^2 area and multiplying by the corrosion rate converted from micrometers to cm to get the volume corroded, and by the density, to get g/cm^2/yr. Reaction rate for water is taken equal to the rate of influx, using the assumed density of 1 g/cm^3 (Assumption 3.2) to convert volume to weight. The remaining conversions involve only years to seconds. Table 5.2.3-2 compiles the results. (See Ref. 11 for details of the calculations.) It is assumed that the Al alloy will last for 200 years, and the degradation rate was adjusted to match that lifetime. See Assumption 3.15.

Table 5.2.3-2. Reaction Rates of Reactants

Reactant	Drip rate	Rate *
A516		1.573E-11
Borated SS		1.169E-13
Al alloy		1.263E-11
LEU SNF		4.419E-14
MOX SNF		4.419E-14
Water	0.5m^3/yr	1.934E-07
Water	0.15m^3/yr	5.803E-08
Water	0.015m^3/yr	5.803E-09

* Moles/cm^2/sec

The final pieces of data needed to characterize the reactants are the surface areas and moles of reactants. These must both be normalized to one kg of solvent for convenient use in EQ6 (other choices may be possible, but would be more awkward). For these purposes the dimensions of the various components of the waste package and fuel are utilized to determine the masses (from volume and density) and to determine the surface areas of the basket metals and the volume of the SNF. The volumes of these solids are then subtracted from the internal volume of the waste package to determine the volume of void space, which is assumed to be filled by J-13 water (Assumption 3.1). The masses of the metals and SNF are then divided by the mass of water, in kg, to achieve the normalization. Similarly, the surface areas of metals are normalized. The surface area of the SNF in cm^2 is taken equal to 39.6 times the weight in grams in accordance with the ratio adopted in CRWMS M&O, 1995 (Ref. 18). Table 5.2.3-3 shows the results of these calculations, which are detailed in Ref. 11.

Table 5.2.3-3. Moles and Surface Areas of Reactants/kg Water

Reactant	Moles	Area, cm^2
A516	21.64	504.16
Borated SS	7.86	156.01
Al alloy	2.36	96.42
LEU SNF	27.21	9.62E+04
MOX SNF	24.77	7.92E+04
Water*	1.00E+06	1

* Values arbitrary

5.2.4 Calculation of Equilibrium Constants for Rhodium Species

Table 5.2.4-1 compiles the results of the calculation of equilibrium constants for Rh species starting from the master basis species in the EQ3/6 data base. Full details of the calculation are provided in Ref. 11.

Table 5.2.4-1. Equilibrium Constants for Rh Species at 25°C

Species	Log K (base 10)
Rh	21.79
RhO	10.06
Rh2O	14.79
Rh2O3	-1.49
RhCl	14.92
RhCl2	6.88
RhCl3	-12.39
RhCl6---	-15.99

5.2.5 Calculations of Volumes and Surface Areas of Basket Materials

The volumes of basket materials, including the void volume, and surface areas are mostly calculated in spreadsheets included in spreadsheet volmas21 in Ref. 11. However, a small portion of these calculations, specifically for the MOX SNF waste package, were done separately in V5moxvol. This spreadsheet is also included in Ref. 11 and included here as Table 5.2.5-1.

Table 5.2.5-1. Calculation of Volumes for PWR MOX Waste Package

Item	Size[1] or Number			
Pellet OD	0.784352			
Guide Tubes/Assembly	25	endfitting mass	12.5	kg
Rods/Assembly	264	endfitting vol	1602.564	cm^3
Rod OD	0.9144			
Assembly Length	406.654	Assy. Volume	84070.78	cm^3
Guide Tube OD	1.22428	12 Assy. Vol.	1008849	cm^3
Active Fuel Length	365.76	Total Fuel Vol.	46656.49	cm^3/assy
Clad ID	0.8001			
Volume for 21 Assemblies		1.765486289	cm^3	
Surface Area of Fuel	238191.5921	cm^2		
[1] cm, converted from inches in Table 5.1.1.1-4				
Density of steel for endfitting, 7.8 g/cm^3, from CRWMS M&O, 1996b (Ref. 28)				

5.3 EQ6 Calculations and Scenarios Modeled

Three basic types of scenarios were simulated. The first simulation is for a case in which the Zircaloy cladding does not fail throughout the period of regulatory concern. In other words the degradation modeling considers only the degradation of the basket materials. Results of this simulation are shown in Figures 5.3.1-1 and 5.3.1-2. The simulation indicates that the iron will degrade to hematite, although goethite is a likely alternative, and virtually no loss of the Fe or Mn from the degraded package. Retention of Ni is very variable, evidently depending strongly on the pH history. Cr, Mo, and Tc are simulated to oxidize to soluble acid radicals and to be flushed from the package. Consequently the pH is modestly decreased.

The second type modeled consisted of cases in which the basket and fuel were exposed to water simultaneously. This is the other extreme in which the Zircaloy is fully breached immediately. For these cases the simulations show very similar results in respect to the basket materials. The fuel degrades mostly to insoluble products. A small proportion of the U is dissolved and flushed away, and a large proportion of the Gd is removed. Tables 5.3.2-1 through 5.3.2-3 and Figures 5.3.2-1 through 5.3.2-8 summarize these results. One set of runs for this type of scenario was made with suppression of hematite with the result that goethite is predicted instead. In view of the observation that goethite more commonly constitutes the bulk of the corrosion products of iron and steel, this simulation may be more realistic. The pH history differs slightly from that when hematite is simulated to form, and does to a minor extent hasten the predicted dissolution of Am and Np. The rare earth elements are comparably affected in the two cases, when account is taken of the fact that any concentration less than about 1.0E-06 molal means that effectively the rare earth element has been flushed from the system.

The final type of situation modeled an intermediate case in which the all the Zircaloy cladding would breach just after all the basket materials had fully degraded. This case isolates the interaction of the SNF from that of the degradation of the metals. Initially the pH rises slightly, evidently owing to the release of positively charged ions (cations), such as UO_2^{++}, at a slightly higher net rate than the release of negatively charged ions (anions). Because electrical neutrality must be maintained, this requires the generation of an equivalent amount of hydroxide ion, OH^-, which means that pH will rise. This situation does not persist for long, however, because as soon as the cation concentrations rise a little, the cations precipitate as insoluble compounds as they are released from the waste. Under that situation, they have no effect on the pH. However, the release of the anions, notably of Mo, Cr, and Tc, continues and the pH decreases to about 6.2, where it stays in a quasi-steady state until all of the waste is degraded. Thereafter, it rises to the normal pH of J-13 water as water continues to course through the degraded waste package. Beyond that time very little is simulated to happen; there is a slow conversion of one uranium and one Gd compound to others with no simulated (within the accuracy of the calculations) further loss of either. A little Gd is dissolved and flushed out at the lowest pHs achieved. To emphasize the potential effect of the low pH period some runs were made at the slowest drip rate. This did lower the minimum pH, but not enough to have much impact on the removal of Gd or U. Tables 5.3.3-1 and 5.3.3-2 summarize these results. Full details of all the calculations are included in Ref. 11.

5.3.1 Degradation of Basket Only

The chemical results of interest to criticality calculations for this scenario consist of the masses and volumes of solids containing Fe, Al, Ni, Mn, Si, and water. The data from the EQ6 runs for the solids, together with their densities, permit calculation of the volumes of solids and the percentage of the void space occupied by each solid. Figures 5.3.1-1 and 5.3.1-2 show the results of these calculations. The void space is calculated as that originally present plus the volume of the basket metals that have been corroded as a function of time. The increase in the volume of hematite over the first 100 years arises primarily from the corrosion of the A516. A small amount of the iron clay, nontronite, is also simulated to occur over this time frame, as is a small volume of pyrolusite, MnO_2. At about 100 years the A516 is predicted to be completely corroded, as is reflected in the sudden change in the rates of change of the space occupied by hematite, nontronite, and pyrolusite. The diaspore, AlOOH, derives from the corrosion of the Al alloy. The pH changes result from complex interactions among all the solid and aqueous species present. Many of these effects are not apparent in Figure 5.3.1-1; for example, the Ni_2SiO_4, derived from corrosion of the borated SS, first forms, then dissolves, then resumes formation at about 165 years. From 100 years to about 14,000 years the pH remains nearly constant as a consequence of the balance between flushing by through-flowing J-13 water as it admixes with water already present, acid production from corrosion of the borated SS, and the solids present, some of which act as buffering agents. During this time frame the diaspore and clay are simulated to dissolve very slowly; hematite and pyrolusite slowly increase. Thereafter, the pH rises quickly to the value in the inflowing J-13 water, and a slow conversion of diaspore and hematite to nontronite, with silica deriving from the J-13 water, takes place. (The loss of hematite is not evident in the figure, but the more detailed output files show this decrease. The shift from dissolution to precipitation of nontronite results from the change in pH.) With the complete corrosion of the borated SS the increase in Ni_2SiO_4 ceases. Full details of the calculations are provided in spreadsheets in Ref. 11.

Essentially all of the Fe and Mn originally present in the basket materials are retained as insoluble solids. About one third of the Ni is retained. A small part of the Fe is simulated to become incorporated into the ferric iron clay, nontronite, as a consequence of the interaction with Al initially present predominantly as the Al alloy and with silica brought in as a solute in the infiltrating J-13 water. Ni_2SiO_4 is simulated to form in very small amount shortly after breach of the WP, but to be dissolved away during the period of lowest pH. Later, as pH rises, the Ni released during further metal corrosion forms a new precipitate and remains insoluble.

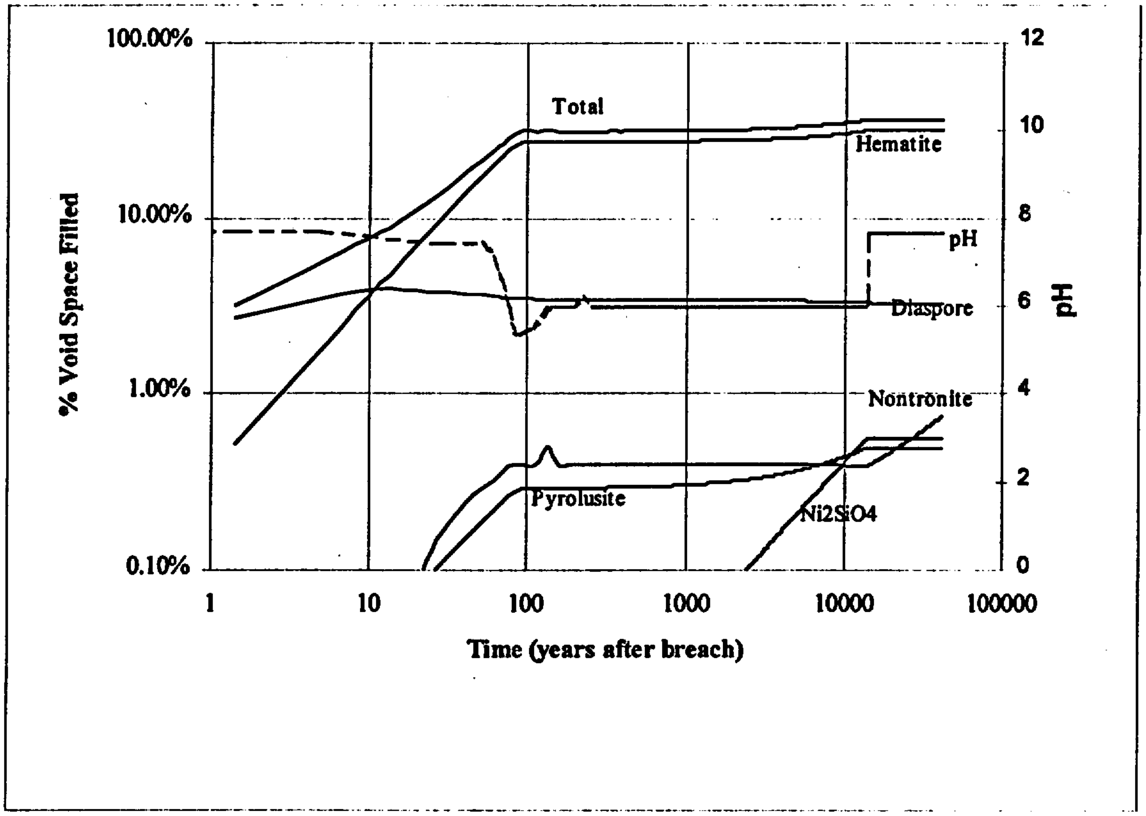

Figure 5.3.1-1. Volume percentages of void space in a 21 PWR LEU waste package occupied by principal minerals precipitated, Zircaloy intact.
This figure shows the simulated history for degradation of the basket materials only. Drip rate was 0.15 m^3/yr.
(Run set PWR0_15. See Ref. 11, file Name.doc for naming conventions.)
(Figure copied from spreadsheet volmas21c.xls, sheet PWR.)

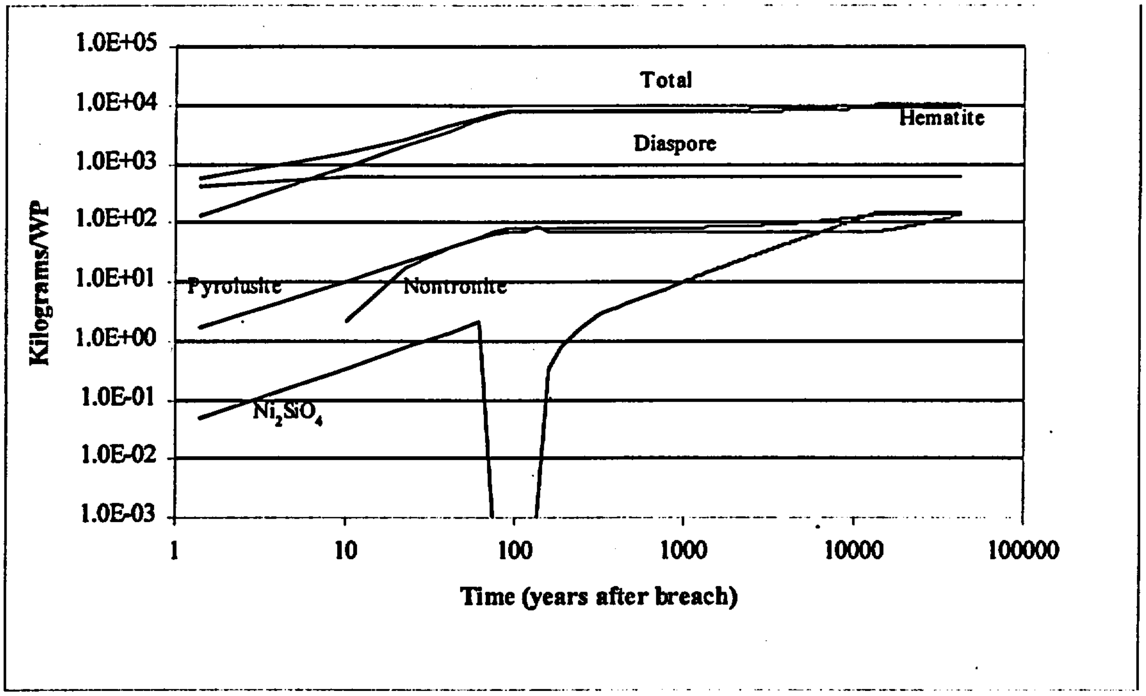

Figure 5.3.1-2. Masses of principal corrosion product solids in a 21 PWR LEU waste package, Zircaloy intact. This figure shows the simulated history for degradation of the basket materials only. Drip rate was 0.15 m^3/yr. (Run set PWR0_15)
(Figure copied from spreadsheet volmas21c.xls, sheet PWR.)

The first case run in this investigation was performed for an average corrosion rate for each of the basket metals and a mean drip rate into the WP of 0.15 m^3/yr (Run PWR0_15ahl). This run indicated complete corrosion of all the metals in the basket by about 1400 years. Because of the simulated acid production arising from the oxidation of the Cr and Mo in the borated SS, the pH decreased. The flushing rate, however, limited this decrease to about pH 5.5. A more conservative case would lower the pH further, as was demonstrated by using the lower drip rate of 0.015 m^3/yr (Run PWR0_15ahsll). In this case the pH decreased to about 5.2, owing to the slower removal of acid from the WP. However, because the borated SS was fully corroded in about 1400 years, the pH subsequently rose to 6.6 by 4400 years, as the acid solution was flushed out and replaced by the admixture of slightly alkaline fresh J-13 water. From chemical principles it was expected that the results from these two runs would provide nearly identical amounts of precipitated solids, unless only small amounts that are sensitive to the pH should form. The limited comparison shown in Table 5.3.1.1-1 bears this out. These indicated, on the basis of chemical principles, that a more conservative simulation would use a slower corrosion rate for the borated SS in order to prolong the period of low pH. This was done, using a corrosion rate of 0.025 micrometer/yr for the borated SS, which was fully corroded at about 13,600 years, and the mean drip rate of 0.15 m^3/yr in the run set PWR0_15ll.

Table 5.3.1.1-1 shows a comparison of some of the output data for these three cases. The main result to be drawn from these runs is that the differences in corrosion rate and drip rate have very minimal effect on the amounts of iron or aluminum retained in the WP as solids, as is shown by the amounts simulated at times after all the borated SS has corroded. Reasons for the more complex behavior for the other solids were discussed above.

Table 5.3.1.1-1. Comparison of PWR LEU Basket Corrosion at Low Drip Rate with Corrosion at Mean Rate

1000s of Years	pH	Hematite	Diaspore	Pyrolusite	Ni_2SiO_4	Smectite
Drip Rate of 0.015m^3/yr[a] Corrosion rate of Borated SS 0.25 micrometer/yr[b]						
0.45	5.23	11.24	2.29	0.25	3.25E-04	4.48E-02
1.04	5.17	12.19	2.29	0.31	1.26E-03	5.52E-02
1.99	5.47	12.73	2.28	0.35	1.74E-03	6.12E-02
3.03	6.07	12.73	2.28	0.35	1.89E-03	6.09E-02
4.01	6.51	12.73	2.28	0.35	2.18E-03	6.02E-02
4.41	6.56	12.73	2.28	0.35	2.37E-03	5.98E-02
Drip Rate of 0.15m^3/yr[a] Corrosion rate of Borated SS 0.25 micrometer/yr[c]						
0.44	5.53	11.23	2.29	0.25	4.52E-04	4.45E-02
Drip Rate of 0.15m^3/yr[a] Corrosion rate of Borated SS 0.025 micrometer/yr[d]						
1.04	6.02	10.68	2.29	0.21	1.10E-01	3.60E-02
1.99	6.02	10.84	2.29	0.22	2.25E-02	3.59E-02
3.03	6.01	11.01	2.29	0.23	3.46E-03	3.59E-02
4.01	6.01	11.17	2.29	0.24	4.59E-03	3.60E-02
4.41	6.01	11.24	2.29	0.25	5.05E-03	3.60E-02
13.60	6.01	12.75	2.29	0.16	1.98E-02	2.01E-01

[a] Units for solids are moles/kg of water in a WP
[b] EQ6 runs PWR0_015ahsl
[c] EQ6 run PWRah0_15
[d] EQ6 run PWR0_15

5.3.2 Simultaneous Degradation of Basket and LEU SNF

Table 5.3.2-1 shows percentages of selected elements of special interest for criticality computations at various times post-breach of the corrosion barriers. These data are for LEU SNF. Mo and Tc are effectively removed as soluble corrosion products from the WP as the fuel degrades. Consequently, they will be absent from the WP, except for very minor amounts of adsorbed species or minute traces left in solution, e.g., as a consequence of incomplete mixing of water within the WP, soon after the SNF is fully degraded. Full data sets are included in Ref. 11.

The data in this table show only the percentages retained as solids. Early in the degradation a few percent of the elements present in the original inventory may be present in solution in the WP, and may later precipitate before these elements are flushed out Thus, occasionally the table shows a decrease in the percentage retained, owing to a partial dissolution of a solid, followed by an increase. Data in Table 5.3.2-1 are for a set of runs in which hematite was not suppressed; the simulation predicts its formation.

Table 5.3.2-1. Percentages of Selected Elements Remaining as Solids in the Degraded PWR LEU Waste Package at Various Times -- Case Corresponds to Simultaneous Degradation of Basket and SNF. Hematite Present^2. Drip Rate 0.15 m^3/yr.

Time^1	U	Np	Pu	Am	Ru	Rh	Ag	Nd	Sm	Eu	Gd
0.000	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00
0.072	100.00	99.79	100.00	90.63	100.00	100.00	98.28	99.93	99.91	99.94	99.84
0.101	100.00	99.49	100.00	50.12	100.00	100.00	96.83	99.90	99.64	99.61	98.98
0.203	100.00	97.62	100.00	0.00	100.00	100.00	91.32	99.49	92.69	90.13	75.79
0.219	100.00	97.56	100.00	0.00	100.00	100.00	92.50	99.54	93.61	91.67	79.25
0.529	100.00	95.72	99.93	0.00	99.94	99.86	91.39	99.27	88.38	90.90	77.76
0.892	99.82	92.94	99.93	0.00	99.94	99.86	90.20	99.15	86.12	88.54	71.86
2.34	99.81	81.57	99.93	0.00	99.94	99.86	85.25	98.76	78.13	80.19	51.07
5.24	99.80	58.17	99.93	0.00	99.94	99.86	75.49	97.92	60.84	62.19	25.07
10.3	99.78	16.83	99.93	0.00	99.94	99.86	58.28	96.41	35.06	30.17	8.82
12.5	99.79	0.00	99.93	0.00	99.94	99.86	50.94	95.77	28.99	16.35	6.27
20.3	99.38	0.00	99.93	0.00	99.94	99.86	26.10	95.39	26.38	7.95	5.29
30.1	98.89	0.00	99.93	0.00	99.94	99.86	0.00	95.35	26.08	7.04	5.18
40.0	98.38	0.00	99.93	0.00	99.94	99.86	0.00	95.33	25.80	6.13	5.07
50.2	97.87	0.00	99.93	0.00	99.94	99.86	0.00	95.30	25.51	5.19	4.96
60.0	97.34	0.00	99.93	0.00	99.94	99.86	0.00	95.28	25.22	4.28	4.86
70.2	96.83	0.00	99.93	0.00	99.94	99.86	0.00	95.24	24.94	3.34	4.75
79.0	96.48	0.00	99.93	0.00	99.94	99.86	0.00	95.22	24.70	2.53	4.67

[1] Time in thousands of years after breach.

[2] Data extracted from spreadsheet PWRSF0_15.xls, sheet minerals.

Figure 5.3.2-1 shows the complete simulated history for these elements for the PWR LEU case in which hematite forms. It shows the rapid removal of Am, and the early flushing out of Np. Eu, Sm, and Gd are decreased to small percentages of their original inventory, but only a small percentage of Nd is removed. Nearly all of the Pu and U are retained. Full details are included in Ref. 11 in files in set PWRSF0_15, and summary data are in Ref. 11 (spreadsheet PWRSF0_15.lastpost.xls, sheet minerals).

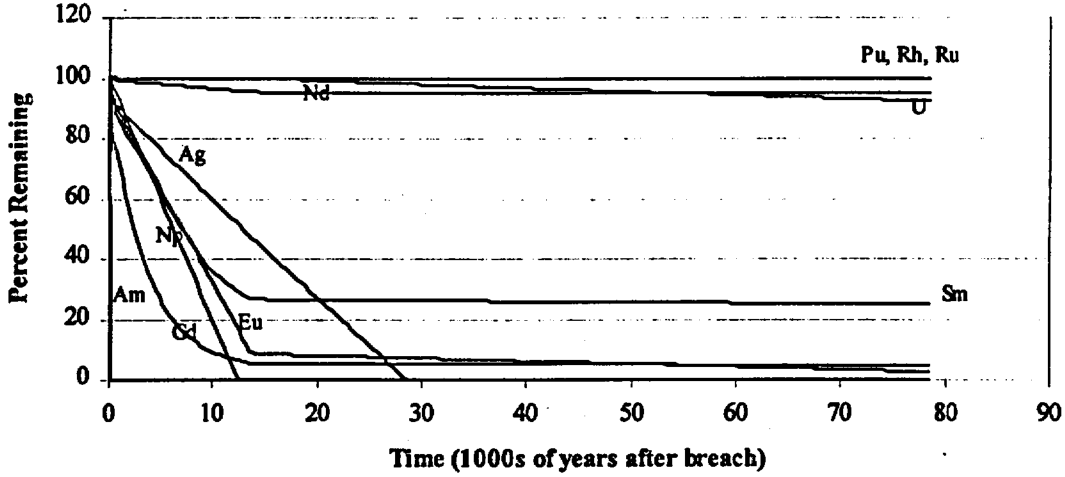

Figure 5.3.2-1. Percent of selected elements remaining in solid phases in a 21 PWR LEU waste package; Zircaloy breached early, hematite present.

This figure shows the entire simulated history of retention of elements of principal interest for criticality during simultaneous degradation of PWR LEU SNF and basket. Hematite is present. Drip rate was 0.15 m^3/yr. The lines for Pu, Rh, and Ru coincide with the 100% line. Am is dissolved out quickly, such that the line for it nearly coincides with the zero time gridline.

(Figure copied from spreadsheet PWRSF0_15.xls, sheet minerals.)

The solubilities of all the lanthanides (Gd, Nd, Sm, and Eu) are all very similar; the different histories reflect differences in their initial inventories in the waste.

The data for the solids, together with their densities, permit calculation of the volumes of solids and the percentage of the void space occupied by each solid. Figure 5.3.2-2 shows the results of these calculations. The void space is calculated as that originally present plus the volume of the basket metals that have been corroded as a function of time. The increase in the volume of hematite over the first 100 years arises primarily from the corrosion of the A516. Unlike the case for the basket only corroding, nontronite, is not simulated to occur. Probably this happens on account of a small effect on the pH, making hematite and/or diaspore a little less soluble, thereby robbing the nontronite of elements that must be at a high enough concentration for it to precipitate. The pH could also affect the silica concentration slightly, thereby allowing too much to be flushed out to permit the formation of silicates. This would apply also to Ni_2SiO_4, which is also simulated to be absent in this case. A small volume of pyrolusite, MnO_2 is still modeled as forming. At about 100 years the A516 is predicted to be completely corroded, as is reflected in the sudden change in the rates of change of the space occupied by the hematite. The diaspore, AlOOH, derives from the corrosion of the Al alloy. The pH changes result from complex interactions among all the solid and aqueous species present. The major solids, hematite and diaspore, remain essentially the same as in the absence of simulated waste degradation. Consequently, virtually all of the Fe and Al initially present in the steel and Al alloy remain in the waste package. The small amounts of Ca, Mg, K, and Na that were predicted to be present in solids in the case of basket degradation only are absent. About one fourth of the Ni is retained as trevorite, $NiFe_2O_4$.

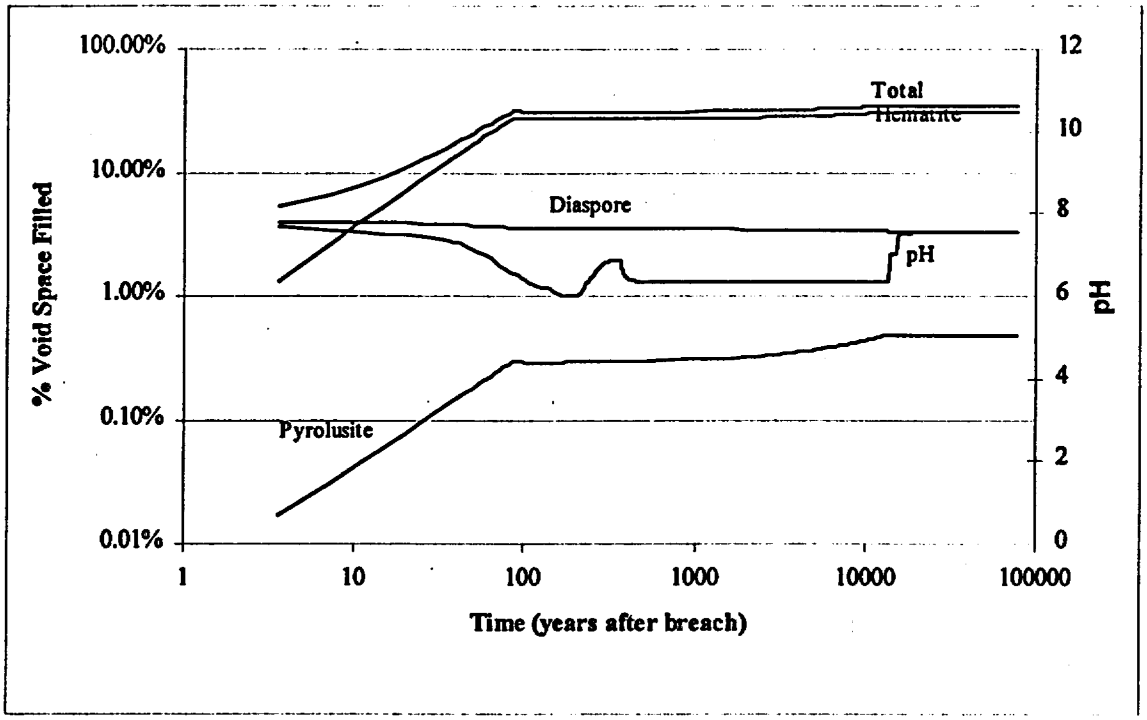

Figure 5.3.2-2. Volume percentages of void space in a 21 PWR LEU waste package occupied by principal minerals precipitated; Zircaloy breached early, hematite present.

This figure shows percentage of void space occupied by most of the solids produced during the degradation of the 21 PWR LEU waste package for simultaneous corrosion of basket and SNF. Hematite is present. Drip rate was 0.15 m^3/yr.

(Figure copied from spreadsheet volmas21c, sheet PWRSF.)

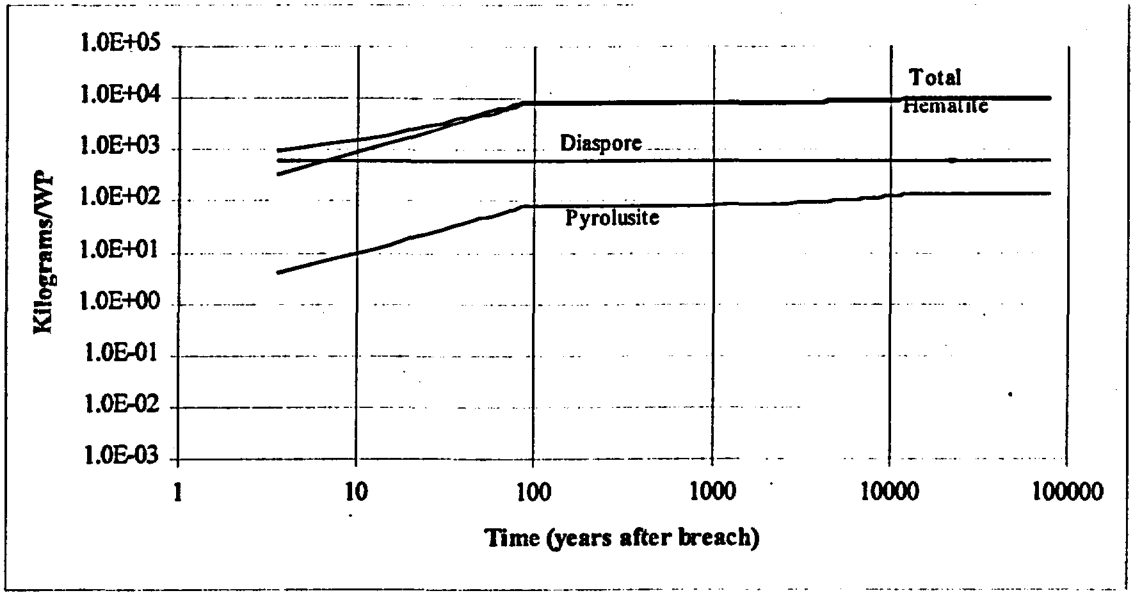

Figure 5.3.2-3. Masses of principal corrosion product solids in a 21 PWR LEU waste package; Zircaloy breached early, hematite present.
This figure shows the total masses of most of the solids produced during the degradation of the 21 PWR LEU waste package for simultaneous corrosion of basket and SNF. Hematite is present. Drip rate was 0.15 m^3/yr.
(Figure copied from spreadsheet volmas21c, sheet PWRSF.)

Table 5.3.2-2 provides the pH and concentrations of U, Np, Pu, Am, Nd, Sm, Eu, Gd, and B at the same times as entered in Table 5.3.2-1. Figure 5.3.2-4 shows the complete time history for the pH and U, Gd, and B concentrations.

Table 5.3.2-2. Concentrations of Selected Elements in the Degraded PWR LEU Waste Package at Various Times – Case Corresponds to Simultaneous Degradation of Basket and SNF. Hematite Present*[2] Drip Rate was 0.15 m^3/yr. Molalities.

Time[1]	pH	U	Np	Pu	Am	B	Nd	Sm	Eu	Gd
0.000	7.64E+00	1.00E-14	1.00E-10	1.00E-14	1.00E-10	1.24E-05	1.00E-14	1.00E-10	1.00E-10	1.00E-14
0.07	6.74E+00	2.21E-05	1.78E-05	1.64E-12	3.19E-06	1.02E-03	8.60E-07	3.96E-06	6.75E-07	1.24E-06
0.101	6.38E+00	1.18E-05	4.08E-05	3.19E-12	1.55E-05	1.10E-03	6.25E-06	2.55E-05	4.69E-06	8.76E-06
0.203	5.98E+00	8.02E-06	1.03E-04	7.47E-12	8.67E-06	1.15E-03	8.43E-05	3.26E-04	6.44E-05	1.17E-04
0.219	6.11E+00	8.57E-06	7.30E-05	5.39E-12	5.29E-06	1.13E-03	2.86E-05	1.11E-04	1.95E-05	3.69E-05
0.529	6.35E+00	1.06E-05	4.08E-05	3.21E-12	4.17E-10	1.10E-03	8.04E-06	3.23E-05	4.65E-06	8.49E-06
0.892	6.35E+00	1.07E-05	3.94E-05	3.09E-12	1.00E-14	1.10E-03	4.91E-06	2.03E-05	3.05E-06	5.88E-06
2.34	6.33E+00	1.04E-05	4.12E-05	3.22E-12	1.00E-14	1.10E-03	5.55E-06	2.28E-05	3.42E-06	5.53E-06
5.24	6.33E+00	1.04E-05	4.15E-05	3.23E-12	1.00E-14	1.10E-03	5.63E-06	2.31E-05	3.46E-06	2.44E-06
10.3	6.33E+00	1.04E-05	4.16E-05	3.24E-12	1.00E-14	1.10E-03	5.69E-06	1.30E-05	3.50E-06	6.24E-07
12.5	6.32E+00	1.03E-05	4.04E-05	3.27E-12	1.00E-14	1.10E-03	5.75E-06	8.85E-06	3.53E-06	3.66E-07
20.3	7.53E+00	1.35E-04	1.00E-14	7.49E-13	1.00E-14	1.24E-05	5.18E-08	1.15E-07	5.10E-08	4.63E-09

30.1	7.53E+00	1.35E-04	1.00E-14	7.49E-13	1.00E-14	1.24E-05	5.18E-08	1.13E-07	5.10E-08	4.53E-09
40.0	7.53E+00	1.35E-04	1.00E-14	7.49E-13	1.00E-14	1.24E-05	5.18E-08	1.12E-07	5.10E-08	4.42E-09
50.2	7.53E+00	1.35E-04	1.00E-14	7.49E-13	1.00E-14	1.24E-05	5.18E-08	1.10E-07	5.10E-08	4.32E-09
60.0	7.53E+00	1.35E-04	1.00E-14	7.49E-13	1.00E-14	1.24E-05	5.18E-08	1.09E-07	5.10E-08	4.22E-09
70.2	7.53E+00	1.35E-04	1.00E-14	7.49E-13	1.00E-14	1.24E-05	5.18E-08	1.07E-07	5.10E-08	4.12E-09
79.0	7.53E+00	1.35E-04	1.00E-14	7.49E-13	1.00E-14	1.24E-05	5.18E-08	1.06E-07	5.10E-08	4.04E-09

[1] Time in thousands of years after breach. * Concentrations equal to or less than 1.00E-14 are reported as 1.00E-14.

[2] Data extracted from spreadsheet PWRSF0_15, sheet elements and PWRSF0_15 EQ6 summary files.

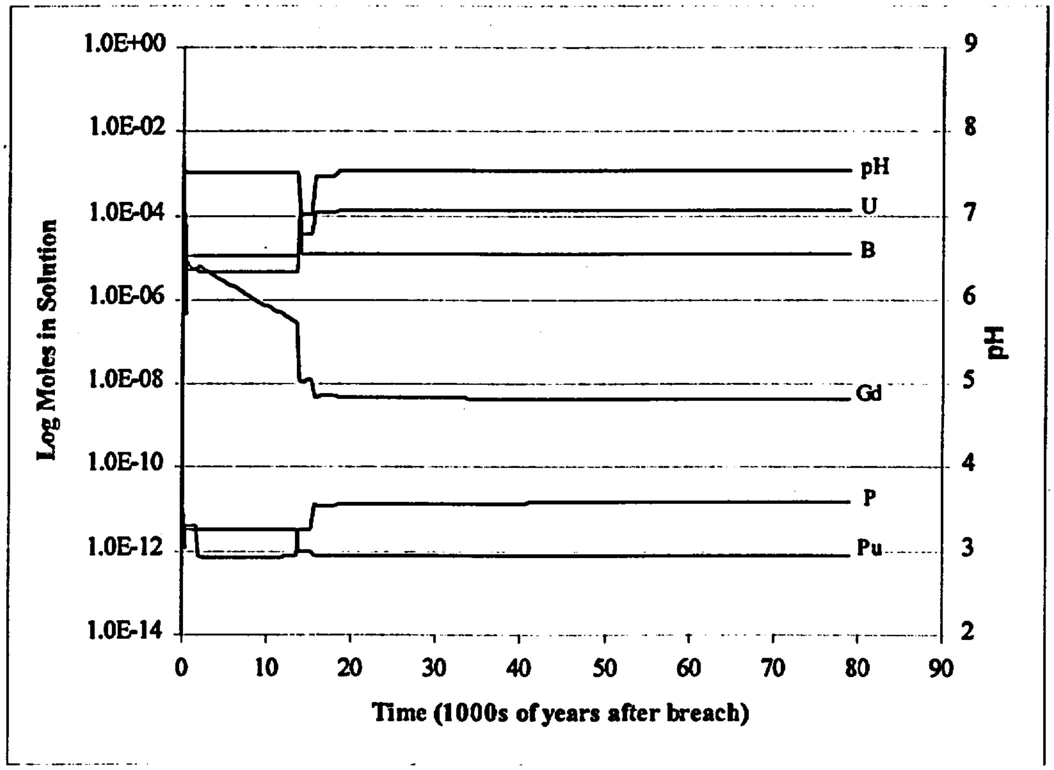

Figure 5.3.2-4. Aqueous concentrations (molalities) of selected elements in a 21 PWR LEU waste package; Zircaloy breached early, hematite present.
This figure shows aqueous concentrations of several of the most significant elements as a function of time following waste package breach for the 21 PWR LEU waste package for simultaneous corrosion of basket and SNF. Hematite is present. Drip rate was 0.15 m^3/yr.
(Figure copied from spreadsheet PWRSF0_15, sheet elements.)

Table 5.3.2-3 and Figure 5.3.2-5 show data for a case that is parallel to that for Table 5.3.2-1, except that in this case hematite was suppressed and goethite is simulated to form instead. Mo and Tc are effectively removed as soluble corrosion products from the WP as the fuel degrades. The runs show minor differences in the solution chemistry, such as the pH, which cause major changes in how long Np and the rare earths remain in the WP. Full details are included in Ref. 11 in files in set PWRnHSF0_15, and summary data are in Ref. 11 (spreadsheet PWRnHSF0_15.lastpost.xls, sheet elements).

Table 5.3.2-3. Concentrations of Selected Elements in the Degraded PWR LEU Waste Package at Various Times -- Case Corresponds to Simultaneous Degradation of Basket and SNF. Hematite Suppressed*[2] Drip Rate was 0.15 m^3/yr. Molalities.

Time[1]	pH	U	Np	Pu	Am	B	Nd	Sm	Eu	Gd
0.00	7.64E+00	1.00E-14	1.00E-14	1.00E-14	1.00E-14	1.24E-05	1.00E-14	1.00E-14	1.00E-14	1.00E-14
0.04	7.33E+00	1.02E-04	5.13E-06	8.33E-13	3.52E-07	7.81E-04	9.55E-08	5.42E-07	8.95E-08	1.56E-07
0.09	6.47E+00	1.32E-05	3.26E-05	2.62E-12	1.28E-05	1.11E-03	3.66E-06	1.52E-05	2.78E-06	5.18E-06
0.12	6.03E+00	8.27E-06	9.06E-05	6.61E-12	1.25E-05	1.15E-03	5.82E-05	2.25E-04	4.39E-05	8.01E-05
0.23	6.06E+00	8.18E-06	7.99E-05	5.86E-12	3.82E-06	1.12E-03	3.49E-05	1.37E-04	2.26e--5	4.31E-05
0.55	6.08E+00	8.12E-06	7.48E-05	5.58E-12	1.86E-10	1.10E-03	3.99E-05	1.56E-04	2.22E-05	3.59E-05
0.90	6.02E+00	7.81E-06	8.37E-05	6.14E-12	1.00E-14	1.10E-03	3.86E-05	1.51E-04	2.26E-05	1.88E-05
1.21	6.02E+00	7.80E-06	8.39E-05	6.16E-12	1.00E-14	1.10E-03	3.88E-05	1.52E-04	2.22E-05	1.13E-05
1.82	6.00E+00	7.72E-06	8.80E-05	6.44E-12	1.00E-14	1.10E-03	4.45E-05	1.06E-04	4.11E-06	4.11E-06
2.37	5.99E+00	7.68E-06	9.03E-05	6.61E-12	1.00E-14	1.10E-03	4.80E-05	6.14E-05	1.60E-05	1.73E-06
4.14	5.95E+00	7.60E-06	9.73E-05	7.11E-12	1.00E-14	1.10E-03	6.03E-05	1.18E-05	1.00E-14	1.40E-07
5.02	5.94E+00	7.58E-06	1.01E-04	7.40E-12	1.00E-14	1.10E-03	6.80E-05	5.04E-06	1.00E-14	4.46E-08
5.70	5.93E+00	7.58E-06	7.72E-05	7.53E-12	1.00E-14	1.10E-03	7.18E-05	3.25E-06	1.00E-14	2.44E-08
10.21	5.92E+00	7.59E-06	1.00E-14	7.80E-12	1.00E-14	1.10E-03	7.99E-05	6.68E-07	1.00E-14	2.29E-09
15.30	6.99E+00	3.31E-05	1.00E-14	1.06E-12	1.00E-14	1.24E-05	2.53E-07	1.32E-09	1.00E-14	2.74E-12
20.16	7.53E+00	1.34E-04	1.00E-14	7.49E-13	1.00E-14	1.24E-05	5.19E-08	3.61E-10	1.00E-14	8.31E-13
30.36	7.53E+00	1.34E-04	1.00E-14	7.49E-13	1.00E-14	1.24E-05	5.19E-08	3.60E-10	1.00E-14	8.28E-13
44.57	7.53E+00	1.34E-04	1.00E-14	7.49E-13	1.00E-14	1.24E-05	5.19E-08	3.59E-10	1.00E-14	8.24E-13

[1] Time in thousands of years after breach. * Concentrations equal to or less than 1.00E-14 are reported as 1.00E-14.
[2] Data extracted from spreadsheet PWRSF0_15nH, sheet elements and PWRSF0_15nH EQ6 summary files.

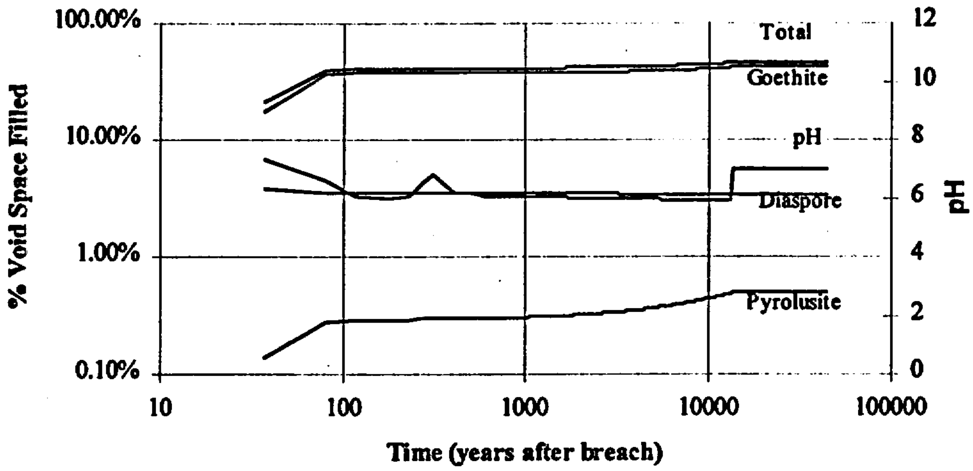

Figure 5.3.2-5. Volume percentages of void space in a 21 PWR LEU waste package occupied by principal minerals precipitated; Zircaloy breached early, goethite present.
This figure shows percentage of void space occupied by most of the solids produced during the degradation of the 21 PWR LEU waste package for simultaneous corrosion of basket and SNF. Goethite is present. Drip rate was 0.15 m^3/yr.
(Figure copied from spreadsheet volmas21c.xls, sheet PWRSFnH.)

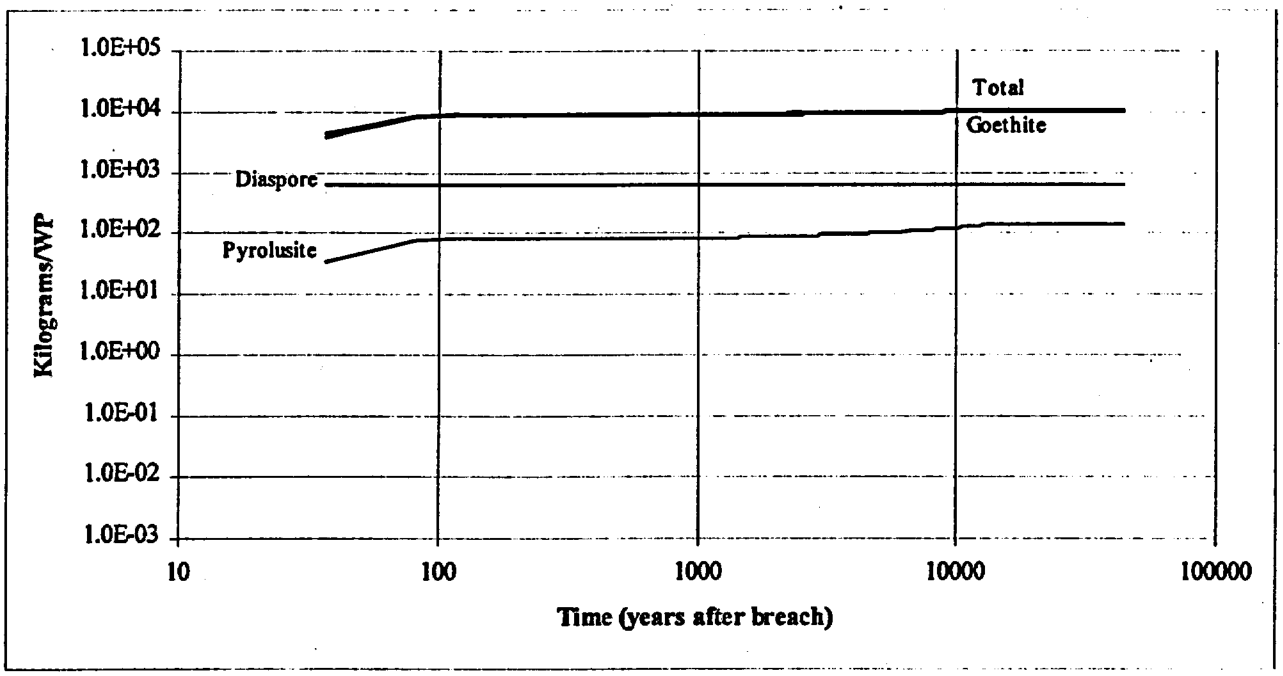

Figure 5.3.2-6. Masses of principal corrosion product solids in a 21 PWR LEU waste package; Zircaloy breached early, goethite present.
This figure shows the total masses of most of the solids produced during the degradation of the 21 PWR LEU waste package for simultaneous corrosion of basket and SNF. Goethite is present. Drip rate was 0.15 m^3/yr.
(Figure copied from spreadsheet volmas21c.xls, sheet PWRSFnH.)

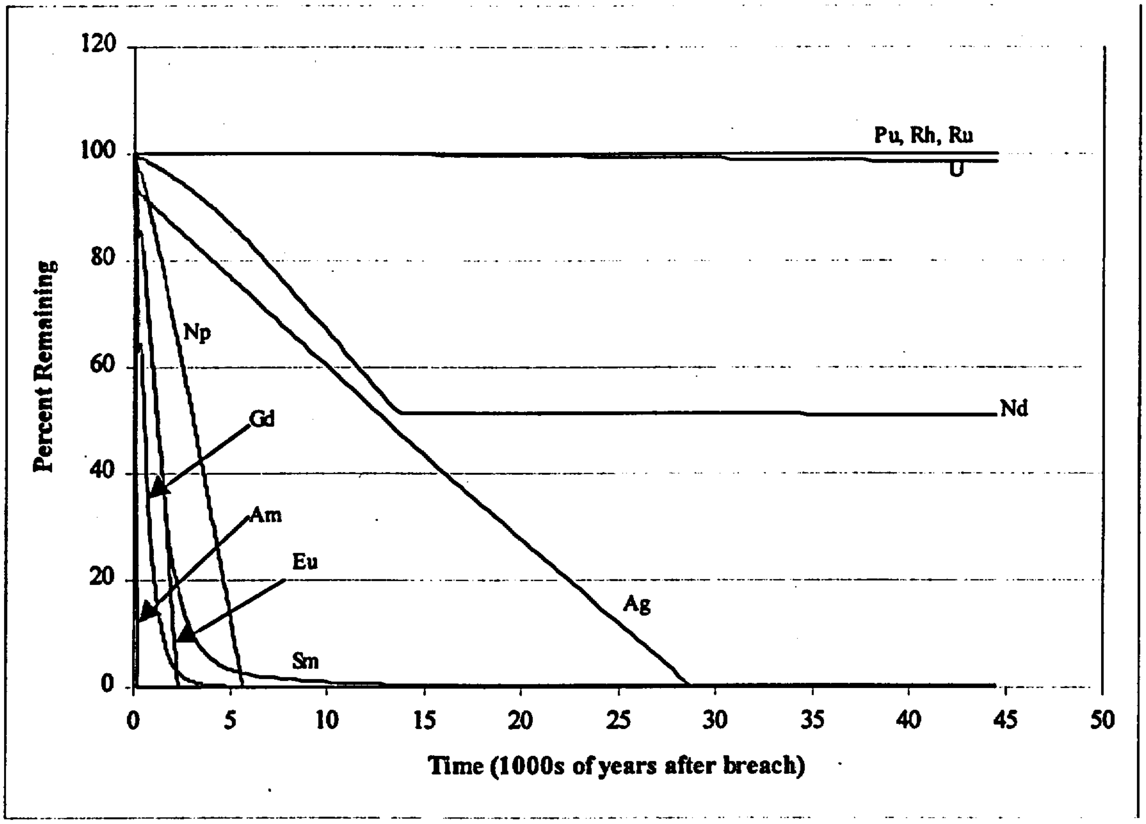

Figure 5.3.2-7. Percent of selected elements remaining in solid phases in a 21 PWR LEU waste package; Zircaloy breached early, goethite present.

This figure shows the entire simulated history of retention of elements of principal interest for criticality during simultaneous degradation of PWR LEU SNF and basket. Goethite is present. Drip rate was 0.15 m^3/yr. The lines for Pu, Rh, and Ru coincide with the 100% line. Am is dissolved out quickly, such that the line for it nearly coincides with the zero time gridline. Drip rate was 0.15 m^3/yr.

(Figure copied from spreadsheet PWRSF0_15nH.xls, sheet minerals.)

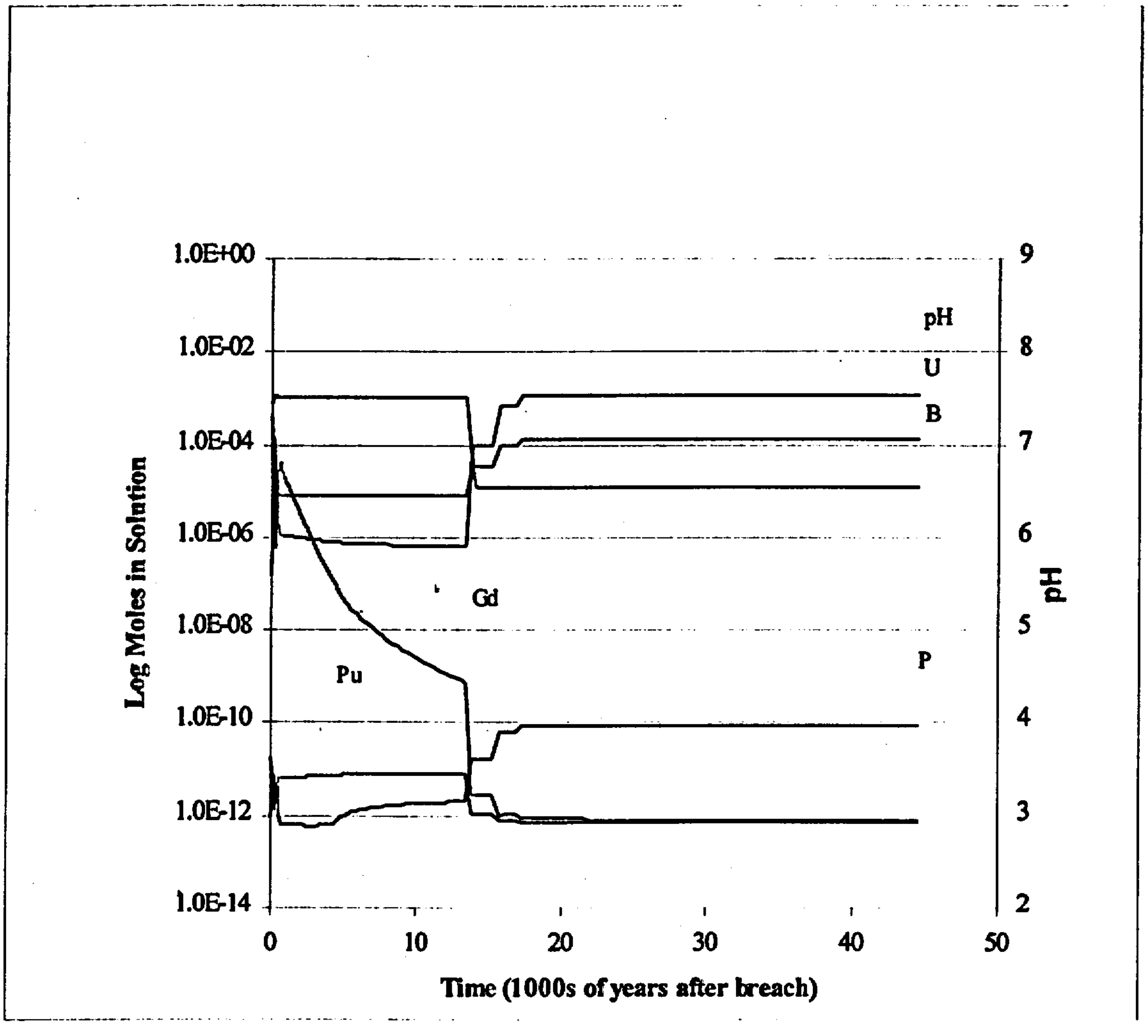

Figure 5.3.2-8. Aqueous concentrations (molalities) of selected elements in a 21 PWR LEU waste package; Zircaloy breached early, goethite present.
This figure shows aqueous concentrations of several of the most significant elements as a function of time following waste package breach for the 21 PWR LEU waste package for simultaneous corrosion of basket and SNF. Goethite is present. Drip rate was 0.15 m^3/yr.
(Figure copied from spreadsheet PWRSF0_15nH.xls, sheet elements.)

Results for a PWR MOX spent fuel package closely resemble those for the PWR LEU fuel. The major differences are in the earlier or larger percentage removal of Ag and the lanthanides for the PWR LEU case. Table 5.3.2-4 and Figure 5.3.2-9 show the percentages of principal isotopes that remain in the WP as a function of time. Full details are included in Ref. 11 in files in set MOXSF0_15, and summary data are in Ref. 11 (spreadsheet MOXSF0_15.lastpost.xls, sheet sum).

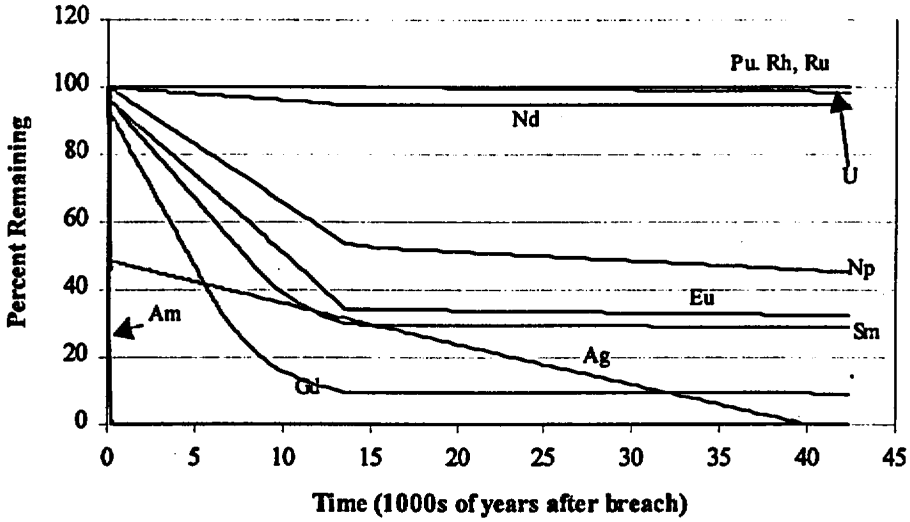

Figure 5.3.2-9. Percent of selected elements remaining in solid phases in a 21 PWR MOX waste package; Zircaloy breached early, hematite present, mean drip rate.
This figure shows the entire simulated history of retention of elements of principal interest for criticality during simultaneous degradation of PWR MOX SNF and basket. Hematite is present. Drip rate was 0.15 m^3/yr. The lines for Pu, Rh, and Ru coincide with the 100% line. Am is dissolved out quickly, such that the line for it nearly coincides with the zero time gridline.
(Figure copied from spreadsheet MOXSF0_15I.lastpost.xls, sheet sum.)

The effect of different infiltration, or drip, rates was investigated partly by using a slower rate following degradation of the basket material, as described in Section 5.3.3, and partly by a relatively short series of runs at a drip rate of 0.5 m^3/yr. The results of this latter set, for PWR MOX SNF, are shown in Figure 5.3.2-10. Comparison with Figure 5.3.2-9 shows that there are essentially no differences for Pu, U, Nd, Rh, and Ru. Am is retained a little longer at the higher infiltration rate, and Ag is initially removed less rapidly, but in the longer term is removed sooner. A closer examination of the output data shows that the rate of removal of Ag for the 0.5 m^3/yr drip rate is very close to 3 1/3 times faster than at the 0.15 m^3/yr drip rate, i.e., in proportion to the drip rate. This is consistent with the removal being controlled by the solubility of the silver solid, AgCl. The lanthanides, most notably the Gd, are simulated to be removed significantly less rapidly at the higher drip rate.

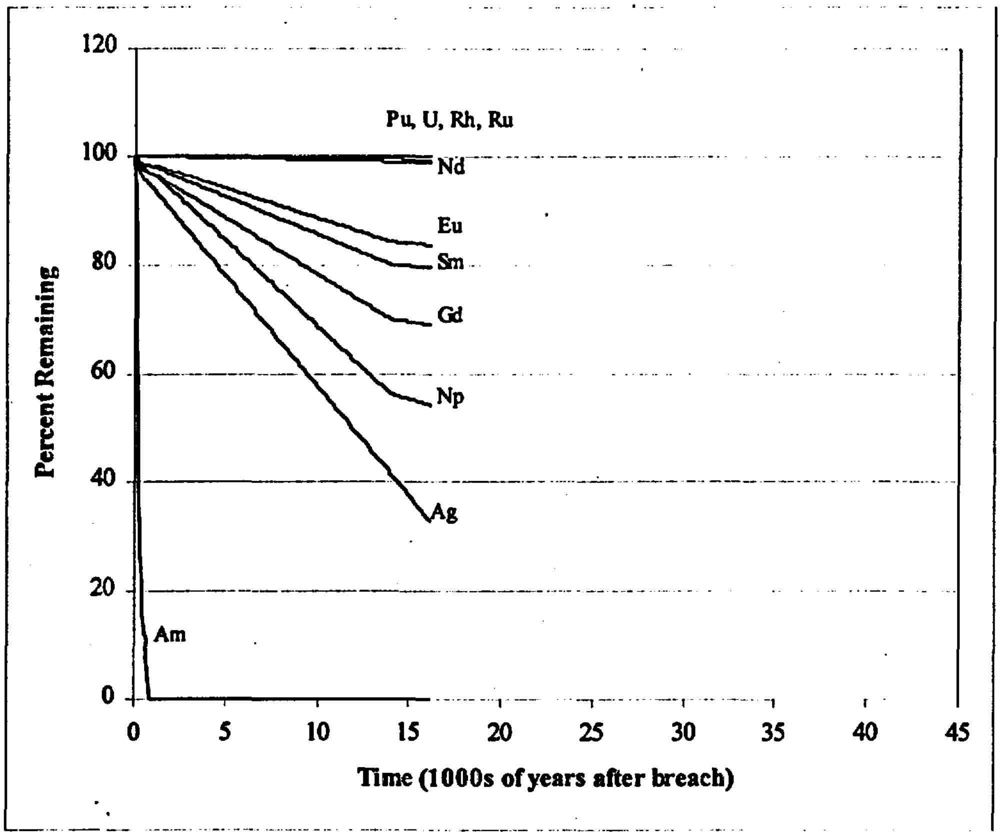

Figure 5.3.2-10. Percent of selected elements remaining in solid phases in a 21 PWR MOX waste package; Zircaloy breached early, hematite present, high drip rate.
This figure shows the entire simulated history of retention of elements of principal interest for criticality during simultaneous degradation of PWR MOX SNF and basket. Hematite is present. Drip rate was 0.5 m^3/yr. The lines for Pu, Rh, and Ru coincide with the 100% line. Am is dissolved out quickly, such that the line for it nearly coincides with the zero time gridline.
(Figure copied from spreadsheet MOXSF0_5.xls, sheet sum.)

5.3.3 Degradation of SNF after Degradation of Basket

Three different scenarios were calculated for the start of degradation of the spent fuel after all the basket materials had corroded. The first considered PWR LEU SNF at the mean drip rate of 0.15 m^3/yr entering the WP, and the second the parallel case for PWR MOX SNF. The case for PWR LEU SNF was run only far enough to confirm that the chemical evolution would be essentially the same as for the case when the basket and SNF degrade simultaneously. The third case was for PWR MOX SNF, but with a minimal drip rate of 0.015 m^3/yr. This case was run to investigate whether a lower drip rate would be more conservative, owing to the expected longer-lasting low pH for a lower drip rate, thereby possibly enabling a greater leaching and removal of Gd absorber from the WP. The simulation did in fact show the expected pH effect (e.g., pH 7.37 for the slow drip rate at 16,700 years as compared with pH 7.53 for the mean drip rate at the same time). However, even in the slow drip rate case the pH rose rapidly enough that the solubility of Gd became minimal and the removal rate from the WP was dominated by the slow drip rate, rather than the approximately 30% higher solubility. Consequently, the rate of removal was substantially slower for a drip rate of 0.015 m^3/yr following complete corrosion of the basket, as shown by a comparison of the data in Tables 5.3.3-2 and 5.3.3-3. The solubility of Pu for the slow drip rate case was only about 3% higher than for the mean drip rate, but that for U was about 40% lower, presumably because of the greater formation of uranyl carbonate complexes at the higher pH for the faster drip rate. (This could not be checked owing to the impracticality of retaining dozens of very large (up to several gigabytes in size) complete output files.) The pH rises following the complete degradation of the basket because of the influx of the slightly alkaline J-13 and lack of any further generation of acid from borated SS corrosion. The case, in which the drip rate decreases upon full corrosion of the basket, would correspond to a rapid climate change to a drier environment that happened to coincide approximately with the end of the degradation of the metals in the basket.

Table 5.3.3-1 shows percentages of selected elements retained as solids at various times post-breach of the corrosion barriers for the first of these cases. The first 13,800 years are the same as for the degradation of the basket materials alone, as discussed in Section 5.3.1. Those details are not repeated here. The rest of the data summarize the chemical evolution after the basket materials are corroded and at which time the Zircaloy cladding is simulated to have breached and the degradation of the PWR LEU SNF begun. Full data sets are included in Ref. 11 (file set PWRSFpd0_15). Figure 5.3.3-1 displays these results graphically.

Table 5.3.3-1. Percentages of Selected Elements Remaining in the Degraded PWR LEU Waste Package at Various Times -- Case Corresponds to Breaching of Zircaloy and Initiation of SNF Degradation After Basket Fully Degraded[2] Drip Rate 0.15 m^3/yr.

Time[1]	U	Np	Pu	Am	Ru	Rh	Ag	Nd	Sm	Eu	Gd
0	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00
0.465	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00
13.8	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00
14.00	100.00	98.54	100.00	21.30	99.99	100.01	94.49	99.90	97.86	97.36	93.34
15.00	99.96	97.18	100.01	0.00	100.00	99.99	90.94	99.86	97.04	96.41	90.96
16.00	99.90	96.53	100.01	0.00	100.00	99.99	87.72	99.85	96.96	96.30	90.74
17.00	99.85	95.87	100.01	0.00	100.00	99.99	84.58	99.85	96.88	96.24	90.52
20.29	99.10	0.00	99.93	0.00	99.94	99.86	26.10	95.39	26.38	7.95	5.29
25.02	98.55	0.00	99.93	0.00	99.94	99.86	11.19	95.36	26.24	7.51	5.23
28.67	98.14	0.00	99.93	0.00	99.94	99.86	0.00	95.36	26.13	7.17	5.19
39.95	96.79	0.00	99.93	0.00	99.94	99.86	0.00	95.33	25.80	6.13	5.07
50.16	95.60	0.00	99.93	0.00	99.94	99.86	0.00	95.30	25.51	5.19	4.96
60.01	94.42	0.00	99.93	0.00	99.94	99.86	0.00	95.28	25.22	4.28	4.86
70.20	93.23	0.00	99.93	0.00	99.94	99.86	0.00	95.24	24.94	3.34	4.75
78.58	92.25	0.00	99.93	0.00	99.94	99.86	0.00	95.22	24.70	2.57	4.67

[1] Time in thousands of years after breach.

[2] Data extracted from spreadsheet PWRSFpd.xls, sheet minerals.

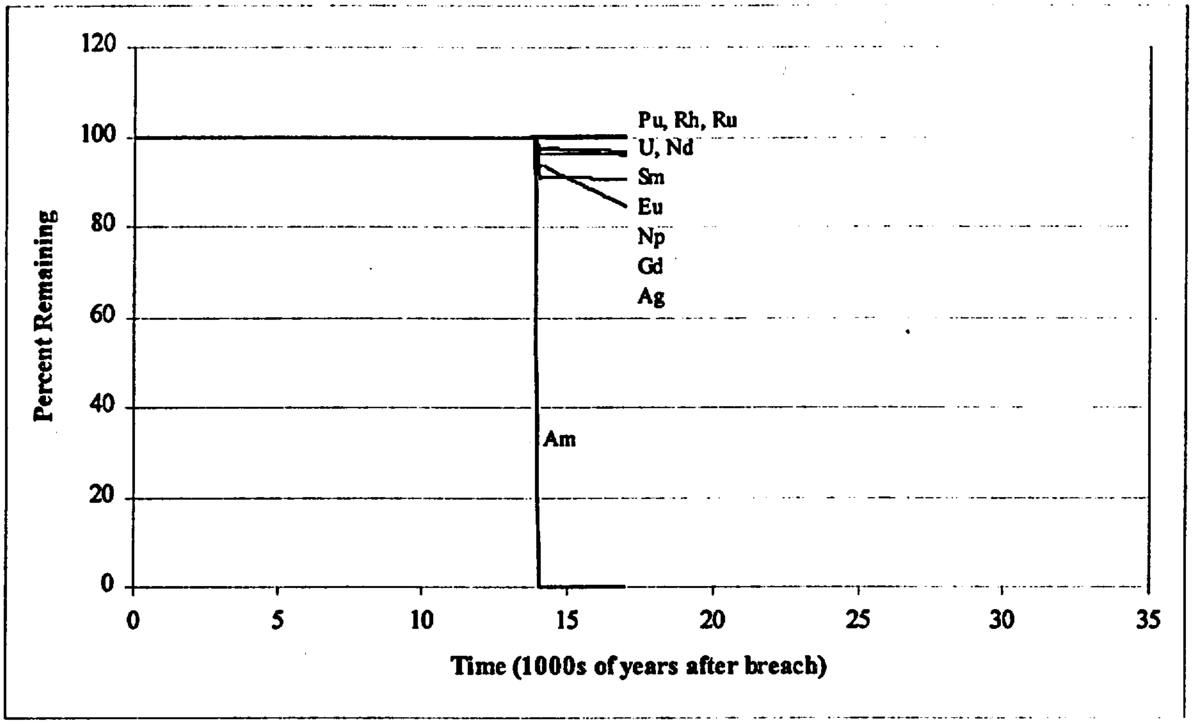

Figure 5.3.3-1. Percent of selected elements remaining in solid phases in a 21 PWR LEU waste package; Zircaloy breached late, mean drip rate.
This figure shows the entire simulated history of retention of elements of principal interest for criticality. This case simulates breach of the Zircaloy cladding only after the basket is completely corroded. Consequently, none of the elements is lost from the WP before that time, about 13,700 years. Hematite is present. Drip rate was 0.15 m^3/yr. The lines for Pu, Rh, and Ru coincide with the 100% line. Am is dissolved out quickly after waste package breach.
(Figure copied from spreadsheet PWRSFpd.xls, sheet minerals.)

Table 5.3.3-2 and Figure 5.3.3-2 show the parallel case for PWR MOX SNF. Full data sets are included in Ref. 11, data set MOXpda0_15.

Table 5.3.3-2. Percentages of Selected Elements Remaining in the Degraded PWR MOX Waste Package at Various Times -- Breaching of Zircaloy and Initiation of SNF Degradation After Basket Fully Degraded. Drip Rate 0.15 m^3/yr.[2]

Time[1]	U	Np	Pu	Am	Ru	Rh	Ag	Nd	Sm	Eu	Gd
0	100	100	100	100	100	100	100	100	100	100	100
0.32	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00
13.69	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00
14.00	99.99	99.10	99.99	5.70	99.99	99.99	50.76	99.86	97.81	98.01	96.04
16.48	99.85	98.42	99.99	0.00	99.99	99.99	47.82	99.84	97.60	97.85	95.70
17.41	99.80	98.18	99.99	0.00	99.99	99.99	46.71	99.84	97.53	97.77	95.59
18.64	99.73	97.85	99.99	0.00	99.99	99.99	45.24	99.83	97.43	97.70	95.40
22.98	99.49	96.68	99.99	0.00	99.99	99.99	40.08	99.82	97.10	97.42	94.85
25.14	99.36	96.11	99.99	0.00	99.99	99.99	37.51	99.81	96.92	97.27	94.55
31.95	98.98	94.27	99.99	0.00	99.99	99.99	29.41	99.80	96.39	96.83	93.67

[1] Time in thousands of years after breach.

[2] Data extracted from spreadsheet PWRpda0_15.xls, sheet minerals.

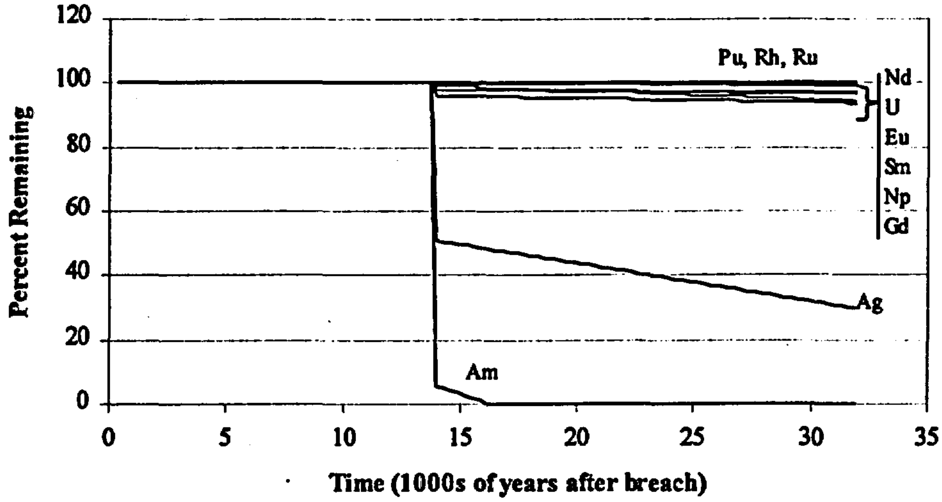

Figure 5.3.3-2. Percent of selected elements remaining in solid phases in a 21 PWR MOX waste package; Zircaloy breached late, mean drip rate.
This figure shows the entire simulated history of retention of elements of principal interest for criticality. This case simulates breach of the Zircaloy cladding only after the basket is completely corroded. Consequently, none of the elements is lost from the WP before that time, about 13,700 years. Hematite is present. Drip rate was 0.15 m^3/yr. The lines for Pu, Rh, and Ru coincide with the 100% line. Am is dissolved out quickly after waste package breach.
(Figure copied from spreadsheet MOXpda1.xls, sheet minerals.)

Table 5.3.3-3 and Figure 5.3.3-3 show the results for the third case, degradation of PWR MOX SNF at a drip rate of 0.015 m^3/yr immediately following the complete corrosion of the basket.

Table 5.3.3-3. Percentages of Selected Elements Remaining in the Degraded PWR MOX Waste Package at Various Times -- Breaching of Zircaloy and Initiation of SNF Degradation After Basket Fully Degraded. Drip Rate 0.015 m^3/yr [2]

Time[1]	U	Np	Pu	Am	Ru	Rh	Ag	Nd	Sm	Eu	Gd
0	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00
0.651	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00
16.70	100.00	99.27	100.00	6.43	99.99	100.00	28.93	99.80	96.83	96.09	92.84
19.98	99.98	99.20	100.00	5.49	99.99	100.00	28.54	99.79	96.80	96.05	92.81
29.82	99.93	98.92	100.00	2.93	99.99	100.00	27.38	99.79	96.73	95.97	92.67
42.93	99.85	98.57	100.00	0.00	99.99	100.00	25.81	99.78	96.63	95.89	92.50
78.96	99.64	97.60	100.00	0.00	99.99	100.00	21.53	99.78	96.35	95.66	92.03
101.90	99.51	96.98	100.00	0.00	99.99	100.00	18.80	99.77	96.16	95.50	91.73
200.20	98.96	94.34	100.00	0.00	99.99	100.00	7.11	99.72	95.39	94.87	90.41
262.50	98.61	92.67	100.00	0.00	99.99	100.00	0.00	99.70	94.91	94.44	89.57
301.70	98.39	91.60	100.00	0.00	99.99	100.00	0.00	99.70	94.60	94.21	89.07
400.50	97.83	88.97	100.00	0.00	99.99	100.00	0.00	99.66	93.82	93.54	87.75
495.60	97.30	86.40	100.00	0.00	99.99	100.00	0.00	99.62	93.07	92.92	86.50

[1] Time in thousands of years after breach.

[2] Data extracted from spreadsheet MOXPdswa.xls, sheet sum.

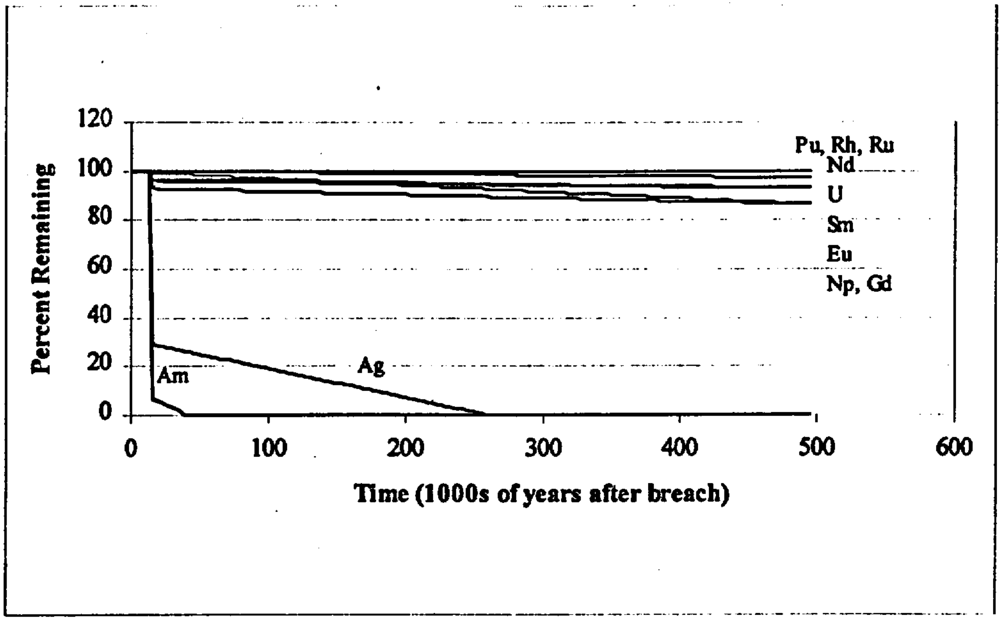

Figure 5.3.3-3. Percent of selected elements remaining in solid phases in a 21 PWR MOX waste package; Zircaloy breached late, low drip rate.
This figure shows the entire simulated history of retention of elements of principal interest for criticality. This case simulates breach of the Zircaloy cladding only after the basket is completely corroded. Consequently, none of the elements is lost from the WP before that time, about 13,700 years. Hematite is present. Drip rate was 0.015 m^3/yr. The lines for Pu, Rh, and Ru coincide with the 100% line. Am is dissolved out quickly after waste package breach.
(Figure copied from spreadsheet MOXPdswa.xls, sheet sum.)

6. Results

A principal objective of the calculations was to assess chemical circumstances that could lead to removal of neutron absorbers from the waste package, thereby increasing the probability that a nuclear criticality could occur within the waste package. This was investigated by setting up some initial cases, examining the results to identify the reasons for the chemical changes during degradation of waste package materials and flushing by J-13 water, and finally setting up additional cases that were expected to lead to a greater removal of neutron absorbers, such as gadolinium, while retaining as much fissile material as possible. In other words successive cases were designed to increase the conservatism. Nevertheless, the differences in the results were in all instances small.

Most of the Fe and Mn initially present in the metals are simulated to be retained. The situation for Ni is more complex. Evidently its retention depends strongly on the pH history, especially during the first several thousand years. The percentage retained may be as low as 6%, e.g., for a fast corrosion rate of the borated SS at a drip rate of 0.15 m^3/yr, or as high as 83%, e.g., for simultaneous degradation of the basket and PWR MOX SNF with a mean corrosion rate for the borated SS and the high drip rate of 0.5 m^3/yr. In most runs the percentage simulated to be retained at very long times was in the range of 25% to 33%. During the early history for cases in which SNF is not exposed to the water the corrosion product is predicted to be Ni_2SiO_4, but later this transforms to trevorite, $NiFe_2O_4$, the only form found after SNF begins to degrade. Another interesting difference is the predicted formation of minor amounts of nontronite clay in the absence of degradation of SNF, but not when the SNF also degrades. This also probably relates to slight differences in pH. Neither of these differences is very significant in view of the small amounts of these solids.

All or most of the Gd, Sm, and Eu are simulated to be removed for those cases in which the borated SS and SNF degrade simultaneously, but most of the Nd is modeled as retained. See Figures 5.3.2-1, 5.3.2-5, and 5.3.2-9. This results not from significant differences in their solubilities, but from the differences in their initial inventories in the SNF. All of the Am is simulated to be removed very quickly, and all of the Np to be flushed out of the LEU SNF WP in less than 15,000 years, and more than half from the MOX SNF WP in 50,000 years. Nearly all of the U is retained, and, within the numerical precision, all of the Pu is kept. The small amounts of Ru and Rh likewise appear to be completely retained. Silver evidently will dissolve slowly and be removed in less than 40,000 years.

For the cases which simulate the complete corrosion of the borated SS prior to the start of the degradation of the SNF, essentially all of the lanthanides, specifically, Nd, Sm, Eu, and Gd would be retained within the WP. Am is still modeled to be removed rapidly, and the Ag is also dissolved and flushed out, but more slowly. The case for a slow drip rate, after basket corrosion, the pH is lower for an extended time and the Gd is modestly more soluble than for the mean drip rate, but the slowness of the flushing results in a slower removal of all elements from the waste package.

Detailed results of specific cases are presented in Section 5.

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8. Attachments

Attachment I. Algorithms for the C Programs (15 pages)

Attachment II. Review of the C Programs in Accordance with QAP-SI-0 (Ref. 27) (1 page)

Attachment III. Pro-Engineer Output (15 pages)

List of Files on the Colorado Trakker Tape (Ref. 11)

```
DATA0N~1 R8     2,298,907 07-29-98 9:08a data0.nuc.R8
dir     txt             0 08-14-98 6:49p dir.txt
DripRate xls       17,920 08-05-98 5:18p DripRate.xls
J13INF~1 XLS       18,432 07-23-98 4:25p J13influx.xls
MOX0_1~1 ALL   30,633,378 07-27-98 6:48p MOX0_15I.allin
MOX0_1~2 ALL   41,591,030 07-27-98 6:49p MOX0_15I.alltab
MOX0_1~1 POS    5,549,999 07-27-98 12:05p MOX0_15I.post
MOX0_15I sum      559,562 07-27-98 12:05p MOX0_15I.sum
MOXcomp2 xls      142,848 07-24-98 9:08a MOXcomp2.xls
MOXPD0~1 ALL   13,767,640 07-27-98 1:04p MOXpd0_15II.allin
MOXPD0~2 ALL   20,773,350 07-27-98 1:05p MOXpd0_15II.alltab
MOXPD0~1 POS    2,120,208 07-27-98 1:05p MOXpd0_15II.post
MOXPD0~1 SUM      215,886 07-27-98 1:05p MOXpd0_15II.sum
MOXPDA~1 ALL   33,508,798 07-27-98 6:54p MOXpda0_15II.allin
MOXPDA~2 ALL  111,730,331 07-27-98 6:58p MOXpda0_15II.allout
MOXPDA~3 ALL   47,075,600 07-27-98 6:59p MOXpda0_15II.alltab
MOXPDA~1 POS    3,804,076 07-27-98 12:49p MOXpda0_15II.post
MOXPDA~1 SUM      384,962 07-27-98 12:49p MOXpda0_15II.sum
MOXpda1  xls      378,368 07-24-98 2:27p MOXpda1.xls
MOXPDS~4 ALL    8,887,342 07-27-98 1:16p MOXpdsw0_15II.allin
MO870F~1 ALL   48,829,470 07-27-98 1:18p MOXpdsw0_15II.allout
MO86C5~1 ALL    7,646,600 07-27-98 1:18p MOXpdsw0_15II.alltab
MOXPDS~1 POS      335,426 07-27-98 1:18p MOXpdsw0_15II.post
MO1B73~1 ALL   33,175,478 08-14-98 6:21p MOXpdsw0_15III.allin
MO2538~1 ALL   49,907,260 07-27-98 1:22p MOXpdsw0_15III.alltab
MOXPDS~2 POS    4,935,831 07-27-98 1:22p MOXpdsw0_15III.post
MOXPdswa xls      534,016 07-24-98 2:26p MOXPdswa.xls
MOXPDS~1 6I        42,673 07-03-98 2:34p MOXpdswa0_015II.6i
MOXPDS~3 ALL   66,476,470 07-07-98 1:51a MOXpdswa0_015II.allin
MOXPDS~2 ALL    9,938,536 07-07-98 1:51a MOXpdswa0_015II.allpost
MOXPDS~1 ALL   93,794,740 07-07-98 1:51a MOXpdswa0_015II.alltab
MOXPDS~1 LAS      995,847 07-08-98 9:56a MOXpdswa0_015II.lastpost
MOXSF0~1 XLS      643,584 07-24-98 2:27p MOXSF0_15I.lastpost.xls
MOXSF0_5 xls    2,028,032 08-10-98 4:55p MOXSF0_5.xls
MOXSF0~1 ALL    3,143,896 07-27-98 7:06p MOXSF0_5I.allin
MOXSF0~2 ALL   54,382,997 07-27-98 7:08p MOXSF0_5I.allout
MOXSF0~3 ALL    4,666,350 07-27-98 7:08p MOXSF0_5I.alltab
MOXSF0~1 POS      487,690 07-27-98 7:27p MOXSF0_5I.post
MOXSF0~1 SUM       53,882 07-27-98 3:33p MOXSF0_5I.sum
MOXSF0~4 ALL   32,979,314 07-27-98 7:09p MOXSF0_5II.allin
```

```
MOF6C9~1 ALL    52,141,180  07-27-98  7:11p MOXSF0_5II.alltab
MOXSF0~2 POS     5,308,209  07-27-98 12:20p MOXSF0_5II.post
MOXSF0~2 SUM       535,198  07-27-98  3:33p MOXSF0_5II.sum
MOC050~1 ALL    32,934,542  07-27-98  7:12p MOXSF0_5III.allin
MO4787~1 ALL    51,970,880  07-27-98  7:14p MOXSF0_5III.alltab
MOXSF0~3 POS     5,308,291  07-27-98  7:27p MOXSF0_5III.post
MOXSF0~3 SUM       535,198  07-27-98  4:52p MOXSF0_5III.sum
Name     doc        22,528  07-29-98  9:58a Name.doc
PWR015~1 SUM        14,083  03-09-98 10:32a PWR0.15I.sum
PWR015~2 SUM        86,995  03-09-98 10:11a PWR0.15II.sum
PWR015~3 SUM       114,512  03-09-98 10:11a PWR0.15III.sum
PWR015~4 SUM       133,600  03-09-98  5:11p PWR0.15IV.sum
PWR0_0~1 ALL     3,761,520  07-28-98 10:03a PWR0_015ahsII.allin
PWR0_0~1 POS       140,018  07-27-98 11:24a PWR0_015ahsII.post
PWR0_0~1 SUM        17,974  07-27-98 11:24a PWR0_015ahsII.sum
PWDD75~1 ALL     7,735,298  07-28-98 10:03a PWR0_15ahI.allin
PW2F2A~1 ALL    35,791,729  07-28-98 10:05a PWR0_15ahI.allout
PW8639~1 ALL     6,074,112  07-28-98 10:05a PWR0_15ahI.alltab
PW50CF~1 ALL     7,167,349  07-28-98 10:05a PWR0_15ahII.allin
PWC730~1 ALL    91,184,486  07-28-98 10:08a PWR0_15ahII.allout
PWD6F6~1 ALL    10,455,892  07-28-98 10:08a PWR0_15ahII.alltab
PW96AE~1 ALL     3,736,279  07-28-98  8:44a PWR0_15I.allin
PW83CE~1 ALL    18,496,900  07-28-98  8:45a PWR0_15I.allout
PWR0_1~1 ALL       135,457  07-24-98  4:12p PWR0_15I.allpost
PWEACD~1 ALL     3,061,890  07-28-98  8:45a PWR0_15I.alltab
PWC45C~1 ALL    27,154,839  07-28-98  8:46a PWR0_15II.allin
PWR0_1~2 ALL       864,661  07-24-98  4:13p PWR0_15II.allpost
PW3B83~1 ALL    20,945,340  07-28-98  8:47a PWR0_15II.alltab
PWCF3D~1 ALL    35,005,754  07-28-98  8:48a PWR0_15III.allin
PWR0_1~3 ALL     1,139,355  07-24-98  4:15p PWR0_15III.allpost
PW7715~1 ALL    28,974,400  07-28-98  8:49a PWR0_15III.alltab
PWCE6C~1 ALL    40,846,302  07-28-98  8:50a PWR0_15IV.allin
PWR0_1~4 ALL     1,331,333  07-24-98  4:18p PWR0_15IV.allpost
PW35A3~1 ALL    33,790,900  07-28-98  8:51a PWR0_15IV.alltab
PWB6A4~1 ALL    26,702,616  07-28-98  8:52a PWR0_15V.allin
PWFAC8~1 ALL    37,957,920  07-28-98  8:53a PWR0_15V.alltab
PWR0_1~1 POS     5,163,595  07-28-98  8:54a PWR0_15V.post
PWR0_15V sum       521,089  07-28-98  8:54a PWR0_15V.sum
PWRSF0~2 XLS       617,984  08-06-98  3:39p PWRSF0_15.xls
PWRSF0~2 ALL     3,377,685  07-28-98  9:27a PWRSF0_15bII.allin
PWRSF0~3 ALL    27,046,348  07-28-98  9:28a PWRSF0_15bII.allout
PWRSF0~4 ALL     3,476,070  07-28-98  9:28a PWRSF0_15bII.alltab
PWRSF0~1 POS       198,701  07-24-98  5:28p PWRSF0_15bII.post
PWRSF0~1 SUM        21,333  05-26-98  6:19p PWRSF0_15bII.sum
PWRSF0~1 ALL    11,703,786  07-28-98  9:49a PWRSF0_15bIII.allin
PW7B4F~1 ALL    11,653,200  07-28-98  9:49a PWRSF0_15bIII.alltab
PWRSF0~2 POS       704,556  07-24-98  5:29p PWRSF0_15bIII.post
PWRSF0~2 SUM        71,759  07-24-98  5:29p PWRSF0_15bIII.sum
PW472C~1 ALL    75,958,315  07-28-98  9:51a PWRSF0_15bIV.allin
PW3B84~1 ALL    70,347,030  07-28-98  9:54a PWRSF0_15bIV.alltab
PWRSF0~3 POS     4,401,969  07-24-98  5:29p PWRSF0_15bIV.post
PWRSF0~3 SUM       440,773  07-24-98  5:29p PWRSF0_15bIV.sum
```

```
PW2C38~1 ALL     9,288,084  07-28-98  9:29a PWRSF0_15cI.allin
PW93B8~1 ALL    53,711,791  07-28-98  9:30a PWRSF0_15cI.allout
PW927F~1 ALL     7,645,820  07-28-98  9:31a PWRSF0_15cI.alltab
PWRSF0~4 POS       362,131  07-24-98  5:29p PWRSF0_15cI.post
PWRSF0~1 XLS       752,128  07-24-98 12:28p PWRSF0_15nH.xls
PWRSFN~3 ALL     9,384,305  07-28-98  4:04p PWRSFnH0_15I.allin
PWRSFN~4 ALL    45,671,501  07-28-98  4:06p PWRSFnH0_15I.allout
PWRSFN~1 POS       291,267  07-28-98  4:06p PWRSFnH0_15I.post
PWRSFN~1 SUM        34,584  07-28-98  4:06p PWRSFnH0_15I.sum
PW3019~1 ALL     5,625,673  07-28-98  4:06p PWRSFnH0_15II.allin
PWRSFN~2 ALL       328,845  07-28-98  4:06p PWRSFnH0_15II.allpost
PWA640~1 ALL     5,632,380  07-28-98  4:06p PWRSFnH0_15II.alltab
PWRSFN~2 SUM        38,896  07-28-98  4:06p PWRSFnH0_15II.sum
PW3BFD~1 ALL    11,235,778  07-28-98  4:14p PWRSFnH0_15III.allin
PWRSFN~1 ALL       669,949  07-28-98  4:14p PWRSFnH0_15III.allpost
PW357D~1 ALL    11,388,130  07-28-98  4:15p PWRSFnH0_15III.alltab
PWRSFN~3 SUM        72,454  07-28-98  4:15p PWRSFnH0_15III.sum
PW3A29~1 ALL    32,046,080  07-28-98  4:16p PWRSFnH0_15IV.allin
PWA060~1 ALL    30,743,050  07-28-98  4:17p PWRSFnH0_15IV.alltab
PWRSFN~2 POS     2,004,348  07-28-98  4:17p PWRSFnH0_15IV.post
PWRSFN~4 SUM       206,019  07-28-98  4:17p PWRSFnH0_15IV.sum
PWRSFpd  xls       672,256  07-24-98 12:30p PWRSFpd.xls
Rhdata   xls        26,624  04-02-98  2:28p Rhdata.xls
V5MOXV~1 XLS        14,848  07-23-98  5:26p V5moxvolorig.xls
VOLMAS~1 XLS     1,847,296  07-23-98  3:54p volmas21c.xls
water    xls        17,920  07-23-98  5:06p water.xls
       118 file(s) 1,775,450,619 bytes
```

Attachment I Scripts and Programs to Perform Simulations

Several of the scripts include adjustable parameters that are changed to suitable values to start specific simulations, e.g. variables $count and $ocount in allpost.bat

bldinput.bat

```
echo "did not run bldinput" >sfile
count=1
bldinput
read status <sfile
if [ "$status" != "go" ]
then
  echo $status
  echo "job terminated"
  exit
fi
echo $count
while [ $count -lt 200 ]
do
  mv bldinput.out input
  eq6dR136.opt
    cat input >> allin
    cat pickup >> allpick
    cat output >> allout
    cat tab >> alltab
  nxtinput
  read status <sfile
  if [ "$status" != "go" ]
  then
    echo $status
    echo "job terminated"
    exit
  fi
  count=`expr $count + 1`
  echo $count
done
exit
```

nxtinput.bat

```
count=1

while [ $count -lt 200 ]

do

  mv bldinput.out input

  eq6dR136.opt

    cat input >> allin

    cat pickup >> allpick

    cat output >> allout

    cat tab >> alltab

  nxtinput

  read status <sfile

  if [ $status != "go" ]
  then
    exit
  fi
  count=`expr $count + 1`
```

```
  echo $count
 done
 rename
 exit
```

bldinput.in

```
root       date        creator       delmaxtime
PWRSF0:15II   05/26/98    Automated        9.56e+08
```

allpost.bat

```
ocount=1

while [ $ocount -lt 5 ]

do

 count=1

 while [ $count -lt 200 ]

 do

  mv bldinput.out input

  eq6dR136.opt

    cat input >> allin
    cat output >> allout
    cat tab >> alltab
  nxtinput
  read status <sfile
  if [ $status != "go" ]
  then
    exit
  fi
  count=`expr $count + 1`
  echo $count
 done
 rm rootname
 postprocC
 cat postproc.out >> allpost
 rm allout
 ocount=`expr $ocount + 1`
done
exit
```

bldinput.c

```
#include <stdio.h>
#include <string.h>
#include <stdlib.h>
#include <math.h>
float  getfloat(char*,int,int);
void setup(),bldpick(),infromstd(),infromlast(),
   strinsert(char*,char*,int,int);
int locate0(char*,FILE*),locateall(char*,FILE*),tobar(char*,int);
float duration,delmaxtime;
char dummy[100],buffer[90],lookahead[90];
char froot[20],cname[20],fname[20];
FILE *fin,*fout,*fp,*ftemp,*fstd,*foutout,*finin,*fsfile;

void main()
{int i,j,k,flag;
fsfile=fopen("sfile","w");
```

```
fprintf(fsfile,"go\n");
flag=1;
fout=fopen("bldinput.out","w");/*file to be moved to input*/
if(flag==1) infromstd();
/*else infromlast();*/}

void infromstd()
{int i,j,k;
char tempstr[20],datestr[10];
fstd=fopen("input","r");/*template for initial input file*/
fin=fopen("bldinput.in","r");/*filename,creator,duration)*/
fgets(dummy,100,fin);/*readthrough labels of setup data*/
fscanf(fin,"%s %s %s %f",froot,datestr,cname,&delmaxtime);
strcpy(fname,froot);
strcat(fname,"1.6i        ");
locate0("|EQ",fstd);
strinsert(dummy,fname,22,strlen(fname));
fputs(dummy,fout);
locate0("|Created",fstd);
strcat(cname,"          ");
strinsert(dummy,datestr,9,8);
strinsert(dummy,cname,30,strlen(cname));
fputs(dummy,fout);
locate0("| starting time",fstd);
i=tobar(dummy,1);
if(i<0)
  {printf("couldn't find |");
  exit(0);}
i=tobar(dummy,i+1);
if(i<0)
  {printf("couldn't find |");
  exit(0);}
i=tobar(dummy,i+1);
if(i<0)
  {printf("couldn't find |");
  exit(0);}
sprintf(tempstr,"%12.5e",delmaxtime);
k=strlen(tempstr);
j=tobar(dummy,i+1);
if(j<0)
  {printf("couldn't find |");
  exit(0);}
strncat(tempstr,"       ",j-i-1-k);
strinsert(dummy,tempstr,i+1,j-i-1);
fputs(dummy,fout);
while(fgets(dummy,90,fstd)!=NULL)fputs(dummy,fout);}

void strinsert(char inline[90],char insert[90],int start,int len)
{int i;
for(i=0;i<len;i++) inline[start+i]=insert[i];}

int locate0(char sstring[50],FILE *fp)
{int i=0;
while(fgets(dummy,90,fp)!=NULL)
  {if(strncmp(dummy,sstring,strlen(sstring))==0)return i;
  i++;
  fputs(dummy,fout);}
return 0;}

int tobar(char line[100],int start)
{int i;
i=start;
while((i<strlen(line))&&(line[i]!='|'))i++;
if(line[i]=='|')return i;
else return -1;}
```

nxtinput.c

```
#include <stdio.h>
#include <string.h>
#include <stdlib.h>
#include <math.h>
double getfloat(char*,int,int),gettobar(char*,int);
void setup(),bldpick(),infromstd(),infromlast(),
   convert(double,double,FILE*,FILE*),
   strinsert(char*,char*,int,int);
int locaterw(char*,FILE*,FILE*),locatero(char*,FILE*),
   locate2(char*,char*,FILE*),tobar(char*,int),findinline(char*),
   puttobar(char*,char*,int),locate1of2(char*,char*,FILE*);
int finished=0;
double mash2oend,duration;
char dummy[100],tdummy[100];
char froot[20],cname[20],fname[20];
FILE *fout,*fpick,*fotemp,*fptemp,*fstd,*foutout,*finin,
   *fttemp,*fs,*fin;

void main()
{int i,j,k,flag;
fs=fopen("sfile","w");
fprintf(fs,"go\n");
flag=1;
fout=fopen("bldinput.out","w");/*file to be moved to input*/
infromlast();}

void infromlast()
{int i,j,k,dot;
char tempstr[30],carbstr[7],*cp,sstring[60],tempstr2[20];
double dmj13,msh2o,msh2ox,xx,yy,moles,dmoles,delmaxtime;
fin=fopen("bldinput.in","r");/*input parameters special to this case*/
fstd=fopen("input","r");/*template from last input file*/
fpick=fopen("pickup","r");/*old pickup file; extract section to bldinput.out*/
foutout=fopen("output","r");/*from last iteration to new input*/
finin=fopen("input","r");/*from last iteration to new input*/
fotemp=fopen("otemp","w");/*store intermediate segments from output*/
fptemp=fopen("ptemp","w");/*store intermediate segments from pickup*/
fgets(dummy,90,fin); /*readthrough labels*/
fscanf(fin,"%s %s %s %lf\n",
     tempstr,tempstr,tempstr,&delmaxtime);/*only 1 param used this prgrm*/
locatero("                    Moles of solvent H2O",foutout);
msh2ox=getfloat(dummy,44,12);  /*optional  parameter from the first block*/
foutout=freopen("output","r",foutout);
strcpy(sstring,"                     Reaction progress");
if(locatero(sstring,foutout)==-1)  /*find output block of interest*/
  {printf("bad output file\n");
  exit(0);}
fputs(dummy,fotemp);        /*and write it to temporary*/
while(fgets(dummy,90,foutout)!=NULL)
  {fputs(dummy,fotemp);
  if(strncmp(dummy,sstring,strlen(sstring))==0)
     {fotemp=freopen("otemp","w",fotemp);
     fputs(dummy,fotemp);}}
fotemp=freopen("otemp","r",fotemp);/* re-open to find water*/
strcpy(sstring,"Mass of solvent H2O");
if(locatero(sstring,fotemp)!=1)
  {printf("Can't find ending water\n");
  fs=fopen("sfile","w");
  fprintf(fs,"cant find ending water");
  exit(0);}/*ending water*/
mash2oend=getfloat(dummy,44,12);
fotemp=freopen("otemp","r",fotemp);/*now reopen for use*/
if(locatero("c pickup file",fpick)==-1)   /*start copying here*/
  {printf("bad pickup file\n");
```

```
  exit(0);}
fputs(dummy,fptemp);
for(i=0;i<2;i++)  /*readwrite through first "|EQ"*/
  {fgets(dummy,90,fpick);
  fputs(dummy,fptemp);}
while(fgets(dummy,90,fpick)!=NULL) /*pickup to ptemp*/
  {fputs(dummy,fptemp);
  if(strncmp(dummy,"|EQ",3)==0) /*read through without copying*/
    while(fgets(dummy,90,fpick)!=NULL)
      if(strncmp(dummy,"c pickup file",strlen("c pickup file"))==0)
        {fptemp=freopen("ptemp","w",fptemp);/*start copying over again*/
        fputs(dummy,fptemp);
        for(i=0;i<2;i++)
          {fgets(dummy,90,fpick);
          fputs(dummy,fptemp);}
        break;}}
fptemp=freopen("ptemp","r",fptemp); /*now reopen for use*/
if(locaterw("|EQ",fstd,fout)==-1)
  {printf("bad input file\n");
  exit(0);}
i=0;
while((i<strlen(dummy))&&(dummy[i]!='.'))i++;
dot=i;
i=0;
while((dummy[dot-i-1]<='9')&&(dummy[dot-i-1]>='0'))i++;
for(j=0;j<i;j++)tempstr[j]=dummy[dot-i+j];
tempstr[i]='\0';
k=atoi(tempstr);
sprintf(tempstr,"%u%s",k+1,".6i");
strinsert(dummy,tempstr,dot-i,strlen(tempstr));
fputs(dummy,fout);
fgets(dummy,90,fotemp);/*get ending value of zi from first line*/
xx=getfloat(dummy,48,22);
if(locaterw("| starting value of zi",fstd,fout)==-1)
  {printf("can't find starting zi in input file\n");
  exit(0);}
sprintf(tempstr,"%15.8lE",xx);
i=tobar(dummy,1);
strinsert(dummy,tempstr,i+1,strlen(tempstr));
fputs(dummy,fout); /*and put into input*/
fgets(dummy,90,fstd);
fputs(dummy,fout);
fgets(tdummy,90,fstd);/*this takes us to entry for starting time*/
if(locatero("       Time increased from",fotemp)==-1)
  {printf("can't find last ending time in output\n");
  exit(0);}
fgets(dummy,90,fotemp);/*this line will have end time of last run*/
xx=getfloat(dummy,31,12);
sprintf(tempstr,"%11.5lE",xx);
i=tobar(tdummy,1);
if(i==-1)
  {printf("cant find slot for starttime\n");
  exit(0);}
strinsert(tdummy,tempstr,i+1,strlen(tempstr));
i=tobar(tdummy,i+1);
i=tobar(tdummy,i+1);
if(i==-1)
  {fs=freopen("sfile","w",fs);
  printf("cant find slot for maxtime\n");
  exit(0);}
/*yy=gettobar(tdummy,i+1); */
sprintf(tempstr,"%12.4lE",xx+delmaxtime);
strinsert(tdummy,tempstr,i+1,strlen(tempstr));
fputs(tdummy,fout); /*and put into input*/
fotemp=freopen("otemp","r",fotemp);/*last read was beyond current interest*/
if(locatero("    Reactant                  Moles     Delta moles",fotemp)==-1)
  {printf("cant find values for reactants in the output file\n");
```

```
  exit(0);}
fgets(tdummy,90,fotemp);
fgets(tdummy,90,fotemp);/*get to first reactant in otemp*/
while((finished==0)&&(strncmp(tdummy,"\n",1)!=0))/*loop to do all reactants*/
  {moles=getfloat(tdummy,29,10);
  dmoles=getfloat(tdummy,42,10);
  locaterw("| moles remaining",fstd,fout);/*next reactant*/
  sprintf(tempstr,"%10.4lE",moles);
  strinsert(dummy,tempstr,20,strlen(tempstr));
  if(strncmp(tdummy,"  J-13 water",12)!=0)
    {sprintf(tempstr2,"%10.4lE",dmoles);
    strinsert(dummy,tempstr2,58,strlen(tempstr2));}
  else
    {dmj13=dmoles;
    finished=1;}                       /*Water is the last reactant*/
  fputs(dummy,fout);
  fgets(tdummy,90,fotemp);}
if(locatero("                    Moles of solvent H2O",fotemp)==-1)
  {fprintf(fs,"cant find moles water in output\n");
  exit(0);}
msh2o=getfloat(dummy,44,12);
k=locatero(" ---  The reaction path has terminated normally",fotemp);
if(k==-1)
  {fputs("abnormal reaction path termination\n",fs);
  exit(0);}
fotemp=freopen("otemp","r",fotemp);/*back to the top again*/
if((k=locate2(" CO3--"," HCO3-",fotemp))==1) strcpy(carbstr,"| CO3--");
else if (k==2) strcpy(carbstr,"| HCO3-");
fttemp=fopen("ttemp","w");/*will later attach to input*/
if(locate1of2("| CO3--","| HCO3-",fptemp)==-1)/*also copies ptemp to ttemp*/
  {fprintf(fs,"cant find line to insert carbonates in pickup\n");
  exit(0);}
strinsert(dummy,carbstr,0,strlen(carbstr));
fputs(dummy,fttemp);
while(fgets(dummy,90,fptemp)!=NULL)fputs(dummy,fttemp);/*rest of ptemp to ttemp*/
fttemp=freopen("ttemp","r",fttemp);
if(locaterw("c pickup file",fstd,fout)==-1)/*transfer the relevant remainder of the
template*/
  {fprintf(fs,"cant find start for pickup info\n");
  exit(0);}
convert(msh2o,dmj13/3,fstd,fttemp);}

int locate1of2(char sstring1[50],char sstring2[50],FILE *fp)
{int found1=0,found2=0;
while((found1==0)&&(found2==0))
  {if(fgets(dummy,90,fp)==NULL)return -1;
  if(found1==0)
     if(strncmp(dummy,sstring1,strlen(sstring1))==0)
       found1=1;
  if(found2==0)
     if(strncmp(dummy,sstring2,strlen(sstring2))==0)
       found2=1;
  if((found1==0)&&(found2==0))fputs(dummy,fttemp);}
if((found1==0)&&(found2==0))return -1;
else return 0;}

void strinsert(char inline[90],char insert[90],int start,int len)
{int i;
for(i=0;i<len;i++) inline[start+i]=insert[i];}

int locate2(char sstring1[50],char sstring2[50],FILE *fp)
{int i,found1=0,found2=0;
double x1=0,x2=0;
char buffer[100];
while((fgets(dummy,90,fp)!=NULL)&&((found1==0)||(found2==0)))
  {strcpy(buffer,dummy);
  if(found1==0)
```

```
      if(strncmp(dummy,sstring1,strlen(sstring1))==0)
        {found1=1;
        x1=getfloat(dummy,28,12);}
   if(found2==0)
      if(strncmp(dummy,sstring2,strlen(sstring2))==0)
        {found2=1;
        x2=getfloat(dummy,28,12);}}
if(x1<x2) return 2;
else return 1;}

int locatero(char sstring[60],FILE *fp)/*read only*/
{while(fgets(dummy,90,fp)!=NULL)
  if(findinline(sstring)==1)return 1;
return -1;}

int locaterw(char sstring[60],FILE *fpin,FILE *fpout)/*read&write*/
{while(fgets(dummy,90,fpin)!=NULL)
  {if(strncmp(dummy,sstring,strlen(sstring))==0)return 1;
  fputs(dummy,fpout);}
return -1;}

void convert(double x,double z,FILE *fins,FILE *finp)
{int i,count=0;
double u,v,w,r;
char buffer[100],temp[50],temp2[50];
r=x/(x+z);
if(mash2oend*r>1)
  {r=1/mash2oend;
   printf("converted to %f\n",r);}
if(locaterw("| elements, moles",finp,fout)==-1)/*readwrite to this point*/
  {printf("cant locate place to put new values of reagents in input\n");
  exit(0);}
fputs(dummy,fout);
fgets(buffer,90,finp);
fputs(buffer,fout);
fgets(buffer,98,finp);
while(strncmp(buffer,"|-------",8)!=0)
  {w=getfloat(buffer,55,21);
  v=w*r;
  u=getfloat(buffer,30,21)-w*(1-r);
  sprintf(temp,"%22.15lE",u);
  strinsert(buffer,temp,29,strlen(temp));
  sprintf(temp,"%22.15lE",v);
  strinsert(buffer,temp,54,strlen(temp));
  fputs(buffer,fout);
  fgets(buffer,90,finp);
  count++;}
fputs(buffer,fout);
for(i=0;i<2;i++)
  {fgets(buffer,100,finp); /*readthrough to species table*/
  fputs(buffer,fout);}
for(i=0;i<count;i++)
  {fgets(buffer,100,finp);
  w=getfloat(buffer,56,22);
  sprintf(temp,"%+20.15lE",w+log10(r));
  strinsert(buffer,temp,56,strlen(temp));
  fputs(buffer,fout);}
while(fgets(buffer,100,finp)!=NULL) fputs(buffer,fout);}

double getfloat(string,start,len)
char string[100];
int start,len;
{char temp[30];
strncpy(temp,string+start,len);
temp[len]='\0';
return atof(temp);}
```

```
double gettobar(char line[100],int start)
{int i;
char temp[30];
i=start;
while((i<strlen(line))&&(line[i]!='|'))
  {temp[i-start]=line[i];
  i++;}
temp[i]='\0';
if(line[i]!='|')return -1;
return atof(temp);}

int puttobar(char line[100],char string[30],int start)
{int i,k;
i=start;
k=strlen(string);
while((i<strlen(line))&&(line[i]!='|')&&(i-start<k))
  {line[i]=string[i-start];
  i++;}
if(line[i]=='|')return i;
else return -1;}

int tobar(char line[100],int start)
{int i;
i=start;
while((i<strlen(line))&&(line[i]!='|'))i++;
if(line[i]=='|')return i;
else return -1;}

int findinline(char sstring[50])
{int i=0;
while(i<100)
  {if(strncmp(dummy+i,sstring,strlen(sstring))==0) return 1;
  else i++;}
return 0;}
```

postprocP.c

```
/* postprocJ.c expanded mineral set*/
#include <stdio.h>
#include <string.h>
#include <stdlib.h>
#include <math.h>
#include <malloc.h>

double getfloat(char*,int,int);
int locate(char*,char*),getreacts(),numreacts;
void msgerr(char*,int,int),getmnrls(),trimb(char*),getelements();
int finished=0;
char dummy[150],reactstrs[20][20];
FILE *fout,*ferr,*fin,*fout,*fallyrs1,*fallyrs2,*fchgyrs1,
  *fchgyrs2,*froot;
float ph,is,mos,mas,hpluss,time,b,gd,ps,pu,u,j13,reactvals[20],
     puo2,npo2,amoh,sodd,haiw,rhabdo,gdpo4,ndpo4,smpo4,gdoh,ndoh,euoh,smco3,laf,
     gdf,ndf,smf,agcl,rh2o3,ruo2,dias,hema,goet,trev,nisi,pyro,smec,nonca,nonk,
     nonmg,nonna,cauo,uo3;
struct OUTREC
   {struct OUTREC *next;
   char data[1000];};

void main()
{int i,j,k,bcount=0,lcount=0,endblock,firstall=1,firstchg=1,
      firsttime=1,newblock=1,fileflag=0;
struct OUTREC *pallyrs1,*pallyrs2,*pallyrs3,
     *pchgyrs1,*pchgyrs2,*pchgyrs3,*p,
     *pfallyrs1,*pfallyrs2,*pfallyrs3,
          *pfchgyrs1,*pfchgyrs2,*pfchgyrs3;
char outs[4][1000], fstr[50],rootstr[50];
```

```
if((froot=fopen("rootname","r"))!=NULL)
  {fscanf(froot,"%s",rootstr);
  fclose(froot);
  strcpy(fstr,rootstr);
  strcat(fstr,".allout");
  if((fin=fopen(fstr,"r"))!=NULL)fileflag=1;}
if(fileflag==0)
 if((fin=fopen("allout","r"))==NULL)
  {printf("Cant open input file\n");
  exit(0);}
if(fileflag==0)fout=fopen("postproc.out","w");
else
  {strcat(rootstr,".postproc");
  fout=fopen(rootstr,"w");}
printf("filename=%s  fileflag=%d\n",fstr,fileflag);
while(finished==0)
  {if((k=locate("                      Time = "," J-13 water"))==1)
    {fgets(dummy,100,fin);
        time=getfloat(dummy,29,11);}
  else if(k==0) msgerr("Missed time",bcount,lcount);
  else break; /*proper end of file */
  if((k=locate("     Reactant                  Moles",
       "      --- Element Totals"))==1)
    {if(firsttime==1)
           {numreacts=getreacts(1);
                firsttime=0;}
         else getreacts(0);}
  else if(k==0) msgerr("Missed reactants",bcount,lcount);
  else msgerr("Unexpected end of file",bcount,lcount);
  getelements();
  if((k=locate("     modified NBS pH scale"," H+"))==1)
     ph=getfloat(dummy,37,8);  /* pH */
  else if(k==0) msgerr("Missed pH",bcount,lcount);
  else msgerr("Unexpected end of file",bcount,lcount);
  if((k=locate("                    Ionic strength"," H+"))==1)
     is=getfloat(dummy,38,13);  /* Ionic strength */
  else if(k==0) msgerr("Missed ionic str",bcount,lcount);
  else msgerr("Unexpected end of file",bcount,lcount);
  if((k=locate("                    Moles of solvent"," H+"))==1)
     mos=getfloat(dummy,44,13);  /* Moles solvent water */
  else if(k==0) msgerr("Missed moles water",bcount,lcount);
  else msgerr("Unexpected end of file",bcount,lcount);
  if((k=locate("                    Mass of solvent"," H+"))==1)
     mas=getfloat(dummy,44,13);  /* Mass solvent water */
  else if(k==0) msgerr("Missed mass water",bcount,lcount);
  else msgerr("Unexpected end of file",bcount,lcount);
  if((k=locate(" H+","        --- Summary of Solid Product Phases---"))==1)
     hpluss=-getfloat(dummy,68,9);  /* H+ */
  else if(k==0) msgerr("Missed H+",bcount,lcount);
  else msgerr("Unexpected end of file",bcount,lcount);
  if(fabs(ph-hpluss)>1.e-4)
    {printf("%f %f\n",ph,hpluss);
        msgerr("pH mismatch",bcount,lcount);}
  getmnrls();
  if((k=locate("       Time increased from",
     "                     Reaction progress"))==1)
         {endblock=1;
         bcount++;}
  else if (k==0) endblock=0;
  else finished==1;
  lcount++;
  printf("%d %d\n",bcount,lcount);
  if ((endblock==0)||(finished==1))
  {sprintf(outs[0],"%11.3e%11.3e%11.3e%11.3e%11.3e%11.3e%11.3e%11.3e%11.3e\n",
     time/365.2486/1000,ph,b,gd,ps,pu,u,is,mos);
  sprintf(outs[1],
```

```
 "%11.3e%11.3e%11.3e%11.3e%11.3e%11.3e%11.3e%11.3e%11.3e%11.3e%11.3e%11.3e%11.3e%11.3e%\
 11.3e%11.3e%11.3e%11.3e%11.3e%11.3e%11.3e%11.3e%11.3e%11.3e%11.3e%11.3e%11.3e%11.3e%\
 11.3e%11.3e%11.3e%11.3e%11.3e%11.3e\n",
      time/365.2486/1000,puo2,npo2,amoh,sodd,haiw,cauo,uo3,rhabdo,gdpo4,ndpo4,smpo4,gdoh,
      ndoh,euoh,smco3,laf,gdf,ndf,smf,agcl,rh2o3,ruo2,dias,hema,goet,trev,nisi,
      pyro,smec,nonca,nonk,nonmg,nonna);
   sprintf(outs[2],"%11.3e",time/365.2486/1000);
   for(i=0;i<numreacts;i++)sprintf(outs[2]+11*(i+1),"%11.3e",reactvals[i]);
   outs[2][11*(numreacts+1)]='\n';
   if(firstall==1)
     {firstall=0;
         pfallyrs1=malloc(sizeof(struct OUTREC));
         pfallyrs2=malloc(sizeof(struct OUTREC));
         pfallyrs3=malloc(sizeof(struct OUTREC));
         pallyrs1=pfallyrs1;
         pallyrs2=pfallyrs2;
         pallyrs3=pfallyrs3;}
   else
     {if((pallyrs1->next=malloc(sizeof(struct OUTREC)))==NULL)
           msgerr("malloc",bcount,lcount);
      if((pallyrs2->next=malloc(sizeof(struct OUTREC)))==NULL)
           msgerr("malloc",bcount,lcount);
      if((pallyrs3->next=malloc(sizeof(struct OUTREC)))==NULL)
           msgerr("malloc",bcount,lcount);
         pallyrs1=pallyrs1->next;
         pallyrs2=pallyrs2->next;
         pallyrs3=pallyrs3->next;}
  strcpy(pallyrs1->data,outs[0]);
  strcpy(pallyrs2->data,outs[1]);
  strcpy(pallyrs3->data,outs[2]);
  pallyrs1->next=NULL;
  pallyrs2->next=NULL;
  pallyrs3->next=NULL;
  if(newblock==1)
    {if(firstchg==1)
           {firstchg=0;
      pfchgyrs1=malloc(sizeof(struct OUTREC));
           pfchgyrs2=malloc(sizeof(struct OUTREC));
           pfchgyrs3=malloc(sizeof(struct OUTREC));
           pchgyrs1=pfchgyrs1;
           pchgyrs2=pfchgyrs2;
           pchgyrs3=pfchgyrs3;}
    else
      {if((pchgyrs1->next=malloc(sizeof(struct OUTREC)))==NULL)
         msgerr("malloc",bcount,lcount);
           pchgyrs2->next=malloc(sizeof(struct OUTREC));
           pchgyrs3->next=malloc(sizeof(struct OUTREC));
           pchgyrs1=pchgyrs1->next;
           pchgyrs2=pchgyrs2->next;
           pchgyrs3=pchgyrs3->next;}
    strcpy(pchgyrs1->data,outs[0]);
    strcpy(pchgyrs2->data,outs[1]);
    strcpy(pchgyrs3->data,outs[2]);
    pchgyrs1->next=NULL;
    pchgyrs2->next=NULL;
    pchgyrs3->next=NULL;
        newblock=0;}}
  if(endblock==1) newblock=1;}
fprintf(fout,"\n\nDATA FOR EACH TIMESTEP Elements\n\n");
fprintf(fout,"%11s%11s%11s%11s%11s%11s%11s%11s%11s\n",
   "1000yr","pH","MolesB","MolesGd","MolesP","MolesPu",
        "MolesU","IonicStr","MlsH20");
p=pfallyrs1;
fputs(p->data,fout);
while((p=p->next)!=NULL) fputs(p->data,fout);
fprintf(fout,"\n\nDATA FOR EACH TIMESTEP Minerals\n\n");
```

```
fprintf(fout,"%11s%11s%11s%11s%11s%11s%11s%11s%11s%11s%11s%11s%11s%11s%11s%11s%11s%11s%11s%\
11s%11s%11s%11s%11s%11s%11s%11s%11s%11s%11s%11s%11s%11s%11s\n",

"1000yr","MlPuO2","MlNpO2","MlAmOHCO3","MlSodd","MlHaiwee","MlCaUO4","MlUO3:2H2O","MlRhabd
o",
   "MlGdPO4","MlNdPO4","MlSmPO4","MlGdOHCO3","MlNdOHCO3","MlEuOHCO3",
   "MlSm2(CO3)3","MlLaF3","MlGdF3","MlNdF3","MlSmF3","MlChlorarg","MlRh2O3",
   "MlRuO2","MlDiaspore","MlHematite","MlGoethite","MlTrevorite","MlNi2SiO4",
   "MlPyrolusi","MlSmectite","MlNontro-Ca","MlNontro-K","MlNontro-Mg",
   "MlNontro-Na");
p=pfallyrs2;
fputs(p->data,fout);
while((p=p->next)!=NULL) fputs(p->data,fout);
fprintf(fout,"\n\nDATA FOR EACH TIMESTEP Reactants\n\n");
  sprintf(outs[3],"%11s","1000yr");
  for(i=0;i<numreacts;i++)sprintf(outs[3]+11*(i+1),"%11s",reactstrs[i]);
fprintf(fout,"%s\n",outs[3]);
p=pfallyrs3;
fputs(p->data,fout);
while((p=p->next)!=NULL) fputs(p->data,fout);
fprintf(fout,"\n\nDATA FOR CHANGING TIMESTEPS Elements\n\n");
fprintf(fout,"%11s%11s%11s%11s%11s%11s%11s%11s%11s\n",
   "1000yr","pH","MolesB","MolesGd","MolesP","MolesPu",
       "MolesU","IonicStr","MlsH20");
p=pfchgyrs1;
fputs(p->data,fout);
while((p=p->next)!=NULL) fputs(p->data,fout);
fprintf(fout,"\n\nDATA FOR CHANGING TIMESTEPS Minerals\n\n");
fprintf(fout,"%11s%11s%11s%11s%11s%11s%11s%11s%11s%11s%11s%11s%11s%11s%11s%11s%11s%11s%11s%\
11s%11s%11s%11s%11s%11s%11s%11s%11s%11s%11s%11s%11s%11s%11s\n",

"1000yr","MlPuO2","MlNpO2","MlAmOHCO3","MlSodd","MlHaiwee","MlCaUO4","MlUO3:2H2O","MlRhabd
o",
   "MlGdPO4","MlNdPO4","MlSmPO4","MlGdOHCO3","MlNdOHCO3","MlEuOHCO3",
   "MlSm2(CO3)3","MlLaF3","MlGdF3","MlNdF3","MlSmF3","MlChlorarg","MlRh2O3",
   "MlRuO2","MlDiaspore","MlHematite","MlGoethite","MlTrevorite","MlNi2SiO4",
   "MlPyrolusi","MlSmectite","MlNontro-Ca","MlNontro-K","MlNontro-Mg",
   "MlNontro-Na");
p=pfchgyrs2;
fputs(p->data,fout);
while((p=p->next)!=NULL) fputs(p->data,fout);
fprintf(fout,"\n\nDATA FOR CHANGING TIMESTEPS Reactants\n\n");
fprintf(fout,"%s\n",outs[3]);
p=pfchgyrs3;
fputs(p->data,fout);
while((p=p->next)!=NULL) fputs(p->data,fout);}

void msgerr(char msgstr[50],int i,int j)
{fprintf(fout,"%s  block count = %d  line count = %d\n",msgstr,i,j);
printf("%s  block count = %d  line count = %d\n",msgstr,i,j);
/*exit(0);*/}

int locate(char sstring[60],char estring[50])
{int i,j;
i=strlen(sstring);
j=strlen(estring);
while(fgets(dummy,100,fin)!=NULL)
  if (strncmp(dummy,sstring,i)==0)return 1;
  else if (strncmp(dummy,estring,j)==0)return 0;
return -1;}

double getfloat(string,start,len)
char string[100];
int start,len;
{char temp[30];
strncpy(temp,string+start,len);
temp[len]='\0';
```

```
return atof(temp);}

void getmnrls()
{int i,k,num=33,founds[33]={0},finished=0,slens[33];
char mnrlstrs[33][20]={" AmOHCO3"," CaUO4"," Chlorargyrite"," Diaspore"," Eu(OH)CO3(s)",
    " GdOHCO3"," Goethite"," Haiweeite"," Hematite"," NdOHCO3"," Ni2SiO4",
    " NpO2"," PuO2"," Pyrolusite"," Rh2O3"," RuO2"," Sm2(CO3)3"," Soddyite",
    " Trevorite"," UO3:2H2O"," Smectite-di","   Nontronite-Ca","   Nontronite-K",
    "   Nontronite-Mg","   Nontronite-Na"," Rhabdophane-ss","   NdPO4:H2O",
    "   GdPO4:H2O","   SmPO4:H2O","   LaF3:0.5H2O","   NdF3:0.5H2O",
    "   GdF3:0.5H2O","   SmF3:0.5H2O"},
    ss[]="           --- Summary of Pure Mineral Saturation States ---";
for(i=0;i<num;i++) slens[i]=strlen(mnrlstrs[i]);
k=strlen(ss);
while((fgets(dummy,100,fin)!=NULL)&&(finished==0))
  {if(strncmp(dummy,ss,k)==0)finished=1;
  else
    for(i=0;i<num;i++)
          if(strncmp(dummy,mnrlstrs[i],slens[i])==0)
                 {founds[i]=1;
                 switch(i)
                   {case 0: amoh=getfloat(dummy,40,12);break;
                        case 1: cauo=getfloat(dummy,40,12);break;
                        case 2: agcl=getfloat(dummy,40,12);break;
                        case 3: dias=getfloat(dummy,40,12);break;
                        case 4: euoh=getfloat(dummy,40,12);break;
                        case 5: gdoh=getfloat(dummy,40,12);break;
                        case 6: goet=getfloat(dummy,40,12);break;
                        case 7: haiw=getfloat(dummy,40,12);break;
                        case 8: hema=getfloat(dummy,40,12);break;
                        case 9: ndoh=getfloat(dummy,40,12);break;
                        case 10: nisi=getfloat(dummy,40,12);break;
                        case 11: npo2=getfloat(dummy,40,12);break;  /* NpO2 */
                        case 12: puo2=getfloat(dummy,40,12);break;  /* PuO2 */
                        case 13: pyro=getfloat(dummy,40,12);break;
                        case 14: rh2o3=getfloat(dummy,40,12);break;
                        case 15: ruo2=getfloat(dummy,40,12);break;
                        case 16: smco3=getfloat(dummy,40,12);break;
                        case 17: sodd=getfloat(dummy,40,12);break;  /* Soddyite */
                        case 18: trev=getfloat(dummy,40,12);break;
                        case 19: uo3=getfloat(dummy,40,12);break;
                        case 20: smec=getfloat(dummy,40,12);break;
                        case 21: nonca=getfloat(dummy,40,12);break;
                        case 22: nonk=getfloat(dummy,40,12);break;
                        case 23: nonmg=getfloat(dummy,40,12);break;
                        case 24: nonna=getfloat(dummy,40,12);break;
                        case 25: rhabdo=getfloat(dummy,40,12);break;
                        case 26: ndpo4=getfloat(dummy,40,12);break;
                        case 27: gdpo4=getfloat(dummy,40,12);break;
                        case 28: smpo4=getfloat(dummy,40,12);break;
                        case 29: laf=getfloat(dummy,40,12);break;
                        case 30: ndf=getfloat(dummy,40,12);break;
                        case 31: gdf=getfloat(dummy,40,12);break;
                        case 32: smf=getfloat(dummy,40,12);}}}

for(i=0;i<num;i++)
  if(founds[i]==0)
   switch(i)
    {case 0: amoh=0;break;
        case 1: cauo=0;break;
         case 2: agcl=0;break;
        case 3: dias=0;break;
        case 4: euoh=0;break;
        case 5: gdoh=0;break;
        case 6: goet=0;break;
        case 7: haiw=0;break;
        case 8: hema=0;break;
```

```
        case 9: ndoh=0;break;
        case 10: nisi=0;break;
        case 11: npo2=0;break;
        case 12: puo2=0;break;
        case 13: pyro=0;break;
        case 14: rh2o3=0;break;
        case 15: ruo2=0;break;
        case 16: smco3=0;break;
        case 17: sodd=0;break;
        case 18: trev=0;break;
        case 19: uo3=0;break;
        case 20: smec=0;break;
        case 21: nonca=0;break;
        case 22: nonk=0;break;
        case 23: nonmg=0;break;
        case 24: nonna=0;break;
        case 25: rhabdo=0;break;
        case 26: ndpo4=0;break;
        case 27: gdpo4=0;break;
        case 28: smpo4=0;break;
        case 29: laf=0;break;
        case 30: ndf=0;break;
        case 31: gdf=0;break;
        case 32: smf=0;}}

void getelements()
{int i,k,num=5,founds[5]={0},finished=0,slens[10};
char elstrs[5][20]={"        B ","      Gd","       P ","      Pu",
    "       U "},ss[]={"   Single ion"};
for(i=0;i<num;i++) slens[i]=strlen(elstrs[i]);
k=strlen(ss);
while((fgets(dummy,100,fin)!=NULL)&&(finished==0))
  {if(strncmp(dummy,ss,k)==0)finished=1;
  else
    for(i=0;i<num;i++)
          if(strncmp(dummy,elstrs[i],slens[i])==0)
                {founds[i]=1;
                switch(i)
                  {case 0:b=getfloat(dummy,57,13);break;
                       case 1: gd=getfloat(dummy,57,13);break;
                       case 2: ps=getfloat(dummy,57,13);break;
                       case 3: pu=getfloat(dummy,57,13);break;
                       case 4: u=getfloat(dummy,57,13);break;}}}
for(i=0;i<num;i++)
  if(founds[i]==0)
   switch(i)
    {case 0:b=0;break;
        case 1: gd=0;break;
        case 2: ps=0;break;
        case 3: pu=0;break;
        case 4: u=0;break;}}


int getreacts(int k)
{int i;
char temps[30];
fgets(dummy,100,fin); /*skip blank line*/
i=0;
fgets(dummy,100,fin); /*now read first line of reactants*/
while(dummy[0]!='\n')
  {if(k==1)
    {strncpy(temps,dummy,25);
    temps[25]='\0';
    trimb(temps);
    strcpy(reactstrs[i],temps);}                    /* name of reactant */
  reactvals[i]=getfloat(dummy,29,11); /* moles of reactant */
  i++;
```

```
  fgets(dummy,100,fin);}
return(i);}

void trimb(char string[30])
{int i=0,j,k;
while(string[i]==' ')i++;
j=strlen(string)-1;
while(string[j]==' ')j--;
for(k=0;k<j-i+1;k++) string[k]=string[k+i];
if(j-i+1<9)string[j-i+1]='\0';
else string[9]='\0';} /*no reactant string name greater than 9chars*/



/*                     Time =
                          =  3.329E+06 days
  J-13 water                 3.9080E+03     .0000E+00    2.3471E+04     .0000E+00
      B          1.405415E-01        1.316626E-05         1.316629E-05
      Gd         1.531378E-03        9.863147E-09         9.863168E-09
      P          1.742931E-04        5.699148E-09         5.699160E-09
      Pu         5.260290E-07        2.183452E-12         2.183456E-12
      U          2.582874E-03        1.098999E-08         1.099001E-08
     modified NBS pH scale           6.6651
                      Ionic strength =  2.596699E-01 molal
                      Moles of solvent H2O =  5.55085E+01
                      Mass of solvent H2O  =  1.00000E+00 kg
 H+                          2.7749E-07     -6.5567       -.1083      -6.6651
 PuO2                         -5.5313   2.9425E-06   8.1213E-04   7.0120E-05
 Soddyite                     -1.5865   2.5912E-02   1.7314E+01   3.4015E+00
 Rhabdophane-ss               -2.1365   7.3031E-03   1.9141E+00    .0000E+00
   GdPO4:H2O                  -2.6521   2.2280E-03   6.0208E-01    .0000E+00
*/
```

lastpost.c

```
/* lastpost.c  processes a file named allpost, which is the result of
   concatenating the results of a sequence of runs of postproc.c representing
         consecutive timesteps which have been sliced into blocks so that the
         output files do not grow too large to handle.  The result of the concatenation
         is a sequence of six table groups, with the groups representing sequential
         timesteps.  This program merges the individual tables accros all the groups,
         resulting in a set of six tables, each covering the entire timespan.
         The present version is also set to print only every tenth line to reduce
         the size of the output file so that it can be easily graphed from a
         spreadsheet.*/

#include <stdio.h>
#include <string.h>
#include <stdlib.h>
#include <malloc.h>

FILE *fin, *fout;

struct OUTREC  /* for linked list of output records */
   {struct OUTREC *next;
   char data[400];};

void main()
{int i, j, count=0,finished=0;
struct OUTREC *pyrs[6],/*used for constructing one linked list for each table*/
    *pfyrs[6],/*used for the start of each linked list*/
               *p;/*used for traversing the linked list to write the output file*/
char outs[400], /*for output line*/
   recstrs[6][100]={"DATA FOR EACH TIMESTEP Elements",
   "DATA FOR EACH TIMESTEP Minerals","DATA FOR EACH TIMESTEP Reactants",
   "DATA FOR CHANGING TIMESTEPS Elements","DATA FOR CHANGING TIMESTEPS Minerals",
```

```
   "DATA FOR CHANGING TIMESTEPS Reactants"}, /*headings for input file tables*/
         dummy[400],/*for reading a line of input data*/
   headstrs[6][400];/*will be used for column headings for each output table.*/
fin=fopen("allpost","r");/*input data  file*/
fout=fopen("lastpost.out","w");/*output file*/
for(i=0;i<6;i++) /*allocate memory for start of each linked list*/
  {pfyrs[i]=malloc(sizeof(struct OUTREC));
   pyrs[i]=pfyrs[i];
   pyrs[i]->next=malloc(sizeof(struct OUTREC));}/*next rec for the first data*/
while((finished==0)&&(fgets(dummy,400,fin)!=NULL))/*outer loop to read all data*/
  for(i=0;i<6;i++)/*inner loop to read each group of six*/
/*starting with the first line read in the above while statement, read through
  lines until the first table heading is reached.  On subsequent passes, it
       will read through the blank lines before the next table*/
               {while((finished==0)&&(strncmp(dummy,recstrs[i],strlen(recstrs[i]))!=0))
       if(fgets(dummy,400,fin)==NULL)/*EOF if we run out of lines*/
         {finished=1;
         break;}
    fgets(dummy,400,fin);/*readthrough a blank line following the table heading*/
    fgets(dummy,400,fin);
    strcpy(headstrs[i],dummy);/*copy the column headings for use in the output*/
    fgets(dummy,400,fin);/*now get the first data line*/
               /*the following test includes whether the input line is blank, which would
               indicate the end of the input table.*/
    while((finished==0)&&(strncmp(dummy,"      ",6)!=0)&&(dummy[0]!='\n'))
      {pyrs[i]=pyrs[i]->next;
      strcpy(pyrs[i]->data,dummy);/*if not blank, copy it to the linked list*/
      pyrs[i]->next=malloc(sizeof(struct OUTREC));/*allocate for the next line*/
      if(i==0)count++;
      if(fgets(dummy,400,fin)==NULL)finished=1;}}/*get the line for the next*/
                                              /*iteration and test for EOF*/
for(i=0;i<6;i++)
  {free(pyrs[i]->next);/*free the last allocation which won't be needed*/
  pyrs[i]->next=NULL;}/*now tag the last link*/
for(i=0;i<6;i++)
  {count=0;
  fprintf(fout,"\n\n%s\n\n",recstrs[i]);/*print table heading*/
  fprintf(fout,"%s\n",headstrs[i]);/*print column headings*/
  p=pfyrs[i];/*point to start of linked list*/
  while((p=p->next)!=NULL) /*skip the first record which has no data*/
    {if (count%10==0) fprintf(fout,"%s",p->data);/*print every tenth line*/
    count++;}}}
```

Attachment II. Review of the C Programs in Accordance with QAP-SI-0, REV 3

Check of Flushing Routine for case Uall5mmr Stage 1 to 2

End of Stage 1, mole solvent = 55.7212 = y
mass solvent = 1.00383

Al moles aqueous= 4.053240E-07
B moles aqueous = 7.355274E-02
Ca moles aqueous = 1.376098E-08

Delta moles J-13 water (added)/3 = 1.144 = z
Initial moles solvent = 55.5088 = x

x/(x+z) = 0.979812

Start of Stage 2, mass solvent = 0.983643,
therefore, reduction factor should be x/(x+z)

Element	Hand calc. of new moles aqueous	Flushing routine calc.
Al	3.971413E-07	3.9717878E-07
B	7.206786E-02	7.207341E-02
Ca	1.348317E-08	1.348421E-08

Attachment III Pro-Engineer Output

```
                    MASS PROPERTIES OF THE PART OUTER_BARRIER

                         VOLUME =  2.5323951e+09 MM^3
                   SURFACE AREA =  5.3536901e+07 MM^2
                        DENSITY =  7.8500000e-06 KILOGRAM / MM^3
                           MASS =  1.9879301e+04 KILOGRAM

      CENTER OF GRAVITY with respect to _OUTER_BARRIER coordinate frame:
X   Y   Z             0.0000000e+00  0.0000000e+00  2.6675000e+03  MM

   INERTIA with respect to _OUTER_BARRIER coordinate frame:  (KILOGRAM * MM^2)

INERTIA TENSOR:
Ixx Ixy Ixz           1.9185547e+11  4.1852897e+06  0.0000000e+00
Iyx Iyy Iyz           4.1852897e+06  1.9185769e+11  0.0000000e+00
Izx Izy Izz           0.0000000e+00  0.0000000e+00  1.2229752e+10

  INERTIA at CENTER OF GRAVITY with respect to _OUTER_BARRIER coordinate frame:
                                                            (KILOGRAM * MM^2)
INERTIA TENSOR:
Ixx Ixy Ixz           5.0403180e+10  4.1852897e+06  0.0000000e+00
Iyx Iyy Iyz           4.1852897e+06  5.0405399e+10  0.0000000e+00
Izx Izy Izz           0.0000000e+00  0.0000000e+00  1.2229752e+10

                 PRINCIPAL MOMENTS OF INERTIA:  (KILOGRAM * MM^2)
I1  I2  I3            1.2229752e+10  5.0399959e+10  5.0408619e+10

      ROTATION MATRIX from _OUTER_BARRIER orientation to PRINCIPAL AXES:
                        0.00000        0.79254        0.60982
                        0.00000       -0.60982        0.79254
                        1.00000        0.00000        0.00000

  ROTATION ANGLES from _OUTER_BARRIER orientation to PRINCIPAL AXES (degrees):
angles about x  y  z  -90.000         37.576         -90.000

                 RADII OF GYRATION with respect to PRINCIPAL AXES:
R1  R2  R3            7.8434706e+02  1.5922620e+03  1.5923988e+03  MM
```

```
                    MASS PROPERTIES OF THE PART OUTER_BARRIER_LID

                          VOLUME =  1.8577509e+08 MM^3
                    SURFACE AREA =  3.8844803e+06 MM^2
                         DENSITY =  7.8500000e-06 KILOGRAM / MM^3
                            MASS =  1.4583344e+03 KILOGRAM

      CENTER OF GRAVITY with respect to _OUTER_BARRIER_LI coordinate frame:
X   Y   Z             0.0000000e+00  0.0000000e+00  5.5000000e+01  MM

 INERTIA with respect to _OUTER_BARRIER_LI coordinate frame:  (KILOGRAM * MM^2)

INERTIA TENSOR:
Ixx Ixy Ixz          2.0187822e+08 -7.9991014e+03  0.0000000e+00
Iyx Iyy Iyz         -7.9991014e+03  2.0187302e+08  0.0000000e+00
Izx Izy Izz          0.0000000e+00  0.0000000e+00  3.9198734e+08

INERTIA at CENTER OF GRAVITY with respect to _OUTER_BARRIER_LI coordinate frame:
                                                              (KILOGRAM * MM^2)
INERTIA TENSOR:
Ixx Ixy Ixz          1.9746676e+08 -7.9991014e+03  0.0000000e+00
Iyx Iyy Iyz         -7.9991014e+03  1.9746156e+08  0.0000000e+00
Izx Izy Izz          0.0000000e+00  0.0000000e+00  3.9198734e+08

                PRINCIPAL MOMENTS OF INERTIA:  (KILOGRAM * MM^2)
I1  I2  I3           1.9745575e+08  1.9747257e+08  3.9198734e+08

      ROTATION MATRIX from _OUTER_BARRIER_LI orientation to PRINCIPAL AXES:
                        0.58778       -0.80902        0.00000
                        0.80902        0.58778        0.00000
                        0.00000        0.00000        1.00000

 ROTATION ANGLES from _OUTER_BARRIER_LI orientation to PRINCIPAL AXES (degrees):
angles about x  y  z     0.000           0.000          54.000

                RADII OF GYRATION with respect to PRINCIPAL AXES:
R1  R2  R3           3.6796484e+02  3.6798052e+02  5.1845069e+02  MM
```

```
                         MASS PROPERTIES OF THE PART INNER_BARRIER

                              VOLUME =  4.2001935e+08 MM^3
                        SURFACE AREA =  4.2217363e+07 MM^2
                             DENSITY =  8.6910000e-06 KILOGRAM / MM^3
                                MASS =  3.6503882e+03 KILOGRAM

           CENTER OF GRAVITY with respect to _INNER_BARRIER coordinate frame:
X   Y   Z              0.0000000e+00  0.0000000e+00  2.3175000e+03  MM

     INERTIA with respect to _INNER_BARRIER coordinate frame:  (KILOGRAM * MM^2)

INERTIA TENSOR:
Ixx Ixy Ixz            2.7081108e+10  5.8084992e+05  0.0000000e+00
Iyx Iyy Iyz            5.8084992e+05  2.7081453e+10  0.0000000e+00
Izx Izy Izz            0.0000000e+00  0.0000000e+00  1.9017120e+09

    INERTIA at CENTER OF GRAVITY with respect to _INNER_BARRIER coordinate frame:
                                                                (KILOGRAM * MM^2)
INERTIA TENSOR:
Ixx Ixy Ixz            7.4755801e+09  5.8084992e+05  0.0000000e+00
Iyx Iyy Iyz            5.8084992e+05  7.4759255e+09  0.0000000e+00
Izx Izy Izz            0.0000000e+00  0.0000000e+00  1.9017120e+09

                    PRINCIPAL MOMENTS OF INERTIA:  (KILOGRAM * MM^2)
I1  I2  I3             1.9017120e+09  7.4751468e+09  7.4763588e+09

          ROTATION MATRIX from _INNER_BARRIER orientation to PRINCIPAL AXES:
                          0.00000         0.80155         0.59792
                          0.00000        -0.59792         0.80155
                          1.00000         0.00000         0.00000

   ROTATION ANGLES from _INNER_BARRIER orientation to PRINCIPAL AXES (degrees):
angles about x  y  z  -90.000           36.721          -90.000

                    RADII OF GYRATION with respect to PRINCIPAL AXES:
R1  R2  R3            7.2177668e+02  1.4310023e+03  1.4311183e+03  MM
```

```
                    MASS PROPERTIES OF THE PART INNER_BARRIER_LID

                          VOLUME =  3.9949611e+07 MM^3
                    SURFACE AREA =  3.3079980e+06 MM^2
                         DENSITY =  8.6910000e-06 KILOGRAM / MM^3
                            MASS =  3.4720207e+02 KILOGRAM

        CENTER OF GRAVITY with respect to _INNER_BARRIER_LI coordinate frame:
X   Y   Z              0.0000000e+00  0.0000000e+00  1.2500000e+01  MM

  INERTIA with respect to _INNER_BARRIER_LI coordinate frame:  (KILOGRAM * MM^2)

INERTIA TENSOR:
Ixx Ixy Ixz          4.4223831e+07 -1.4361281e+02  0.0000000e+00
Iyx Iyy Iyz         -1.4361281e+02  4.4223738e+07  0.0000000e+00
Izx Izy Izz          0.0000000e+00  0.0000000e+00  8.8302901e+07

INERTIA at CENTER OF GRAVITY with respect to _INNER_BARRIER_LI coordinate frame:
                                                             (KILOGRAM * MM^2)
INERTIA TENSOR:
Ixx Ixy Ixz          4.4169581e+07 -1.4361281e+02  0.0000000e+00
Iyx Iyy Iyz         -1.4361281e+02  4.4169487e+07  0.0000000e+00
Izx Izy Izz          0.0000000e+00  0.0000000e+00  8.8302901e+07

                PRINCIPAL MOMENTS OF INERTIA:  (KILOGRAM * MM^2)
I1  I2  I3           4.4169383e+07  4.4169685e+07  8.8302901e+07

       ROTATION MATRIX from _INNER_BARRIER_LI orientation to PRINCIPAL AXES:
                         1.00000         0.00000         0.00000
                         0.00000         1.00000         0.00000
                         0.00000         0.00000         1.00000

 ROTATION ANGLES from _INNER_BARRIER_LI orientation to PRINCIPAL AXES (degrees):
angles about x  y  z    0.000           0.000           0.000

                RADII OF GYRATION with respect to PRINCIPAL AXES:
R1  R2  R3           3.5667241e+02  3.5667363e+02  5.0430856e+02  MM
```

```
                       MASS PROPERTIES OF THE PART A_GUIDE

                         VOLUME =  8.1003148e+06 MM^3
                   SURFACE AREA =  1.6793636e+06 MM^2
                        DENSITY =  7.8500000e-06 KILOGRAM / MM^3
                           MASS =  6.3587471e+01 KILOGRAM

          CENTER OF GRAVITY with respect to _A_GUIDE coordinate frame:
X   Y   Z           3.6660000e+02  4.9600063e+00  5.6565000e+02  MM

      INERTIA with respect to _A_GUIDE coordinate frame:  (KILOGRAM * MM^2)

INERTIA TENSOR:
Ixx Ixy Ixz          2.7129351e+07 -1.1562354e+05 -1.3185962e+07
Iyx Iyy Iyz         -1.1562354e+05  3.8391375e+07 -1.7840276e+05
Izx Izy Izz         -1.3185962e+07 -1.7840276e+05  1.1266213e+07

     INERTIA at CENTER OF GRAVITY with respect to _A_GUIDE coordinate frame:
                                                         (KILOGRAM * MM^2)
INERTIA TENSOR:
Ixx Ixy Ixz          6.7823439e+06  0.0000000e+00  0.0000000e+00
Iyx Iyy Iyz          0.0000000e+00  9.5000587e+06  0.0000000e+00
Izx Izy Izz          0.0000000e+00  0.0000000e+00  2.7187744e+06

               PRINCIPAL MOMENTS OF INERTIA:  (KILOGRAM * MM^2)
I1  I2  I3           2.7187744e+06  6.7823439e+06  9.5000587e+06

         ROTATION MATRIX from _A_GUIDE orientation to PRINCIPAL AXES:
                      0.00000        1.00000        0.00000
                      0.00000        0.00000        1.00000
                      1.00000        0.00000        0.00000

     ROTATION ANGLES from _A_GUIDE orientation to PRINCIPAL AXES (degrees):
angles about x  y  z  -90.000          0.000          -90.000

               RADII OF GYRATION with respect to PRINCIPAL AXES:
R1  R2  R3          2.0677632e+02  3.2659094e+02  3.8652480e+02  MM
```

```
                       MASS PROPERTIES OF THE PART B_GUIDE

                          VOLUME =  9.2015813e+05 MM^3
                    SURFACE AREA =  2.0845188e+05 MM^2
                         DENSITY =  7.8500000e-06 KILOGRAM / MM^3
                            MASS =  7.2232413e+00 KILOGRAM

          CENTER OF GRAVITY with respect to _B_GUIDE coordinate frame:
X   Y   Z          -5.0176971e+00 -4.0669703e+01  5.6565000e+02  MM

      INERTIA with respect to _B_GUIDE coordinate frame:  (KILOGRAM * MM^2)

INERTIA TENSOR:
Ixx Ixy Ixz         3.0974608e+06 -1.4792327e+03  2.0501439e+04
Iyx Iyy Iyz        -1.4792327e+03  3.0817724e+06  1.6616935e+05
Izx Izy Izz         2.0501439e+04  1.6616935e+05  1.6172545e+04

     INERTIA at CENTER OF GRAVITY with respect to _B_GUIDE coordinate frame:
                                                           (KILOGRAM * MM^2)
INERTIA TENSOR:
Ixx Ixy Ixz         7.7436565e+05 -5.1984314e+00  0.0000000e+00
Iyx Iyy Iyz        -5.1984314e+00  7.7044277e+05  0.0000000e+00
Izx Izy Izz         0.0000000e+00  0.0000000e+00  4.0432634e+03

                PRINCIPAL MOMENTS OF INERTIA:  (KILOGRAM * MM^2)
I1  I2  I3          4.0432634e+03  7.7044276e+05  7.7436565e+05

          ROTATION MATRIX from _B_GUIDE orientation to PRINCIPAL AXES:
                       0.00000        0.00133       -1.00000
                       0.00000        1.00000        0.00133
                       1.00000        0.00000        0.00000

     ROTATION ANGLES from _B_GUIDE orientation to PRINCIPAL AXES (degrees):
angles about x  y  z  -90.000        -89.924        -90.000

               RADII OF GYRATION with respect to PRINCIPAL AXES:
R1  R2  R3          2.3659195e+01  3.2659094e+02  3.2742134e+02  MM
```

```
                         MASS PROPERTIES OF THE PART CORNER_GUIDE

                              VOLUME =  5.3367510e+06 MM^3
                        SURFACE AREA =  1.1033308e+06 MM^2
                             DENSITY =  7.8500000e-06 KILOGRAM / MM^3
                                MASS =  4.1893495e+01 KILOGRAM

          CENTER OF GRAVITY with respect to _CORNER_GUIDE coordinate frame:
X    Y    Z             6.3802932e+01  6.3802932e+01  5.6690000e+02  MM

     INERTIA with respect to _CORNER_GUIDE coordinate frame:  (KILOGRAM * MM^2)

INERTIA TENSOR:
Ixx Ixy Ixz             1.8364056e+07 -2.5468842e+04 -1.5152828e+06
Iyx Iyy Iyz            -2.5468842e+04  1.8364056e+07 -1.5152828e+06
Izx Izy Izz            -1.5152828e+06 -1.5152828e+06  8.2531813e+05

   INERTIA at CENTER OF GRAVITY with respect to _CORNER_GUIDE coordinate frame:
                                                                (KILOGRAM * MM^2)
INERTIA TENSOR:
Ixx Ixy Ixz             4.7299676e+06  1.4507179e+05  0.0000000e+00
Iyx Iyy Iyz             1.4507179e+05  4.7299676e+06  0.0000000e+00
Izx Izy Izz             0.0000000e+00  0.0000000e+00  4.8423687e+05

                    PRINCIPAL MOMENTS OF INERTIA:  (KILOGRAM * MM^2)
I1   I2   I3            4.8423687e+05  4.5848958e+06  4.8750394e+06

        ROTATION MATRIX from _CORNER_GUIDE orientation to PRINCIPAL AXES:
                              0.00000         0.70711         0.70711
                              0.00000        -0.70711         0.70711
                              1.00000         0.00000         0.00000

   ROTATION ANGLES from _CORNER_GUIDE orientation to PRINCIPAL AXES (degrees):
angles about x  y  z  -90.000           45.000          -90.000

                    RADII OF GYRATION with respect to PRINCIPAL AXES:
R1   R2   R3            1.0751168e+02  3.3081976e+02  3.4112674e+02  MM
```

```
                  MASS PROPERTIES OF THE PART CORNER_STIFFENER

                         VOLUME =  2.9468916e+05 MM^3
                   SURFACE AREA =  6.7354628e+04 MM^2
                        DENSITY =  7.8500000e-06 KILOGRAM / MM^3
                           MASS =  2.3133099e+00 KILOGRAM

      CENTER OF GRAVITY with respect to _CORNER_STIFFENER coordinate frame:
X   Y   Z           5.7762779e+00  5.7762321e+00  5.0000000e+00  MM

 INERTIA with respect to _CORNER_STIFFENER coordinate frame:  (KILOGRAM * MM^2)

INERTIA TENSOR:
Ixx Ixy Ixz         7.2799223e+03  3.1343997e+03 -6.6811605e+01
Iyx Iyy Iyz         3.1343997e+03  7.2799238e+03 -6.6811075e+01
Izx Izy Izz        -6.6811605e+01 -6.6811075e+01  1.4405625e+04

INERTIA at CENTER OF GRAVITY with respect to _CORNER_STIFFENER coordinate frame:
                                                               (KILOGRAM * MM^2)
INERTIA TENSOR:
Ixx Ixy Ixz         7.1449063e+03  3.2115836e+03  0.0000000e+00
Iyx Iyy Iyz         3.2115835e+03  7.1449066e+03  0.0000000e+00
Izx Izy Izz         0.0000000e+00  0.0000000e+00  1.4251258e+04

               PRINCIPAL MOMENTS OF INERTIA:  (KILOGRAM * MM^2)
I1  I2  I3          3.9333229e+03  1.0356490e+04  1.4251258e+04

      ROTATION MATRIX from _CORNER_STIFFENER orientation to PRINCIPAL AXES:
                      0.70711        0.70711        0.00000
                     -0.70711        0.70711        0.00000
                      0.00000        0.00000        1.00000

 ROTATION ANGLES from _CORNER_STIFFENER orientation to PRINCIPAL AXES (degrees):
angles about x  y  z   0.000          0.000          -45.000

               RADII OF GYRATION with respect to PRINCIPAL AXES:
R1  R2  R3          4.1234704e+01  6.6909747e+01  7.8489161e+01  MM
```

```
                        MASS PROPERTIES OF THE PART A-PLATE

                         VOLUME =  9.4683638e+06 MM^3
                   SURFACE AREA =  2.7698904e+06 MM^2
                        DENSITY =  7.7600000e-06 KILOGRAM / MM^3
                           MASS =  7.3474503e+01 KILOGRAM

           CENTER OF GRAVITY with respect to _A-PLATE coordinate frame:
X   Y   Z             6.0800000e+02  5.7236467e+02  3.5000000e+00  MM

       INERTIA with respect to _A-PLATE coordinate frame:  (KILOGRAM * MM^2)

INERTIA TENSOR:
Ixx Ixy Ixz           3.1940321e+07 -2.5568959e+07 -1.5635374e+05
Iyx Iyy Iyz          -2.5568959e+07  3.6301009e+07 -1.4718973e+05
Izx Izy Izz          -1.5635374e+05 -1.4718973e+05  6.8238930e+07

      INERTIA at CENTER OF GRAVITY with respect to _A-PLATE coordinate frame:
                                                             (KILOGRAM * MM^2)
INERTIA TENSOR:
Ixx Ixy Ixz           7.8690770e+06  0.0000000e+00  0.0000000e+00
Iyx Iyy Iyz           0.0000000e+00  9.1392304e+06  0.0000000e+00
Izx Izy Izz           0.0000000e+00  0.0000000e+00  1.7007707e+07

                PRINCIPAL MOMENTS OF INERTIA:  (KILOGRAM * MM^2)
I1  I2  I3            7.8690770e+06  9.1392304e+06  1.7007707e+07

          ROTATION MATRIX from _A-PLATE orientation to PRINCIPAL AXES:
                        1.00000        0.00000        0.00000
                        0.00000        1.00000        0.00000
                        0.00000        0.00000        1.00000

     ROTATION ANGLES from _A-PLATE orientation to PRINCIPAL AXES (degrees):
angles about x  y  z     0.000          0.000          0.000

                RADII OF GYRATION with respect to PRINCIPAL AXES:
R1  R2  R3            3.2726048e+02  3.5268459e+02  4.8112127e+02  MM
```

```
                         MASS PROPERTIES OF THE PART B-PLATE

                          VOLUME =  9.4683638e+06 MM^3
                    SURFACE AREA =  2.7698904e+06 MM^2
                         DENSITY =  7.7600000e-06 KILOGRAM / MM^3
                            MASS =  7.3474503e+01 KILOGRAM

           CENTER OF GRAVITY with respect to _B-PLATE coordinate frame:
X   Y   Z             6.0800000e+02 -3.5000000e+00  5.6808797e+02  MM

       INERTIA with respect to _B-PLATE coordinate frame:  (KILOGRAM * MM^2)

INERTIA TENSOR:
Ixx Ixy Ixz           3.1584049e+07  1.5635374e+05 -2.5377909e+07
Iyx Iyy Iyz           1.5635374e+05  6.7882658e+07  1.4608993e+05
Izx Izy Izz          -2.5377909e+07  1.4608993e+05  3.6301009e+07

     INERTIA at CENTER OF GRAVITY with respect to _B-PLATE coordinate frame:
                                                          (KILOGRAM * MM^2)
INERTIA TENSOR:
Ixx Ixy Ixz           7.8711674e+06  0.0000000e+00  0.0000000e+00
Iyx Iyy Iyz           0.0000000e+00  1.7009798e+07  0.0000000e+00
Izx Izy Izz           0.0000000e+00  0.0000000e+00  9.1392304e+06

                PRINCIPAL MOMENTS OF INERTIA:  (KILOGRAM * MM^2)
I1  I2  I3            7.8711674e+06  9.1392304e+06  1.7009798e+07

          ROTATION MATRIX from _B-PLATE orientation to PRINCIPAL AXES:
                        1.00000        0.00000        0.00000
                        0.00000        0.00000       -1.00000
                        0.00000        1.00000        0.00000

     ROTATION ANGLES from _B-PLATE orientation to PRINCIPAL AXES (degrees):
angles about x  y  z   90.000          0.000          0.000

                RADII OF GYRATION with respect to PRINCIPAL AXES:
R1  R2  R3            3.2730395e+02  3.5268459e+02  4.8115084e+02  MM
```

```
                    MASS PROPERTIES OF THE PART C-PLATE

                     VOLUME =  5.6873676e+06 MM^3
               SURFACE AREA =  1.6669370e+06 MM^2
                    DENSITY =  7.7600000e-06 KILOGRAM / MM^3
                       MASS =  4.4133972e+01 KILOGRAM

         CENTER OF GRAVITY with respect to _C-PLATE coordinate frame:
X   Y   Z             3.6530000e+02 -3.5000000e+00  5.6136232e+02  MM

      INERTIA with respect to _C-PLATE coordinate frame:  (KILOGRAM * MM^2)

INERTIA TENSOR:
Ixx Ixy Ixz           1.8635063e+07  5.6427490e+04 -9.0503620e+06
Iyx Iyy Iyz           5.6427490e+04  2.6511938e+07  8.6713022e+04
Izx Izy Izz          -9.0503620e+06  8.6713022e+04  7.8783166e+06

     INERTIA at CENTER OF GRAVITY with respect to _C-PLATE coordinate frame:
                                                       (KILOGRAM * MM^2)
INERTIA TENSOR:
Ixx Ixy Ixz           4.7266876e+06  0.0000000e+00  0.0000000e+00
Iyx Iyy Iyz           0.0000000e+00  6.7146853e+06  0.0000000e+00
Izx Izy Izz           0.0000000e+00  0.0000000e+00  1.9883582e+06

              PRINCIPAL MOMENTS OF INERTIA:  (KILOGRAM * MM^2)
I1  I2  I3            1.9883582e+06  4.7266876e+06  6.7146853e+06

         ROTATION MATRIX from _C-PLATE orientation to PRINCIPAL AXES:
                         0.00000        1.00000        0.00000
                         0.00000        0.00000        1.00000
                         1.00000        0.00000        0.00000

     ROTATION ANGLES from _C-PLATE orientation to PRINCIPAL AXES (degrees):
angles about x  y  z  -90.000          0.000          -90.000

              RADII OF GYRATION with respect to PRINCIPAL AXES:
R1  R2  R3            2.1225640e+02  3.2725926e+02  3.9005543e+02  MM
```

```
                    MASS PROPERTIES OF THE PART D-PLATE

                       VOLUME =  6.7403340e+06 MM^3
                 SURFACE AREA =  2.7422246e+06 MM^2
                      DENSITY =  2.7130000e-06 KILOGRAM / MM^3
                         MASS =  1.8286526e+01 KILOGRAM

          CENTER OF GRAVITY with respect to _D-PLATE coordinate frame:
X   Y   Z          6.0720000e+02  5.7121092e+02  2.5000000e+00  MM

      INERTIA with respect to _D-PLATE coordinate frame:  (KILOGRAM * MM^2)

INERTIA TENSOR:
Ixx Ixy Ixz         7.9171812e+06 -6.3424854e+06 -2.7758947e+04
Iyx Iyy Iyz        -6.3424854e+06  9.0107564e+06 -2.6113658e+04
Izx Izy Izz        -2.7758947e+04 -2.6113658e+04  1.6927633e+07

     INERTIA at CENTER OF GRAVITY with respect to _D-PLATE coordinate frame:
                                                          (KILOGRAM * MM^2)
INERTIA TENSOR:
Ixx Ixy Ixz         1.9505042e+06  0.0000000e+00  0.0000000e+00
Iyx Iyy Iyz         0.0000000e+00  2.2685491e+06  0.0000000e+00
Izx Izy Izz         0.0000000e+00  0.0000000e+00  4.2189772e+06

               PRINCIPAL MOMENTS OF INERTIA:  (KILOGRAM * MM^2)
I1  I2  I3          1.9505042e+06  2.2685491e+06  4.2189772e+06

          ROTATION MATRIX from _D-PLATE orientation to PRINCIPAL AXES:
                           1.00000       0.00000       0.00000
                           0.00000       1.00000       0.00000
                           0.00000       0.00000       1.00000

     ROTATION ANGLES from _D-PLATE orientation to PRINCIPAL AXES (degrees):
angles about x  y  z    0.000          0.000          0.000

               RADII OF GYRATION with respect to PRINCIPAL AXES:
R1  R2  R3          3.2659373e+02  3.5221552e+02  4.8032809e+02  MM
```

```
                         MASS PROPERTIES OF THE PART E-PLATE

                          VOLUME =  6.7403340e+06 MM^3
                    SURFACE AREA =  2.7422246e+06 MM^2
                         DENSITY =  2.7130000e-06 KILOGRAM / MM^3
                            MASS =  1.8286526e+01 KILOGRAM

            CENTER OF GRAVITY with respect to _E-PLATE coordinate frame:
X   Y   Z             6.0720000e+02 -2.5000000e+00  5.6693716e+02  MM

         INERTIA with respect to _E-PLATE coordinate frame:  (KILOGRAM * MM^2)

INERTIA TENSOR:
Ixx Ixy Ixz          7.8287520e+06  2.7758947e+04 -6.2950313e+06
Iyx Iyy Iyz          2.7758947e+04  1.6839204e+07  2.5918278e+04
Izx Izy Izz         -6.2950313e+06  2.5918278e+04  9.0107564e+06

        INERTIA at CENTER OF GRAVITY with respect to _E-PLATE coordinate frame:
                                                             (KILOGRAM * MM^2)
INERTIA TENSOR:
Ixx Ixy Ixz          1.9510238e+06  0.0000000e+00  0.0000000e+00
Iyx Iyy Iyz          0.0000000e+00  4.2194967e+06  0.0000000e+00
Izx Izy Izz          0.0000000e+00  0.0000000e+00  2.2685491e+06

                  PRINCIPAL MOMENTS OF INERTIA:  (KILOGRAM * MM^2)
I1  I2  I3           1.9510238e+06  2.2685491e+06  4.2194967e+06

            ROTATION MATRIX from _E-PLATE orientation to PRINCIPAL AXES:
                          1.00000        0.00000        0.00000
                          0.00000        0.00000       -1.00000
                          0.00000        1.00000        0.00000

         ROTATION ANGLES from _E-PLATE orientation to PRINCIPAL AXES (degrees):
angles about x  y  z   90.000          0.000          0.000

                  RADII OF GYRATION with respect to PRINCIPAL AXES:
R1  R2  R3          3.2663723e+02  3.5221552e+02  4.8035766e+02  MM
```

```
                    MASS PROPERTIES OF THE PART SIDE_COVER

                          VOLUME =  5.0144801e+05 MM^3
                    SURFACE AREA =  1.1595236e+05 MM^2
                         DENSITY =  7.8500000e-06 KILOGRAM / MM^3
                            MASS =  3.9363668e+00 KILOGRAM

           CENTER OF GRAVITY with respect to _SIDE_COVER coordinate frame:
X   Y   Z            3.6660000e+02  4.0888533e+01  5.0000000e+00  MM

     INERTIA with respect to _SIDE_COVER coordinate frame:  (KILOGRAM * MM^2)

INERTIA TENSOR:
Ixx Ixy Ixz          9.5276543e+03 -5.9005088e+04 -7.2153605e+03
Iyx Iyy Iyz         -5.9005088e+04  6.3752055e+05 -8.0476132e+02
Izx Izy Izz         -7.2153605e+03 -8.0476132e+02  6.4678578e+05

   INERTIA at CENTER OF GRAVITY with respect to _SIDE_COVER coordinate frame:
                                                               (KILOGRAM * MM^2)
INERTIA TENSOR:
Ixx Ixy Ixz          2.8481431e+03  1.3046996e-02  0.0000000e+00
Iyx Iyy Iyz          1.3046996e-02  1.0839191e+05  0.0000000e+00
Izx Izy Izz          0.0000000e+00  0.0000000e+00  1.1117445e+05

                PRINCIPAL MOMENTS OF INERTIA:  (KILOGRAM * MM^2)
I1   I2   I3         2.8481431e+03  1.0839191e+05  1.1117445e+05

          ROTATION MATRIX from _SIDE_COVER orientation to PRINCIPAL AXES:
                        1.00000        0.00000        0.00000
                        0.00000        1.00000        0.00000
                        0.00000        0.00000        1.00000

    ROTATION ANGLES from _SIDE_COVER orientation to PRINCIPAL AXES (degrees):
angles about x  y  z    0.000          0.000          0.000

                RADII OF GYRATION with respect to PRINCIPAL AXES:
R1   R2   R3         2.6898814e+01  1.6593983e+02  1.6805626e+02  MM
```

```
                         MASS PROPERTIES OF THE PART TUBE

                           VOLUME =  2.0879658e+07 MM^3
                     SURFACE AREA =  8.3616621e+06 MM^2
                          DENSITY =  7.8500000e-06 KILOGRAM / MM^3
                             MASS =  1.6390531e+02 KILOGRAM

             CENTER OF GRAVITY with respect to _TUBE coordinate frame:
X   Y   Z             1.1320000e+02 -1.1320001e+02  2.2876201e+03  MM

       INERTIA with respect to _TUBE coordinate frame:  (KILOGRAM * MM^2)

INERTIA TENSOR:
Ixx Ixy Ixz           1.1472196e+09  2.1003221e+06 -4.2444686e+07
Iyx Iyy Iyz           2.1003221e+06  1.1472196e+09  4.2444692e+07
Izx Izy Izz          -4.2444686e+07  4.2444692e+07  7.1055817e+06

     INERTIA at CENTER OF GRAVITY with respect to _TUBE coordinate frame:
                                                          (KILOGRAM * MM^2)
INERTIA TENSOR:
Ixx Ixy Ixz           2.8736905e+08  0.0000000e+00  0.0000000e+00
Iyx Iyy Iyz           0.0000000e+00  2.8736905e+08  0.0000000e+00
Izx Izy Izz           0.0000000e+00  0.0000000e+00  2.9049375e+06

                  PRINCIPAL MOMENTS OF INERTIA:  (KILOGRAM * MM^2)
I1   I2   I3          2.9049375e+06  2.8736905e+08  2.8736905e+08

            ROTATION MATRIX from _TUBE orientation to PRINCIPAL AXES:
                        0.00000         1.00000         0.00000
                        0.00000         0.00000         1.00000
                        1.00000         0.00000         0.00000

      ROTATION ANGLES from _TUBE orientation to PRINCIPAL AXES (degrees):
angles about x  y  z  -90.000           0.000          -90.000

                  RADII OF GYRATION with respect to PRINCIPAL AXES:
R1   R2   R3         1.3312876e+02  1.3241082e+03  1.3241082e+03  MM
```