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7. Checker	Doug Walker	Douglas A Walker	11/16/99
8. Lead	Peter Gottlieb	Peter Gottlieb	12/6/99
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1. PURPOSE

The Monitored Geologic Repository Waste Package Operations of the Civilian Radioactive Waste Management System Management & Operating Contractor (CRWMS M&O) performed calculations to provide input for disposal of spent nuclear fuel (SNF) from the Navy (Refs. 1 and 2). The Navy SNF has been considered for disposal at the potential Yucca Mountain site. For some waste packages, the containment may breach (Ref. 3), allowing the influx of water. Water in the waste package may moderate neutrons, increasing the likelihood of a criticality event within the waste package. The water may gradually leach the fissile components and neutron absorbers out of the waste package. In addition, the accumulation of silica (SiO_2) in the waste package over time may further affect the neutronics of the system.

This study presents calculations of the long-term geochemical behavior of waste packages containing the Enhanced Design Alternative (EDA) II inner shell, Navy canister, and basket components. The calculations do not include the Navy SNF in the waste package. The specific study objectives were to determine the chemical composition of the water and the quantity of silicon (Si) and other solid corrosion products in the waste package during the first million years after the waste package is breached.

The results of this calculation will be used to ensure that the type and amount of criticality control material used in the waste package design will prevent criticality.

This calculation was prepared under procedure AP-3.12Q, Revision 0, ICN 0.

2. METHOD

The method used for this calculation involves the following steps:

- Use EQ3 to determine a starting fluid composition for EQ6 calculations.
- Use EQ6 to trace the progress of reactions as the chemistry of the waste package evolves.
- Evaluate available data on the range of dissolution rates for the materials involved.
- Use the "solid-centered flow-through" mode (SCFT) in EQ6 (Section 4.2).
- Use EQ6 to determine the concentrations in solution as a function of time.
- Use EQ6 to determine the composition and amounts of solids (precipitated minerals or corrosion products, and unreacted waste package materials).

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

3. ASSUMPTIONS

All assumptions are for preliminary design. All assumptions are used throughout Section 5.

3.1 All of the voids in the waste package will be completely filled with an aqueous solution. The basis for this assumption is that it provides the maximum degradation rate with the potential for the fastest flushing of the neutron absorber (when present) out of the waste package and is thereby conservative.

3.2 The aqueous solution that enters the waste package will have the composition of J-13 well water (as given in Ref. 4) for $\sim 1 \times 10^6$ years. The basis for this assumption is that the groundwater composition is controlled largely by transport through the host rock, over pathways of hundreds of meters. The host rock is several million years old, therefore its composition is not expected to change substantially over one million years. 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 water is not expected to breach the waste package until after that perturbed period. Therefore, the early perturbation is not relevant to the calculations reported in this document.

3.3 The density of the incoming water is 1.0 g/cm^3. The basis for this assumption is that for dilute solutions, the density is very close to that for pure water, and any differences are insignificant in respect to other uncertainties in the data and calculations. Moreover, the density is only used initially in EQ3/6 to convert concentrations of dissolved substances from parts per million to moles per kilogram.

3.4 The composition of the aqueous solution that will enter the waste package will not be altered by contact with the drift liner, except for the first few thousand years. The basis for this assumption is that the drift liner at the top of the drift is expected to collapse with the roof support well before 1,000 years. In addition, the water flowing through the 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.

3.5 The corrosion-resistant outer shell of the waste package will react slowly with the infiltrating water (and water already in the waste package) as to have negligible effect on the chemistry. The basis for this assumption is that the outer shell is fabricated from Alloy 22 (see nomenclature in Section 5.1.1), which corrodes very slowly compared to (1) other reactants in the waste package and (2) the rate at which soluble corrosion products will likely be flushed out of the waste package.

3.6 The calculations can satisfactorily be performed with the thermodynamic database containing data for a temperature of 25 °C. The basis for this assumption is that even though the initial breach may occur when the waste package contents are at temperatures

≥ 50 °C (Ref. 11), at times > 25,000 years, the waste package temperatures are likely to be closer to 25 °C.

3.7 The chromium and molybdenum (Cr and Mo) will oxidize fully to chromate (or dichromate) and molybdate, respectively. The basis for this assumption is that the available thermodynamic data indicate that in the presence of air the chromium and molybdenum will both oxidize to the VI 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. In fact, oxidation to the VI state may not occur at a significant rate with respect to the time frame of interest, or there may exist stable $Cr^{(III)}$ solids (not present in the EQ3/6 thermodynamic database) that substantially lower aqueous Cr concentration. For the present analyses, however, the assumption is made that over the times of concern the oxidation will occur.

3.8 The gases in solution in the waste package will remain in equilibrium with the ambient atmosphere outside the waste package. The basis for this assumption is that it is assumed that there will be 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 normal atmosphere in open air or rock gas that seeps out of the adjacent tuff. Under these conditions, the partial pressure of CO_2 exerts important controls on the pH and carbonate concentration in the solution.

3.9 The precipitated solids that are deposited remain in place, and are not mechanically eroded or entrained as colloids in the advected water. The basis for this assumption is that the result conservatively maximizes the size of potential deposits inside the waste package.

3.10 The corrosion rates used in this study encompass rates for degradation are enhanced by microbes, and the degradation rates will not be controlled principally by bacteria. The bases for this assumption are (1) steel corrosion rates measured under environmental conditions inherently include exposure to bacteria, and (2) the lack of organic nutrients available for bacterial corrosion will limit the involvement of bacteria. It is assumed that bacteria act as catalysts, particularly for processes such as the reduction of sulfate, but this catalytic effect is not expected to significantly change the types of solids formed in the waste package.

3.11 Sufficient decay heat is retained within the waste package over times of interest to cause convective circulation and mixing of the water inside the waste package. The basis for this assumption is discussed in Reference 12.

3.12 The water flow rate into and out of the waste package is equal to the rate at which water drips onto the waste package. The basis for this assumption is that 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 waste package than to assume that a significant portion will instead be diverted around the remains.

3.13 A number of minor assumptions have been made about the geometry of the Navy waste package. These assumptions are outlined and referenced in the spreadsheet "navy4.xls" (Ref. 10). The bases for these assumptions about the waste package geometry are that the assumptions are always intended to obtain the greatest accuracy in the representation, and where inadequate information is available to choose among competing representations of waste package geometry, the choice that appears to lead to greatest conservatism is always made.

4. USE OF COMPUTER SOFTWARE AND MODELS

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

EQ3/6 Software Package–The EQ3/6 software package originated in the mid-1970s at Northwestern University (Ref. 5). Since 1978, Lawrence Livermore National Laboratory (LLNL) has been responsible for maintenance of EQ3/6. The software has most recently been maintained under the sponsorship of the Civilian Radioactive Waste Management Program of the United States Department of Energy (DOE). The major components of the EQ3/6 package include EQ3NR, a speciation-solubility code; EQ6, a reaction-path code, which simulates water/rock interaction or fluid mixing in either a reaction-progress mode (time independent) or a time mode; EQPT, a data file preprocessor; EQLIB, a supporting software library; and several 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 represents the consequences of irreversible reactions between an aqueous solution and a set of solid or fluid reactants. It can also represent fluid mixing and the consequences of changes in temperature. This code operates both in a reaction-progress frame (independent of time) 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 perform 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 Microsoft Windows and the UNIX operating systems. Further information on the codes of the EQ3/6 package is provided in References 5, 6, 7, and 8.

Solid-Centered Flow-Through Mode–EQ6 version 7.2b, as distributed by LLNL, does not contain an SCFT mode. To add this mode, it was necessary to change the EQ6 source code and recompile the source. By using a variant of the "special reactant" type built into EQ6, it was possible to add the functionality of SCFT mode in a very simple and straightforward manner. The new mode is induced with a "special-special" reactant. The EQ6 input file nomenclature for this new mode is jcode=5; in the Daveler format, it is indicated by the reactant type DISPLACER. The jcode=5 is immediately trapped and converted to jcode=2, and a flag is set to indicate the existence of the DISPLACER reactant. Apart from the input trapping, the distinction between the DISPLACER and SPECIAL reactants is seen only in one 9-line block of the EQ6 FORTRAN source code (in the reacts subroutine), where the total moles of elements in the rock-plus-water system (mte array) is adjusted by adding in the DISPLACER reactant, and subtracting out a commensurate amount of the total aqueous elements (mteaq array).

4.1 SOFTWARE APPROVED FOR QUALITY ASSURANCE (QA) WORK

The software package, EQ3/6 Version 7.2b (Ref. 13) was used to provide the following:

- A general overview of the expected chemical reactions
- The degradation products from corrosion of the waste forms and canisters
- An indication of the minerals and their amounts likely to precipitate within the waste package.

The software specifications are as follow:

- Software name: EQ3/6
- Software version/revision number: Version 7.2b
- Computer sofware configuration identifier (CSCI): UCRL-MA-110662 V 7.2b
- Computer type: personal computer (PC) (Ref. 14).

The input and output files attributes for the various EQ6 calculations are documented in Attachment II. The calculation files described in Sections 5 and 6 are such that an independent repetition of the software used may be performed.

The EQ3/6 software used was: (a) appropriate for the calculations performed, (b) used only within the range of validation as documented in Reference 13 and, (c) obtained from the Software Configuration Manager in accordance with appropriate procedures.

4.2 SOFTWARE ROUTINES

Spreadsheet analyses were performed with Microsoft Excel version 97, installed on a PC. The specific spreadsheets used for results reported in this document are included in the electronic media (Ref. 10). Spreadsheet "navy4".xls contains two worksheets that convert various data values into a form suitable for input to EQ6. Excel spreadsheets "density_navy4.xls" and "navy aqueous all element.xls" manipulates data from EQ6 output files for presentation in the results tables in Section 5.

4.3 MODELS

None used.

5. CALCULATION

The calculations begin with selection of data for compositions, amounts, surface areas, and reaction rates of the various components of the Navy waste packages. These quantities are recalculated to the form required for entry into EQ6. For example, weight percentages of elements in the stainless steel are converted to moles based on 100 g/mole; the degradation rate in micrometers/year is converted into moles per square centimeter per second, etc. Spreadsheets (Ref. 10) 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 (Section 5.1.1.4). The EQ6 output provides the results of the chemical degradation of the waste package and its components. In the calculations, the degradation of the waste package occurs in one stage. The results include the compositions and amounts of solid products and of substances in solution. Details of the results are presented below.

In all tables from this document, the number of digits reported does not necessarily reflect the accuracy or precision of the calculation. In most tables, two to four digits after the decimal place have been retained to prevent round-off errors in subsequent calculations.

The existing database supplied with the EQ3/6 computer package is sufficiently accurate for the purposes of this calculation. The data have been carefully scrutinized by many experts over the course of several decades and carefully selected by LLNL for incorporation into the data base (Refs. 5, 6, 7, and 8). These databases are periodically updated and/or new databases added, such as one including extensive data on the lanthanides (Ref 9). 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 the electronic files labeled data0 that accompany this calculation, for details (Ref. 10). Nevertheless, the quality of data needs to be verified in the future.

5.1 CALCULATION INPUTS

5.1.1 Waste Package Materials and Performance Parameters

This section provides a brief overview of the physical and chemical characteristics of the Navy SNF waste package (without the SNF) and describes how the waste package is represented in the EQ6 inputs. The conversion of the waste package physical description, into parameters suitable for the EQ6 input files, is performed by the spreadsheet "navy4.xls."

Material nomenclature used throughout this document includes SB-575 N06022 (referred to as Alloy 22), SA-240 S31603 (referred to as 316L) and SA-240 316 NG (referred to as 316NG).

5.1.1.1 Physical and Chemical Form of the Navy Waste Package

The Navy waste package considered in the calculations is comprised of

- The stainless steel inner shell of the waste package (316NG)
- The stainless steel basket components (316L)
- The Navy SNF canister (316L), consisting of the shield plug, shell, and bottom.

Table 5-1 provides the composition, molar volume, density, and degradation rate of the stainless steel used in the calculations. The properties of the 316NG in the inner shell of the waste package is assumed to be the same as 316L.

Table 5-1. 316L Stainless Steel Composition and Degradation Rate

Element	Amount [a] (wt%)	Value Used (wt%)	Moles [b]
C	0.03 (max)	0.03	2.4977E-03
Mn	2.00 (max)	2.00	3.6405E-02
P	0.045 (max)	0.045	1.4528E-03
S	0.03 (max)	0.03	9.3557E-04
Si	1.00 (max)	1.00	3.5606E-02
Cr	16.00-18.00	17.00	3.2695E-01
Ni	10.00-14.00	12.00	2.0446E-01
Mo	2.00-3.00	2.50	2.6058E-02
N	0.10 (max)	0.10	7.1394E-03
Fe	Balance	65.295	1.1692
Total		100.00	1.8107
Molar Volume (cm^3/mole)[c]	12.53		
Density (g/cm^3)[a]	7.98		
Degradation Rate (µm/y)[d]	0.1		
Degradation Rate (moles/(cm^2-s))[e]	2.53E-14		

NOTES:
[a] Ref. 15
[b] Normalized to 100 g/mole; calculations in "navy4.xls" (Ref. 10).
[c] Molecular weight (assumed to be 100 g/mole) divided by density
[d] Ref. 16
[e] Conversion based on 100 g/mole and 365.25 d/y; calculations in "navy4.xls" (Ref. 10)

All EQ6 calculations are based on 1 liter of water; therefore, all the values of moles and surface area must be divided by the void volume expressed in liters. Three different void volumes were chosen for the calculations. Table 5-2 provides the calculated and normalized EQ6 input values for the components of the Navy waste package considered in the calculation (Ref. 10). The calculation of the normalized moles and surface area are presented in Excel spreadsheet "navy4.xls" (Ref. 10). The dimensions of the 316NG inner shell come from spreadsheet "navy4.xls" (Ref. 10, sketch SK-0146); the 316L Navy canister dimensions come from Reference 1; the 316L basket values of mass and surface area come from Reference 2. The waste package void volumes were calculated in spreadsheet "navy4.xls" based on waste package dimensions from Reference 1.

Table 5-2. Calculated and Normalized EQ6 Input Values for Materials in the Navy Waste Package

Calculated or Normalized EQ6 Input Parameter	Void Fraction in Waste Package[a]	Component			
		316NG Inner Shell of Waste Package	316L Navy Canister Shield Plug	316L Navy Canister Shell and Bottom	316L Basket
Mass (lb)	N/A	38,359	13,964	15,681	30,000
Mass (kg)	N/A	17,399	6,334	7,113	13,608
Normalized moles[b]	0.7	24.54	8.93	10.03	19.20
	0.3	65.91	23.99	26.94	51.55
	0.05	395.44	143.96	161.66	309.27
Surface area (in^2)	N/A	52,522	9480	92,139	178,000
Surface area (cm^2)	N/A	338,848	61159	594,446	1,148,385
Normalized surface area (cm^2)[b]	0.7	47.80	8.63	83.85	161.99
	0.3	128.35	23.1668	225.17	435.00
	0.05	770.12	139.00	1,351.04	2,610.01
Low drip rate (0.015 m^3/y) of incoming water in units of normalized moles/(cm^2·s)	0.7	6.705E-11			
	0.3	1.800E-10			
	0.05	1.080E-09			
Medium drip rate (0.15 m^3/y) of incoming water in units of normalized moles/(cm^2·s)	0.7	6.705E-10			
	0.3	1.800E-09			
	0.05	1.080E-08			
High drip rate (0.5 m^3/y) of incoming water in units of normalized moles/(cm^2·s)	0.7	2.235E-09			
	0.3	6.002E-09			
	0.05	3.601E-08			

NOTES [a] Void volume fraction corresponds to the following volumes: 0.7 x 618,000 in^3 = 432,600 in^3 (7,089 liters); 0.3 x 537,000 in^3 = 161,100 in^3 (2,640 liters); 0.05 x 537,000 in^3 = 26,850 in^3 (440 liters)

[b] Normalized moles and areas are calculated by dividing the moles and areas by the void volume; calculations in "navy4.xls" (Ref. 10)

5.1.1.2 Kinetics of SiO_2 Dissolution and Precipitation

At high drip rates, the precipitation rate of SiO_2 may be slower than the residence time in the waste package. To account for this in the calculations, the reaction kinetics of SiO_2 dissolution were added to the EQ6 input files. EQ6 automatically calculates the rate of precipitation based on the rate of dissolution. The changes in the dissolution rate as a function of pH were estimated in spreadsheet "quartz.xls" and plotted as the solid line in Figure 5-1. The choice of the dissolution rate (1×10^{-6} moles/($cm^2 \cdot s$)) at low pH values and the slope of the curve in the high pH range (0.3) came from Figure 2 of Reference 17. Figure 5-1 provides experimental values of quartz dissolution at 25 °C from Tables I and III of Reference 18. For the range of pH values (5 to 8) encountered in the EQ6 calculations, the EQ6 dissolution rate used in the EQ6 calculation fits the experimental data fairly well.

Besides the dissolution rate, a precipitation surface area equal to the basket surface area (Table 5-2) and a small value representing the initial moles of SiO_2 (1×10^{-5}) were added to the EQ6 input file.

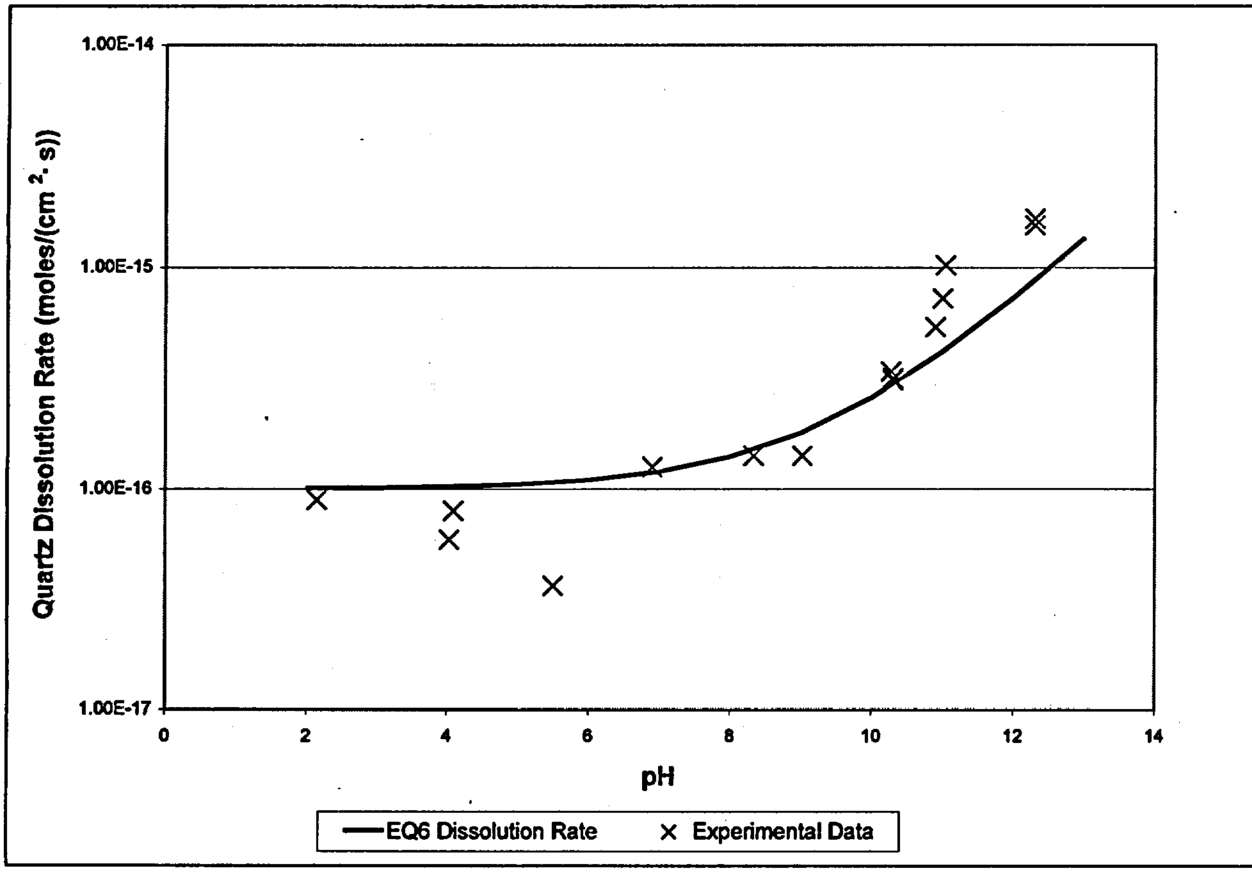


Figure 5-1. Quartz Dissolution Rate as a Function of pH at 25 °C.

5.1.1.3 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 the J-13 well (Assumption 3.2). This water has been analyzed repeatedly over a span of at least two decades (Ref. 4). Table 5-3 contains the EQ3NR input file constraints for J-13 well water composition based on Reference 4 and based on the assumptions of carbon dioxide fugacity found in Reference 19. Table 5-3 is in the format required by EQ3NR. For an explanation of terms used in the input file see Reference 7. Table 5-4 provides the elemental molal (moles/kg) composition for J-13 well water calculated by EQ3NR and included in the EQ6 input files for this calculation.

Table 5-3. EQ3NR Input File Constraints for J-13 Well Water Composition

Species	Basis Switch/Constraint	Concentration	Units or Type
redox		-0.7	log fO_2
Na+		4.580E+01	mg/l
SiO_2(aq)		6.097E+01	mg/l
Ca++		1.300E+01	mg/l
K+		5.040E+00	mg/l
Mg++		2.010E+00	mg/l
Li+		4.800E-02	mg/l
H+		8.1	pH
HCO_3-	CO_2(g)	-3	log fCO_2
O_2(aq)		5.600E+00	mg/l
F-		2.180E+00	mg/l
Cl-		7.140E+00	mg/l
NO_3-	NH_3(aq)	8.780E+00	mg/l
SO_4--		1.840E+01	mg/l
$B(OH)_3$(aq)		7.660E-01	mg/l
Al+++	Diaspore	0	mineral
Mn++	Pyrolusite	0	mineral
Fe++	Goethite	0	mineral
HPO_4--		1.210E-01	mg/L
CrO_4--		1.000E-16	molality
MoO_4--		1.000E-16	molality

NOTES: [a] Refs. 4 and 19. For definition of terms, see Ref. 7.
[b] The concentration of 1.0E-16 is added as a trace to ensure numerical stability.

Table 5-4. EQ3/6 Input File Elemental Molar Composition for J-13 Well Water

Element	Mole/kg	Element	Mole/kg
O	5.55E+01	P	1.26E-06
Al	2.55E-08	K	1.29E-04
B	1.24E-05	Li	6.92E-06
Ca	3.24E-04	Mg	8.27E-05
Cl	2.01E-04	Mn	3.05E-16
Cr	1.00E-16	Mo	1.00E-16
F	1.15E-04	N	1.42E-04
Fe	3.60E-12	Na	1.99E-03
H	1.11E+02	S	1.92E-04
C	2.09E-03	Si	1.02E-03

5.1.1.4 Drip Rate of Water into a Waste Package

It is assumed (Assumption 3.122) that the drip rate into 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 (Ref. 20). Specifically, percolation rates of 40 mm/year and 8 mm/year correlate with drip rates onto the waste package of 0.15 m^3/year and 0.015 m^3/year, respectively. The choice of these particular percolation and drip rates is discussed in detail in Reference 21.

For the present study, the range of allowed drip rates was extended to include an upper value of 0.5 m^3/year. The upper value corresponds to the 95 percentile upper limit for a percolation rate of 40 mm/year (Ref. 20). The values of drip rate, converted to the units appropriate for EQ6 input, are provided in Table 5-2 for each of the three void volumes.

5.1.1.5 Densities and Molecular Weights of Solids

For input to criticality calculations, one must convert moles of solids to solid volumes. The molecular weights and molar volumes of the solids are found in file data0.nuc.r8a in Reference 10.

5.1.1.6 Atomic Weights

Atomic weights were taken from Reference 22 and are listed in Reference 10 (spreadsheet "density_navy4.xls", sheet "density").

5.2 EQ6 CALCULATIONS AND SCENARIOS REPRESENTED

The rationale for selection of scenarios in EQ6 simulations is to provide a range of possible conditions in the waste package during degradation. The internal degradation configurations are based on the assumption that groundwater drips onto the upper surface of the waste package and penetrates it. Groundwater accumulates inside the waste package, which could dissolve and flush corrosion products out of the waste package. The scenarios included three different drip rates and three different void volumes. Six cases of EQ6 simulations were run, with different void volumes and water fluxes through the waste package. Table 5-5 summarizes the conditions of each case.

Table 5-5. Conditions of All Cases

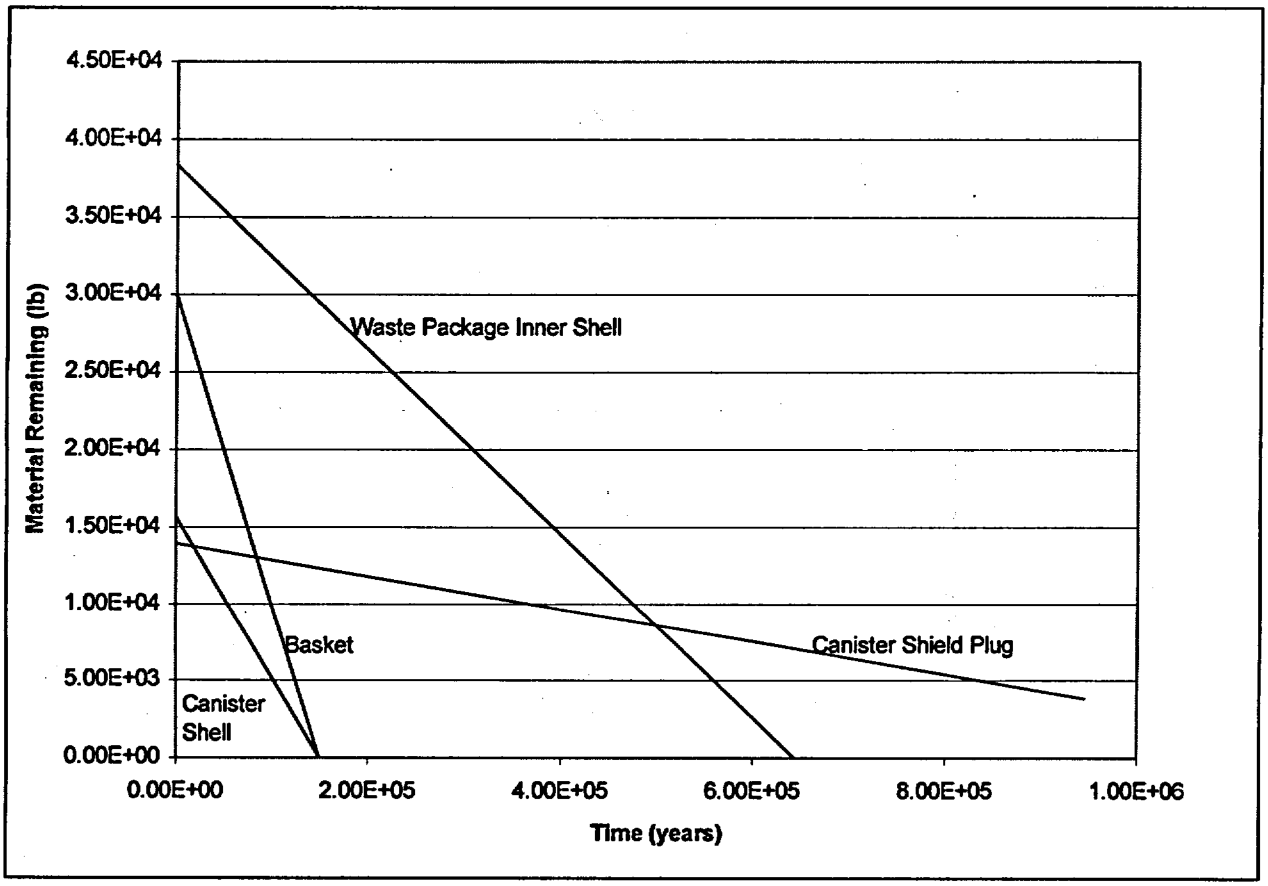
Case	File Name[a]	Void Volume Fraction	Drip Rate of Incoming Water (m^3/y)	Time (y)
1	V49s1002	0.7	0.015	946,400
2	V40{st}1002	0.05	0.015	207,520
3	V41{stu}1002	0.3	0.015	953,140
4	V41{stu}1003	0.3	0.15	998,640
5	V41{stuvwxy}1004	0.3	0.5	1,054,200
6	V40{stu}1004	0.05	0.5	65,692

NOTE: [a] In the cases that have file names with brackets, the letters within the brackets (such as s, t, u, etc.) indicate the specific file names for the EQ6 runs that were required for that case. For example, Case 2 consisted of runs with the file names V40s1002 and V40t1002.

The EQ6 input file corresponding to each run is included in the electronic media accompanying this calculation (Ref. 10). Each input file has the form of #.6i, where the "#" represents the name of the run (e.g., V49s1002.6i is the EQ6 input file name for Case 1). EQ6 generates four different types of text output files. Reference 10 contains tab delimited text files with the names like #.elem_*.txt. The text files list total moles of elements in aqueous phase (#.elem_aqu.txt.), total moles of each element produced by minerals (#.elem_min.txt), and total moles of each element, which is the sum of aqueous, mineral, and unreacted reactants (#.elem_tot.txt).

The file name, in column 2 of Table 5-5, provides most of the important run conditions. The third character of the file name indicates the void volume as 0, 1, and 9 for very low, low, and high void volumes, respectively. The actual void volumes are listed in the table notes of Table 5-2. The characters within the brackets (such as s, t, u, etc.) indicate the specific file names for the EQ6 runs that were required for that case. For example, Case 2 consisted of runs with the file names V40s1002 and V40t1002. The last character indicates the choice of drip rate of the incoming water, with 2, 3, and 4 corresponding to 0.015 m^3/year, 0.15 m^3/year, and 0.5 m^3/year, respectively.

Figure 5-2 provides a plot of the undegraded mass of each component in the waste package versus time for all cases. Since the degradation rate is independent of operating conditions, such as pH, water drip rate, or void volume, the data plotted in Figure 5-2 applies to all cases. By one millions years, everything has fully degraded, except the canister shield plug, which is initially 15 inches thick and therefore takes the longest to fully degrade.



SOURCE: File V49s1002.txt (Ref. 10); conversion from moles to pounds in Excel spreadsheet "components report.xls" (Ref. 10).

Figure 5-2. Unreacted Mass Remaining Versus Time for All Cases

The concentrations of each element in the aqueous phase at selected times are presented in Tables 5-6 through 5-11. The aqueous concentrations from the EQ6 output files "#.elem_aqu.txt" were converted from moles/liter to mg/liter in spreadsheet "navy aqueous all elements.xls." The mass of each element, the total mass, and the density of the corrosion products are presented at selected times in Tables 5-12 through 5-17. The mass and density of the corrosion products were calculated in spreadsheet "density_navy4.xls," using values from the EQ6 output files "#.elem_min.txt," and using the grams-to-pounds conversion from Reference 23.

Table 5-6. Concentration (mg/l) in Aqueous Phase and pH at Selected Times for Case 1 (V49s1002)

	Year						
Element	12,700	31,751	101,600	300,890	499,540	701,180	946,400
O	8.91E+05	8.91E+05	8.91E+05	8.89E+05	8.89E+05	8.88E+05	8.88E+05
Al	4.20E-16	4.20E-16	4.20E-16	6.97E-13	6.97E-13	7.54E-15	7.54E-15
B	0.13	0.13	0.13	0.13	0.13	0.13	0.13
Ca	13.01	13.01	13.00	11.76	11.76	12.60	12.60
Cl	7.14	7.14	7.14	7.14	7.14	7.14	7.14
Cr	1938.00	1938.00	1938.00	361.77	361.77	55.31	55.31
F	2.18	2.18	2.18	2.06	2.06	2.14	2.14
Fe	1.26E-06	1.26E-06	1.26E-06	3.75E-07	3.75E-07	8.60E-08	8.60E-08
H	1.12E+05	1.12E+05	1.12E+05	1.12E+05	1.12E+05	1.12E+05	1.12E+05
C	0.44	0.44	0.44	0.51	0.51	1.69	1.69
P	5.17E+00	5.17E+00	5.17E+00	4.21E-01	4.21E-01	2.24E-03	2.24E-03
K	5.04	5.04	5.04	5.04	5.04	5.04	5.04
Li	0.05	0.05	0.05	0.05	0.05	0.05	0.05
Mg	2.01	2.01	2.01	2.01	2.01	2.01	2.01
Mn	8.35E-06	8.35E-06	8.35E-06	8.26E-07	8.26E-07	4.15E-09	4.15E-09
Mo	285.00	285.00	285.00	53.20	53.20	8.13	8.13
N	13.38	13.38	13.38	4.11	4.11	2.31	2.31
Na	45.80	45.80	45.80	45.80	45.80	45.80	45.80
Ni	1293.88	1293.88	1293.88	212.93	212.93	1.35	1.35
S	9.56	9.56	9.56	6.78	6.78	6.24	6.24
Si	54.31	54.31	54.31	19.60	19.60	12.20	12.20
$NO3^-$	59.25	59.25	59.25	18.20	18.20	10.22	10.22
$SO4^{--}$	28.65	28.65	28.65	20.31	20.31	18.69	18.69
$HCO3^-$	2.26	2.26	2.26	2.60	2.60	8.59	8.59
pH	5.29	5.29	5.29	5.70	5.70	6.81	6.81

Table 5-7. Concentration (mg/l) in Aqueous Phase and pH at Selected Times for Case 2 (V40{st}1002)

Element	Year			
	10,247	29,954	100,110	207,520
O	8.91E+05	8.91E+05	8.91E+05	8.89E+05
Al	4.20E-16	4.20E-16	4.20E-16	6.97E-13
B	0.13	0.13	0.13	0.13
Ca	13.00	13.00	13.00	11.76
Cl	7.14	7.14	7.14	7.14
Cr	1937.95	1937.95	1937.95	361.76
F	2.18	2.18	2.18	2.06
Fe	1.26E-06	1.26E-06	1.26E-06	3.75E-07
H	1.12E+05	1.12E+05	1.12E+05	1.12E+05
C	0.44	0.44	0.44	0.51
P	5.17	5.17	5.17	0.421
K	5.04	5.04	5.04	5.04
Li	0.05	0.05	0.05	0.05
Mg	2.01	2.01	2.01	2.01
Mn	8.35E-06	8.35E-06	8.35E-06	8.26E-07
Mo	285.00	285.00	285.00	53.20
N	13.38	13.38	13.38	4.11
Na	45.80	45.80	45.80	45.80
Ni	1293.88	1293.88	1293.88	212.93
S	9.56	9.56	9.56	6.78
Si	54.31	54.31	54.31	19.60
$NO3^{-}$	59.24	59.24	59.24	18.20
$SO4^{--}$	28.65	28.65	28.65	20.31
$HCO3^{-}$	2.26	2.26	2.26	2.60
pH	5.29	5.29	5.29	5.70

Table 5-8. Concentration (mg/l) in Aqueous Phase and pH at Selected Times for Case 3 (V41{stu}1002)

Element	Year						
	11,824	30,742	101,680	299,730	499,570	699,990	953,140
O	8.91E+05	8.91E+05	8.91E+05	8.89E+05	8.89E+05	8.88E+05	8.88E+05
Al	4.20E-16	4.20E-16	4.20E-16	6.97E-13	6.97E-13	7.53E-15	7.53E-15
B	0.13	0.13	0.13	0.13	0.13	0.13	0.13
Ca	13.01	13.00	13.00	11.76	11.76	12.60	12.60
Cl	7.14	7.14	7.14	7.14	7.14	7.14	7.14
Cr	1937.95	1937.95	1937.95	361.76	361.75	55.31	55.31
F	2.18	2.18	2.18	2.06	2.06	2.14	2.14
Fe	1.26E-06	1.26E-06	1.26E-06	3.75E-07	3.75E-07	8.60E-08	8.60E-08
H	1.12E+05	1.12E+05	1.12E+05	1.12E+05	1.12E+05	1.12E+05	1.12E+05
C	0.44	0.44	0.44	0.51	0.51	1.69	1.69
P	5.17E+00	5.17E+00	5.17E+00	4.21E-01	4.21E-01	2.24E-03	2.24E-03
K	5.04	5.04	5.04	5.04	5.04	5.04	5.04
Li	0.05	0.05	0.05	0.05	0.05	0.05	0.05
Mg	2.01	2.01	2.01	2.01	2.01	2.01	2.01
Mn	8.35E-06	8.35E-06	8.35E-06	8.26E-07	8.26E-07	4.15E-09	4.15E-09
Mo	285.00	285.00	285.00	53.20	53.20	8.13	8.13
N	13.38	13.38	13.38	4.11	4.11	2.31	2.31
Na	45.80	45.80	45.80	45.80	45.80	45.80	45.80
Ni	1293.88	1293.88	1293.88	212.93	212.93	1.35	1.35
S	9.56	9.56	9.56	6.78	6.78	6.24	6.24
Si	54.31	54.31	54.31	19.60	19.60	12.20	12.20
NO3-	59.24	59.24	59.24	18.20	18.20	10.22	10.22
SO4--	28.65	28.65	28.65	20.31	20.31	18.69	18.69
HCO3-	2.26	2.26	2.26	2.60	2.60	8.59	8.59
pH	5.29	5.29	5.29	5.70	5.70	6.81	6.81

Table 5-9. Concentration (mg/l) in Aqueous Phase and pH at Selected Times for Case 4 (V41{stu}1003)

Element	Year						
	10,179	40,194	99,962	299,700	499,620	699,660	998,370
O	8.88E+05	8.88E+05	8.88E+05	8.88E+05	8.88E+05	8.88E+05	8.88E+05
Al	9.19E-15	9.19E-15	9.19E-15	2.28E-18	2.28E-18	2.07E-18	2.07E-18
B	0.13	0.13	0.13	0.13	0.13	0.13	0.13
Ca	12.19	12.19	12.19	12.71	12.71	12.88	12.88
Cl	7.14	7.14	7.14	7.14	7.14	7.14	7.14
Cr	193.79	193.79	193.79	36.18	36.18	5.53	5.53
F	2.10	2.10	2.10	2.15	2.15	2.17	2.17
Fe	2.85E-07	2.85E-07	2.85E-07	6.79E-08	6.79E-08	6.64E-08	6.64E-08
H	1.12E+05	1.12E+05	1.12E+05	1.12E+05	1.12E+05	1.12E+05	1.12E+05
C	0.55	0.55	0.55	7.70	7.70	20.98	20.98
P	1.78E-01	1.78E-01	1.78E-01	1.85E-04	1.85E-04	5.24E-05	5.24E-05
K	5.04	5.04	5.04	5.04	5.04	5.04	5.04
Li	0.05	0.05	0.05	0.05	0.05	0.05	0.05
Mg	2.01	2.01	2.01	2.01	2.01	0.46	0.46
Mn	4.08E-07	4.08E-07	4.08E-07	1.32E-10	1.32E-10	2.11E-11	2.11E-11
Mo	28.50	28.50	28.50	5.32	5.32	0.81	0.81
N	3.12	3.12	3.12	2.20	2.20	2.02	2.02
Na	45.80	45.80	45.80	45.80	45.80	45.80	45.80
Ni	91.20	91.20	91.20	0.03	0.03	0.00	0.00
S	6.48	6.48	6.48	6.21	6.21	6.15	6.15
Si	26.06	26.06	26.06	21.77	21.77	22.45	22.44
NO3-	13.83	13.83	13.83	9.72	9.72	8.92	8.92
SO4--	19.43	19.43	19.43	18.59	18.59	18.43	18.43
HCO3-	2.78	2.78	2.78	39.10	39.10	106.58	106.58
pH	5.83	5.83	5.83	7.56	7.56	8.01	8.01

Table 5-10. Concentration (mg/l) in Aqueous Phase and pH at Selected Times for Case 5 (V41{stuvwxy}1004)

Element	Year						
	10,024	29,993	100,000	299,550	499,630	699,510	1,054,200
O	8.88E+05	8.88E+05	8.88E+05	8.88E+05	8.88E+05	8.88E+05	8.88E+05
Al	2.98E-17	2.98E-17	2.98E-17	9.30E-19	9.30E-19	7.42E-19	7.42E-19
B	0.13	0.13	0.13	0.13	0.13	0.13	0.13
Ca	12.59	12.59	12.59	12.85	12.85	12.91	12.91
Cl	7.14	7.14	7.14	7.14	7.14	7.14	7.14
Cr	58.14	58.14	58.14	10.85	10.85	1.66	1.66
F	2.14	2.14	2.14	2.17	2.17	2.17	2.17
Fe	9.29E-08	9.29E-08	9.29E-08	6.64E-08	6.64E-08	6.65E-08	6.65E-08
H	1.12E+05	1.12E+05	1.12E+05	1.12E+05	1.12E+05	1.12E+05	1.12E+05
C	1.39	1.39	1.39	18.45	18.45	22.75	22.75
P	3.51E-03	3.51E-03	3.51E-03	6.09E-05	6.09E-05	4.76E-05	4.76E-05
K	5.04	5.04	5.04	5.04	5.04	5.04	5.04
Li	0.05	0.05	0.05	0.05	0.05	0.05	0.05
Mg	2.01	2.01	2.01	0.55	0.55	0.35	0.35
Mn	7.08E-09	7.08E-09	7.08E-09	2.56E-11	2.56E-11	1.88E-11	1.88E-11
Mo	8.55	8.55	8.55	1.60	1.60	0.24	0.24
N	2.33	2.33	2.33	2.05	2.05	1.99	1.99
Na	45.80	45.80	45.80	45.80	45.80	45.80	45.80
Ni	1.73	1.73	1.73	0.00	0.00	0.00	0.00
S	6.24	6.24	6.24	6.16	6.16	6.14	6.14
Si	21.76	21.76	21.76	24.05	24.05	24.70	24.70
NO3-	10.29	10.29	10.29	9.06	9.06	8.82	8.82
SO4--	18.71	18.71	18.71	18.46	18.46	18.41	18.41
HCO3-	7.05	7.05	7.05	93.70	93.70	115.58	115.58
pH	6.69	6.69	6.69	7.96	7.96	8.05	8.05

Table 5-11. Concentration (mg/l) in Aqueous Phase and pH at Selected Times for Case 6 (V40{stu}1004)

	Year		
Element	9,998	29,953	65,692
O	8.88E+05	8.88E+05	8.88E+05
Al	2.98E-17	2.98E-17	2.98E-17
B	0.13	0.13	0.13
Ca	12.59	12.59	12.59
Cl	7.14	7.14	7.14
Cr	58.14	58.14	58.14
F	2.14	2.14	2.14
Fe	9.29E-08	9.29E-08	9.29E-08
H	1.12E+05	1.12E+05	1.12E+05
C	1.39	1.39	1.39
P	3.51E-03	3.51E-03	3.51E-03
K	5.04	5.04	5.04
Li	0.05	0.05	0.05
Mg	2.01	2.01	2.01
Mn	7.08E-09	7.08E-09	7.08E-09
Mo	8.55	8.55	8.55
N	2.33	2.33	2.33
Na	45.80	45.80	45.80
Ni	1.73	1.73	1.73
S	6.24	6.24	6.24
Si	21.76	21.76	21.76
NO3-	10.29	10.29	10.29
SO4--	18.71	18.71	18.71
HCO3-	7.05	7.05	7.05
pH	6.69	6.69	6.69

Table 5-12. Mass of Corrosion Products in Waste Package (lb), Density, and pH at Selected Times for Case 1 (V49s1002)

Element	Year						
	12,700	31,751	101,600	300,890	499,540	701,180	946,400
O	1.42E+03	3.54E+03	1.13E+04	1.99E+04	2.41E+04	2.74E+04	2.83E+04
Al	3.00E-04	7.34E-04	2.33E-03	6.86E-03	1.14E-02	1.60E-02	2.16E-02
B	2.00E-18	1.14E-18	1.43E-18	3.38E-16	0.00E+00	0.00E+00	0.00E+00
Ca	1.77E-02	1.23E-02	9.38E-04	6.17E+00	1.43E+01	2.10E+01	2.42E+01
Cl	0.00E+00	6.01E-17	2.10E-16	0.00E+00	1.14E-13	1.40E-14	1.43E-14
Cr	0.00E+00	2.26E-12	5.67E-11	0.00E+00	1.32E-08	1.29E-10	1.32E-10
F	1.66E-03	1.13E-03	2.17E-16	5.85E-01	1.36E+00	1.99E+00	2.29E+00
Fe	3.13E+03	7.82E+03	2.50E+04	4.37E+04	5.28E+04	5.98E+04	6.15E+04
H	6.79E-05	1.66E-04	5.26E-04	1.55E-03	2.58E-03	3.62E-03	4.88E-03
C	0.00E+00	1.01E-11	7.71E-12	0.00E+00	0.00E+00	0.00E+00	0.00E+00
P	8.13E-03	5.55E-03	1.25E-13	2.86E+00	6.64E+00	9.73E+00	1.12E+01
K	1.45E-05	3.54E-05	1.12E-04	3.26E-04	5.40E-04	7.20E-04	9.72E-04
Li	0.00E+00	0.00E+00	1.01E-18	0.00E+00	1.18E-15	3.29E-16	3.37E-16
Mg	5.05E-05	1.24E-04	3.91E-04	1.17E-03	1.94E-03	2.66E-03	3.59E-03
Mn	9.58E+01	2.39E+02	7.66E+02	1.34E+03	1.62E+03	1.83E+03	1.88E+03
Mo	6.50E-16	0.00E+00	0.00E+00	3.25E-16	0.00E+00	1.22E-16	0.00E+00
N	0.00E+00	1.90E-16	6.86E-15	0.00E+00	9.57E-13	2.22E-14	2.27E-14
Na	1.26E-05	3.09E-05	9.80E-05	2.80E-04	4.65E-04	6.18E-04	8.34E-04
Ni	3.17E+01	7.84E+01	2.50E+02	5.80E+02	8.58E+02	1.13E+03	1.44E+03
S	0.00E+00	5.81E-15	1.52E-13	0.00E+00	8.70E-11	4.03E-12	4.12E-12
Si	8.86E+00	2.21E+01	7.04E+01	1.39E+02	2.06E+02	2.71E+02	3.44E+02
Total Mass (lb)	4.68E+03	1.17E+04	3.74E+04	6.56E+04	7.96E+04	9.05E+04	9.36E+04
Density (g/cm^3)	5.258	5.258	5.258	5.263	5.263	5.262	5.261
pH	5.29	5.29	5.29	5.70	5.70	6.81	6.81

Table 5-13. Mass of Corrosion Products in Waste Package (lb), Density, and pH at Selected Times for Case 2 (V40{st}1002)

Element	Year			
	10,247	29,954	100,110	207,520
O	1.14E+03	3.34E+03	1.12E+04	1.79E+04
Al	2.34E-04	6.83E-04	2.28E-03	4.73E-03
B	1.24E-19	0.00E+00	0.00E+00	0.00E+00
Ca	9.45E-05	2.76E-04	9.21E-04	2.33E+00
Cl	4.66E-18	0.00E+00	0.00E+00	2.07E-15
Cr	8.74E-13	0.00E+00	3.50E-16	2.38E-10
F	4.25E-18	0.00E+00	0.00E+00	2.21E-01
Fe	2.52E+03	7.37E+03	2.46E+04	3.94E+04
H	5.30E-05	1.55E-04	5.16E-04	1.07E-03
C	5.34E-12	0.00E+00	0.00E+00	0.00E+00
P	1.92E-15	0.00E+00	1.63E-18	1.08E+00
K	1.13E-05	3.30E-05	1.10E-04	2.24E-04
Li	1.71E-20	1.14E-20	1.14E-20	2.13E-17
Mg	3.94E-05	1.15E-04	3.84E-04	8.05E-04
Mn	7.73E+01	2.26E+02	7.55E+02	1.21E+03
Mo	0.00E+00	0.00E+00	0.00E+00	3.03E-17
N	1.03E-16	0.00E+00	0.00E+00	1.73E-14
Na	9.86E-06	2.88E-05	9.61E-05	1.93E-04
Ni	2.51E+01	7.34E+01	2.45E+02	4.48E+02
S	2.33E-15	0.00E+00	8.43E-18	1.57E-12
Si	7.10E+00	2.07E+01	6.93E+01	1.07E+02
Total Mass (lb)	3.78E+03	1.10E+04	3.69E+04	5.90E+04
Density (g/cm^3)	5.258	5.258	5.258	5.263
pH	5.29	5.29	5.29	5.70

Table 5-14. Mass of Corrosion Products in Waste Package (lb), Density, and pH at Selected Times for Case 3 (V41{stu}1002)

Element	Year						
	11,824	30,742	101,680	299,730	499,570	699,990	953,140
O	1.32E+03	3.43E+03	1.14E+04	1.98E+04	2.41E+04	2.74E+04	2.84E+04
Al	2.73E-04	7.04E-04	2.32E-03	6.83E-03	1.14E-02	1.59E-02	2.17E-02
B	0.00E+00	0.00E+00	7.46E-19	1.24E-16	1.26E-16	1.84E-16	2.93E-16
Ca	4.57E-03	2.84E-04	9.37E-04	6.12E+00	1.43E+01	2.10E+01	2.43E+01
Cl	0.00E+00	6.71E-17	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Cr	8.65E-13	2.59E-11	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
F	4.23E-04	8.84E-17	3.00E-18	5.80E-01	1.36E+00	1.99E+00	2.30E+00
Fe	2.91E+03	7.57E+03	2.50E+04	4.36E+04	5.28E+04	5.98E+04	6.16E+04
H	6.19E-05	1.59E-04	5.25E-04	1.55E-03	2.58E-03	3.61E-03	4.92E-03
C	0.00E+00	0.00E+00	0.00E+00	4.78E-12	0.00E+00	0.00E+00	0.00E+00
P	2.07E-03	5.72E-14	0.00E+00	2.84E+00	6.64E+00	9.72E+00	1.13E+01
K	1.32E-05	3.40E-05	1.12E-04	3.24E-04	5.40E-04	7.19E-04	9.79E-04
Li	0.00E+00	3.42E-19	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Mg	4.60E-05	1.19E-04	3.91E-04	1.16E-03	1.94E-03	2.65E-03	3.61E-03
Mn	8.91E+01	2.32E+02	7.67E+02	1.34E+03	1.62E+03	1.83E+03	1.89E+03
Mo	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.54E-17	4.54E-17
N	7.95E-17	3.13E-15	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Na	1.15E-05	2.97E-05	9.77E-05	2.79E-04	4.65E-04	6.16E-04	8.39E-04
Ni	2.92E+01	7.55E+01	2.49E+02	5.78E+02	8.58E+02	1.13E+03	1.45E+03
S	2.18E-15	6.94E-14	3.04E-17	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Si	8.21E+00	2.13E+01	7.04E+01	1.38E+02	2.05E+02	2.71E+02	3.46E+02
Total Mass (lb)	4.36E+03	1.13E+04	3.75E+04	6.55E+04	7.96E+04	9.05E+04	9.37E+04
Density (g/cm^3)	5.258	5.258	5.258	5.263	5.263	5.262	5.261
pH	5.29	5.29	5.29	5.70	5.70	6.81	6.81

Table 5-15. Mass of Corrosion Products in Waste Package (lb), Density, and pH at Selected Times for Case 4 (V41{stu}1003)

Element	Year						
	10,179	40,194	99,962	299,700	499,620	699,660	998,640
O	1.21E+03	4.77E+03	1.19E+04	2.15E+04	2.65E+04	3.05E+04	3.20E+04
Al	2.32E-03	9.16E-03	2.28E-02	6.83E-02	1.14E-01	1.59E-01	2.27E-01
B	6.40E-19	0.00E+00	0.00E+00	7.46E-19	2.13E-19	0.00E+00	1.07E-19
Ca	2.72E+00	1.07E+01	2.67E+01	5.43E+01	7.35E+01	8.95E+01	1.01E+02
Cl	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	7.84E-15	2.24E-17
Cr	0.00E+00	0.00E+00	3.41E-15	0.00E+00	0.00E+00	6.96E-13	0.00E+00
F	2.58E-01	1.02E+00	2.53E+00	5.15E+00	6.97E+00	8.48E+00	9.56E+00
Fe	2.51E+03	9.89E+03	2.46E+04	4.36E+04	5.28E+04	5.98E+04	6.19E+04
H	5.26E-04	2.07E-03	5.16E-03	1.55E-02	2.58E-02	8.30E-01	5.07E+00
C	0.00E+00	4.86E-11	0.00E+00	4.41E-11	1.02E-10	2.89E-11	1.62E-10
P	1.26E+00	4.98E+00	1.24E+01	2.52E+01	3.41E+01	4.15E+01	4.68E+01
K	1.07E-04	4.24E-04	1.05E-03	3.07E-03	5.12E-03	8.87E-03	1.27E-02
Li	0.00E+00	2.40E-19	0.00E+00	0.00E+00	0.00E+00	2.15E-16	2.05E-19
Mg	3.91E-04	1.54E-03	3.83E-03	1.13E-02	1.89E-02	2.87E+01	1.82E+02
Mn	7.67E+01	3.03E+02	7.54E+02	1.34E+03	1.62E+03	1.83E+03	1.90E+03
Mo	0.00E+00	9.08E-17	0.00E+00	2.27E-17	3.03E-17	4.73E-18	0.00E+00
N	8.84E-18	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.23E-14	0.00E+00
Na	9.23E-05	3.64E-04	9.05E-04	2.63E-03	4.39E-03	7.59E-03	1.08E-02
Ni	1.54E+02	6.06E+02	1.51E+03	3.52E+03	5.21E+03	6.50E+03	6.88E+03
S	0.00E+00	1.52E-17	3.54E-17	0.00E+00	0.00E+00	2.00E-12	1.01E-17
Si	3.68E+01	1.45E+02	3.61E+02	8.44E+02	1.25E+03	1.60E+03	1.93E+03
Total Mass (lb)	3.98E+03	1.57E+04	3.91E+04	7.09E+04	8.75E+04	1.00E+05	1.05E+05
Density (g/cm^3)	5.250	5.251	5.251	5.244	5.239	5.229	5.195
pH	5.83	5.83	5.83	7.56	7.56	8.01	8.01

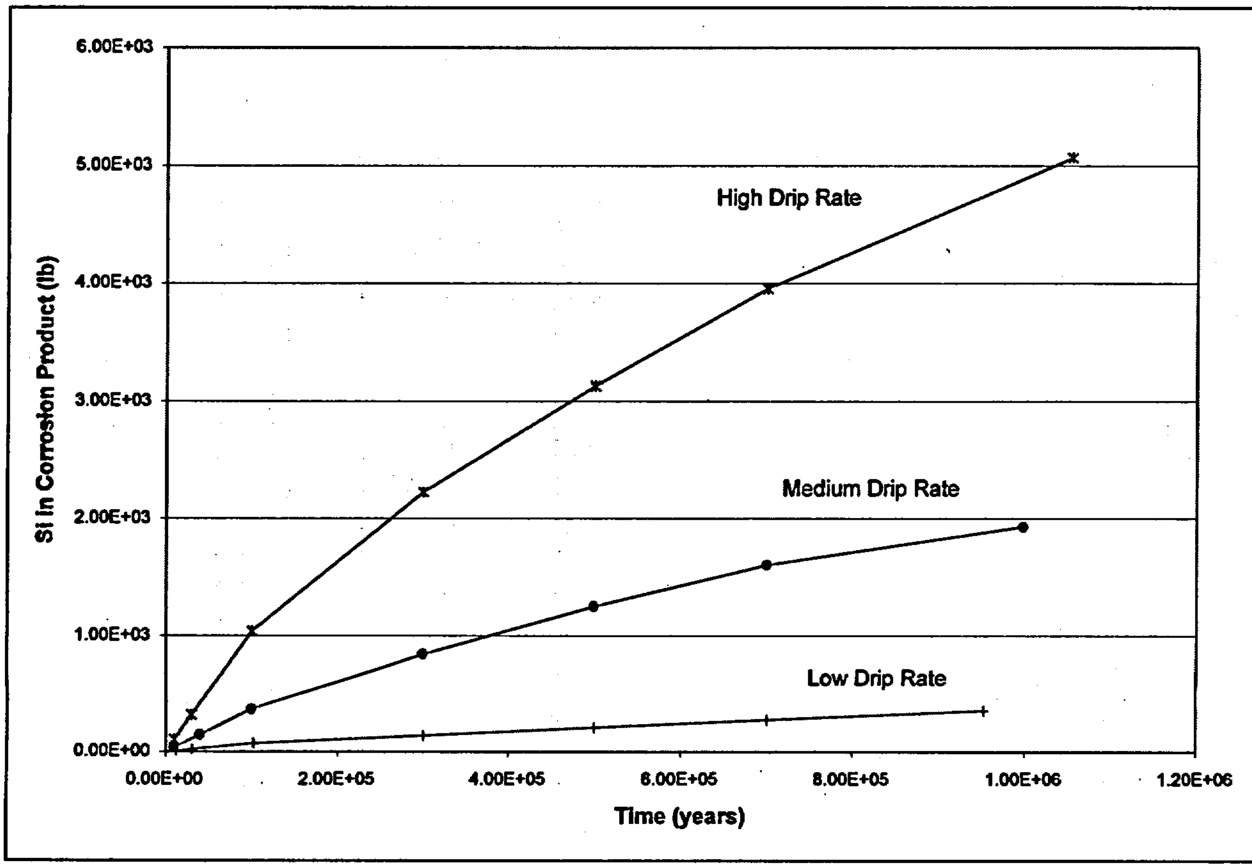
Table 5-16. Mass of Corrosion Products in Waste Package (lb), Density, and pH at Selected Times for Case 5 (V41{stuvwxy}1004)

Element	Year						
	10,024	29,993	100,080	299,550	500,190	699,590	1,054,200
O	1.35E+03	4.03E+03	1.34E+04	2.45E+04	3.04E+04	3.51E+04	3.82E+04
Al	7.61E-03	2.28E-02	7.60E-02	2.27E-01	3.80E-01	5.31E-01	8.00E-01
B	3.20E-19	0.00E+00	0.00E+00	2.13E-19	0.00E+00	1.07E-19	2.13E-19
Ca	4.52E+00	1.35E+01	4.51E+01	9.14E+01	1.24E+02	1.53E+02	1.89E+02
Cl	5.59E-18	5.59E-18	5.59E-18	0.00E+00	0.00E+00	5.59E-18	1.12E-17
Cr	0.00E+00	0.00E+00	0.00E+00	1.64E-17	1.64E-17	0.00E+00	0.00E+00
F	4.28E-01	1.28E+00	4.27E+00	8.66E+00	1.17E+01	1.45E+01	1.79E+01
Fe	2.47E+03	7.38E+03	2.46E+04	4.36E+04	5.28E+04	5.98E+04	6.23E+04
H	1.72E-03	5.16E-03	1.72E-02	6.73E+00	1.57E+01	2.50E+01	4.30E+01
C	0.00E+00	0.00E+00	0.00E+00	7.82E-11	4.64E-11	7.22E-11	7.22E-11
P	2.09E+00	6.26E+00	2.09E+01	4.24E+01	5.73E+01	7.07E+01	8.77E+01
K	3.43E-04	1.03E-03	3.43E-03	1.24E-02	2.07E-02	3.05E-02	4.59E-02
Li	1.03E-19	1.03E-19	1.03E-19	1.71E-19	0.00E+00	2.74E-19	0.00E+00
Mg	1.27E-03	3.79E-03	1.26E-02	2.42E+02	5.65E+02	8.98E+02	1.55E+03
Mn	7.56E+01	2.26E+02	7.55E+02	1.34E+03	1.62E+03	1.83E+03	1.91E+03
Mo	7.57E-18	7.57E-18	1.51E-17	0.00E+00	0.00E+00	1.42E-18	0.00E+00
N	2.21E-18	2.21E-18	6.63E-18	4.42E-18	4.42E-18	6.63E-18	6.63E-18
Na	2.94E-04	8.80E-04	2.94E-03	1.06E-02	1.77E-02	2.61E-02	3.93E-02
Ni	4.34E+02	1.30E+03	4.34E+03	7.73E+03	9.42E+03	1.07E+04	1.12E+04
S	1.52E-17	0.00E+00	0.00E+00	2.53E-17	0.00E+00	0.00E+00	0.00E+00
Si	1.04E+02	3.11E+02	1.04E+03	2.22E+03	3.13E+03	3.95E+03	5.06E+03
Total Mass (lb)	4.43E+03	1.33E+04	4.43E+04	7.97E+04	9.81E+04	1.13E+05	1.21E+05
Density (g/cm^3)	5.215	5.215	5.215	5.146	5.085	5.036	4.934
pH	6.69	6.69	6.69	7.96	7.96	8.05	8.05

Table 5-17. Mass of Corrosion Products in Waste Package (lb), Density, and pH at Selected Times for Case 6 (V40{stu}1004)

Element	Year		
	10,024	29,979	65,692
O	1.35E+03	4.02E+03	8.82E+03
Al	7.61E-03	2.28E-02	4.99E-02
B	0.00E+00	0.00E+00	0.00E+00
Ca	4.52E+00	1.35E+01	2.96E+01
Cl	9.32E-19	0.00E+00	0.00E+00
Cr	0.00E+00	4.37E-17	0.00E+00
F	4.28E-01	1.28E+00	2.80E+00
Fe	2.47E+03	7.38E+03	1.62E+04
H	1.72E-03	5.15E-03	1.13E-02
C	2.38E-12	1.12E-11	5.86E-12
P	2.09E+00	6.26E+00	1.37E+01
K	3.43E-04	1.03E-03	2.25E-03
Li	3.99E-20	4.56E-20	0.00E+00
Mg	1.27E-03	3.79E-03	8.30E-03
Mn	7.56E+01	2.26E+02	4.95E+02
Mo	0.00E+00	3.78E-18	7.57E-18
N	7.37E-19	1.10E-18	0.00E+00
Na	2.94E-04	8.80E-04	1.93E-03
Ni	4.34E+02	1.30E+03	2.85E+03
S	2.53E-18	1.69E-18	2.53E-18
Si	1.04E+02	3.11E+02	6.82E+02
Total Mass (lb)	4.43E+03	1.33E+04	2.91E+04
Density (g/cm^3)	5.215	5.215	5.215
pH	6.69	6.69	6.69

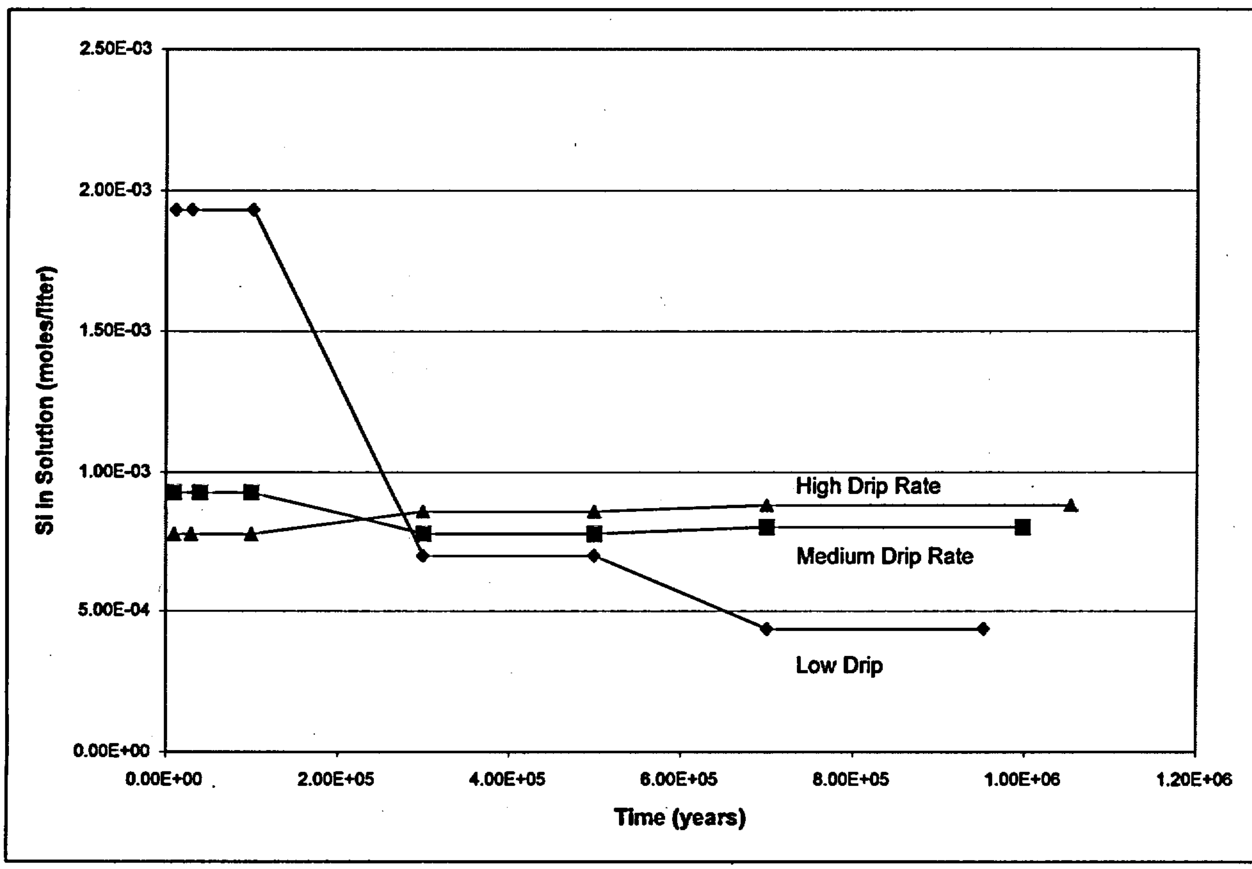
The aqueous concentrations in Table 5-6 and Table 5-8 (Cases 1 and 3, same drip rate, different void volumes) are nearly identical, as are the data in Table 5-12 and Table 5-14, indicating that the void volume has no effect on the composition of the aqueous or solid products formed. The choice of drip rate, on the other hand, does have an impact on the results. Figure 5-3 shows the quantity of silicon (Si) in the solid corrosion product versus time for three different drip rates. The higher the drip rate, the higher quantity of Si formed in the corrosion product.



NOTE: Cases 3, 4, and 5; plotted values come from EQ6 output files "#.elem_min.txt" (Ref. 10); conversions from moles/liter to total pounds in "density_navy4.xls."

Figure 5-3. Silicon in Solid Corrosion Product Versus Time for Three Drip Rates at 0.3 Void Fraction

Figure 5-4 is a plot of the Si in solution (moles/l) for the same three cases as in Figure 5-3. For early times, the highest concentration of Si in solution occurs in the lowest drip rate case. And in fact, the concentration for the low drip rate case is higher that for the incoming water (1.02×10^{-3} moles/l) for the first 150,000 years. This is due to the formation of amorphous SiO_2 in the low drip rate case at early times. Amorphous SiO_2 is more soluble than chalcedony, a fine grained quartz (SiO_2). Allowing amorphous SiO_2 to form (rather than suppressing it) is conservative in that more SiO_2 solids are formed. If amorphous SiO_2 were suppressed, more chalcedony would form, and the equilibrium concentration of Si in the water at early times would be lower. In addition, the high concentration of Si in solution at early times is due to the corrosion of the basket and canister shell and the release of 1 wt% Si from the steel into solution and into the corrosion products. At later times, the aqueous concentrations of Si in the high drip rate cases are higher than those in the low drip rate cases. This is due to the kinetics of SiO_2. At the higher drip rates, SiO_2 has a lower residence time in the waste package, and the formation of chalcedony is inhibited. This leads to a higher concentration at later times for the high drip rate cases.



NOTE: Cases 3, 4, and 5; plotted values from EQ6 output files "#.elem_aqu.txt" (Ref. 10).

Figure 5-4. Silicon Concentration in Solution Versus Time for Three Drip Rates at 0.3 Void Fraction

6. RESULTS

The results of this Calculation are based on a combination of qualified and unqualified technical information. Therefore, use of any unqualified technical information or result from the Calculation as input in documents supporting construction, fabrication, or procurement, or as part of a verified design to be released to another organization, is required to be identified and controlled in accordance with appropriate procedures.

A principal objective of this calculation was to determine the aqueous concentrations and the quantity of solid corrosion products that would form as a result of the degradation of a Navy waste package that does not contain SNF. Emphasis was placed on aqueous Si concentrations and solid SiO_2 formation, because of the importance of silica in the criticality calculations. Water with a composition of J-13 well water is assumed to drip in through an opening at the top of the waste package, pooling inside and eventually overflowing, allowing removal of soluble components through continual dilution. This calculation selected six EQ6 cases and examined the effects of varying the void volume and the drip rate.

Results indicated that void volume had no effect on the aqueous concentration or solid corrosion products. The highest quantity of corrosion products were formed at the highest drip rates. The aqueous concentrations of Si were higher at early times for the low drip rate cases. At later times, the concentration of Si was higher for the high drip rate cases due to kinetic effects of chalcedony formation.

7. ATTACHMENTS

Attachment I. Document Input Reference Sheets (6 pages)

Attachment II. Listing of Files on Electronic Media (3 pages)
(Reference 10 contains the electronic media for this calculation.)

8. REFERENCES

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DOCUMENT INPUT REFERENCE SYSTEM

1. Document Identifier No./Rev.: CAL-EDC-MD-000007 REV 00	Change: N/A	Title: EQ6 CALCULATIONS FOR CHEMICAL DEGRADATION OF NAVY WASTE PACKAGES

Input Document			4. Input Status	5. Section Used in	6. Input Description	7. TBV/TBD Priority	8. TBVDue To		
2a.	2. Technical Product Input Source Title and Identifier(s) with Version	3. Section					Unqual.	From Uncontrolled Source	Un-Confirmed
1	Naples, E.M. 1999. Thermal, Shielding, and Structural Information on the Naval Spent Nuclear Fuel Canister. Letter from E.M. Naples (Department of the Navy) to D.C. Haught (YMSCO), August 6, 1999, with enclosures, Detailed Information. ACC: MOL.19991001.0133.	Encl. 3 and 3B	TBV-3746	1, 5	Navy canister dimensions	3	X	N/A	N/A
2	Naples, E.M.; Johnson, K.E; 1999. Request to Perform Geochemistry Calculations for Waste Packages Containing Naval Spent Nuclear Fuel. Letter from E.M. Naples, (Department of the Navy) to D.C. Haught (YMSCO) with table, "Components in the Naval Spent Fuel Canister System for Corrosion Calculations." ACC: MOL.19991103.0342.	Entire	N/A - Reference Only	1	Navy Spent fuel Reference	N/A	N/A	N/A	N/A
		Entire	TBV-3754	5.1.1.1	316L basket values of mass and surface area	3	X	N/A	N/A
3	CRWMS M&O 1998. "Disruptive Events." Chapter 10 of *Total System Performance Assessment-Viability Assessment (TSPA-VA) Analyses Technical Basis Document.* B00000000-01717-4301-00010 REV 01. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19981008.0010.	10.5.1.2	N/A - Reference Only	1	Discussion of degradation scenarios	N/A	N/A	N/A	N/A
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1. Document Identifier No./Rev.: CAL-EDC-MD-000007 REV 00	Change: N/A	Title: EQ6 CALCULATIONS FOR CHEMICAL DEGRADATION OF NAVY WASTE PACKAGES

Input Document			4. Input Status	5. Section Used in	6. Input Description	7. TBV/TBD Priority	8. TBVDue To		
2a.	2. Technical Product Input Source Title and Identifier(s) with Version	3. Section					Unqual.	From Uncontrolled Source	Un-Confirmed
5	Wolery, T.J. 1992. *EQ3/6, A Software Package for Geochemical Modeling of Aqueous Systems. Package Overview and Installation Guide (Version 7.0).* UCRL-MA-110662 PT I. Livermore, California: Lawrence Livermore National Laboratory. TIC: 205087.	Entire	N/A – Reference Only	3, 4	Discussion of EQ3/6 software	N/A	N/A	N/A	N/A
6	Daveler, S.A. and Wolery, T.J. 1992. *EQPT, A Data File Preprocessor for the EQ3/6 Software Package. User's Guide, and Related Documentation (Version 7.0).* UCRL-MA-110662 PT II. Livermore, California: Lawrence Livermore National Laboratory. TIC: 205240.	Entire	N/A – Reference Only	3, 4	Discussion of EQ3/6 software	N/A	N/A	N/A	N/A
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DOCUMENT INPUT REFERENCE SYSTEM

1. Document Identifier No./Rev.: CAL-EDC-MD-000007 REV 00		Change: N/A	Title: EQ6 CALCULATIONS FOR CHEMICAL DEGRADATION OF NAVY WASTE PACKAGES						
Input Document			4. Input Status	5. Section Used in	6. Input Description	7. TBV/TBD Priority	8. TBVDue To		
2a.	2. Technical Product Input Source Title and Identifier(s) with Version	3. Section					Unqual.	From Uncontrolled Source	Un-Confirmed
9	Spahiu, K. and Bruno, J. 1995. *A Selected Thermodynamic Database for REE to be Used in HLNW Performance Assessment Exercises.* SKB Technical Report 95-35. Stockholm, Sweden: Swedish Nuclear Fuel and Waste Management Company. TIC: 225493.	Entire	TBV-3748	3, 5	SKB thermodynamic data supplied with EQ3/6 code package; basis for rare-earth data in data0	3	N/A	X	N/A
10	CRWMS M&O 1999. *Electronic Media for EQ6 Calculations for Chemical Waste Packages, CAL-EDC-MD-000007 REV 00.* Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19991116.0353.	Entire	N/A – Reference Only	3, 4. 5	EQ6 database files and geometry calculations	N/A	N/A	N/A	N/A
11	DOE (U.S. Department of Energy) 1998. *Total System Performance Assessment.* Volume 3 of *Viability Assessment of a Repository at Yucca Mountain.* DOE/RW-0508. Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: MOL.19981007.0030.	Fig 3-20 to 3-22, pp 3-34 to 3-37	N/A - Reference Only	3	Discussion of temperature at which initial breach of waste package will occur	N/A	N/A	N/A	N/A
12	CRWMS M&O 1996. *Second Waste Package Probabilistic Criticality Analysis: Generation and Evaluation of Internal Criticality Configurations.* BBA000000-01717-2200-00005 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19960924.0193.	7.3.3 , Att. 6	N/A - Reference Only	3	Basis for assumption of convective circulation and mixing of water inside waste package	N/A	N/A	N/A	N/A

OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT
DOCUMENT INPUT REFERENCE SYSTEM

1. Document Identifier No./Rev.: CAL-EDC-MD-000007 REV 00	Change: N/A	Title: EQ6 CALCULATIONS FOR CHEMICAL DEGRADATION OF NAVY WASTE PACKAGES

Input Document							8. TBVDue To		
2a.	2. Technical Product Input Source Title and Identifier(s) with Version	3. Section	4. Input Status	5. Section Used in	6. Input Description	7. TBV/TBD Priority	Unqual.	From Uncontrolled Source	Un-Confirmed
13	CRWMS M&O 1998. *Software Qualification Report (SQR), Addendum to Existing LLNL Document UCRL-MA-110662 Part IV: Implementation of a Solid-Centered Flow-Through Mode for EQ6 Version 7.2b*. CSCI: UCRL-MA-110662 V 7.2b. SCR: LSCR198. MI: 30084-M04-001 (Addendum only). Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19990920.0169.	Entire	N/A - Reference Only	4	Software Qualification	N/A	N/A	N/A	N/A
14	CRWMS M&O 1998. *EQ3/6 Software Installation and Testing Report for Pentium Based Personal Computers (PCs)*. CSCI: LLYMP9602100. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19980813.0191.	Entire	N/A - Reference Only	4	Documentation of installation and test report for EQ3/6 software	N/A	N/A	N/A	N/A
15	CRWMS M&O 1999. *Waste Package Materials Properties*. BBA000000-01717-0210-00017 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19990407.0172.	5.3	TBV-3749	5	Composition and density of 316L stainless steel	3	N/A	X	N/A
16	CRWMS M&O 1997. *Criticality Evaluation of Degraded Internal Configurations for the PWR AUCF WP Designs*. BBA000000-01717-0200-00056 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19971231.0251.	pp. 11-13	TBV-3750	5	Degradation rate of 316L stainless steel	3	N/A	X	N/A

OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT
DOCUMENT INPUT REFERENCE SYSTEM

1. Document Identifier No./Rev.: CAL-EDC-MD-000007 REV 00		Change: N/A	Title: EQ6 CALCULATIONS FOR CHEMICAL DEGRADATION OF NAVY WASTE PACKAGES						
Input Document			4. Input Status	5. Section Used in	6. Input Description	7. TBV/TBD Priority	8. TBVDue To		
2a.	2. Technical Product Input Source Title and Identifier(s) with Version	3. Section					Unqual.	From Uncontrolled Source	Un-Confirmed
17	Brady, P.V. and Walther, J.V. 1989. "Controls on Silicate Dissolution Rates in Neutral and Basic pH Solutions at 25 °C." *Geochimica et Cosmochimica Acta, 53,* 2823-2830. New York, New York: Pergamon Press. TIC: 235216.	Fig. 2	TBV–3751	5	Quartz dissolution rate at low pH; slope of log(dissolution rate) versus pH at high pH	3	N/A	X	N/A
18	Brady, P.V. and Walther, J.V. 1990. "Kinetics of Quartz Dissolution at Low Temperatures." *Chemical Geology, 82*, 253-264. Amsterdam, Netherlands: Elsevier Science Publishers. TIC: 235349.	Table I and III	N/A – Reference Only	5	Experimental data of quartz dissolution rate versus pH	N/A	N/A	N/A	N/A
19	CRWMS M&O 1998. "Near-Field Geochemical Environment." Chapter 4 of *Total System Performance Assessment-Viability Assessment (TSPA-VA) Analyses Technical Basis Document.* B00000000-01717-4301-00004 REV 01. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19981008.0004.	Fig. 4-27	TBV-3752	5	Carbon dioxide fugacity in water	3	X	N/A	N/A
20	CRWMS M&O 1998. *Complete Draft VA UZ Abstraction/Test Document.* B00000000-01717-2200-00201. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19980428.0202.	Fig 2.3-110, Tables 2.3-49 & -50	TBV-3753	5	Correlation between percolation rate and drip rate	3	X	N/A	N/A
21	CRWMS M&O 1998. *EQ6 Calculations for Chemical Degradation of PWR LEU and PWR MOX Spent Fuel Waste Packages.* BBA000000-01717-0210-00009 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19980701.0483.	5.1.1.3	N/A – Reference Only	5	Justification for drip rates	N/A	N/A	N/A	N/A

OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT DOCUMENT INPUT REFERENCE SYSTEM										
1. Document Identifier No./Rev.: CAL-EDC-MD-000007 REV 00		Change: N/A	Title: EQ6 CALCULATIONS FOR CHEMICAL DEGRADATION OF NAVY WASTE PACKAGES							
Input Document			4. Input Status	5. Section Used in	6. Input Description	7. TBV/TBD Priority	8. TBVDue To			
2a.	2. Technical Product Input Source Title and Identifier(s) with Version	3. Section					Unqual.	From Uncontrolled Source	Un-Confirmed
22	Walker, F.W.; Parrington, J.R.; and Feiner, F. 1989. *Nuclides and Isotopes, Fourteenth Edition: Chart of the Nuclides.* San Jose, California: General Electric Company. TIC: 201637.	List of Elements	N/A - Accepted Data (Fact)	5	Atomic weights	N/A	N/A	N/A	N/A
23	Lide, D.R. and Frederikse, H.P.R., eds. 1997. *CRC Handbook of Chemistry and Physics, 78th edition.* Boca Raton, Florida: CRC Press. TIC: 243741.	p. 1-29	N/A - Accepted Data (Fact)	5	Grams-to-pounds conversion	N/A	N/A	N/A	N/A

Attachment II. Listing of Files on Electronic Media.

This attachment contains the MS-DOS directory for files placed on the electronic media (Ref. 10). The files are of 6 types:

1) Excel files (extension = xls), called out in the text and tables;
2) EQ6 input files (extension = 6i), as discussed in Section 5.3.1, have 8-character names V???????.6i;
3) Tab-delimited text files (extension = txt), with names V???????.elem????.txt. as discussed in Section 5.3.2; these contain total aqueous moles (#.elem_aqu.txt), total moles in minerals, aqueous phase, and remaining special reactants (#.elem_tot.txt), and the total moles in minerals alone (#.elem_min.txt). The #.elem_tot.txt and #.elem_min.txt also have the volume in cm^3 of the minerals and total solids (including special reactants) in the system;
4) FORTRAN source files (extension = for) for the version of EQ6 used in the calculations; and
5) MS-DOS/Win95/Win98 executables (extension = exe) for the version of EQ6 and runeq6 used in the calculations, and the autoexec.bat file that sets up the environment;
6) EQ6 data files used for the calculations, with the text file data0.nuc.R8a, and the binary version data1.nuc.

```
Below are listed the contents of the directories within the
electronic attachment:
The first column is the DOS file name.  The second column is the
size of the file (bytes).
The third and fourth columns are the date and time of the last
update.
The fifth column is the file name.
```

```
Directory of D:\

EQ6_6I~5        <DIR>         11-09-99 12:41p EQ6_6i_txt
EXCELF~7        <DIR>         11-09-99 12:41p excel files
PROGRA~9        <DIR>         11-09-99 12:39p program files

Directory of D:\EQ6_6i_txt

V40S1002 6I         40,225  09-16-99  6:10p V40s1002.6i
V40S1~10 TXT       145,131  09-16-99  5:01p v40s1002.elem_aqu.txt
V40S1~12 TXT       134,434  09-16-99  5:01p v40s1002.elem_min.txt
V40S1~14 TXT       134,447  09-16-99  5:01p v40s1002.elem_tot.txt
V40S1002 TXT       175,779  09-16-99  6:37p V40S1002.TXT
V40S1004 6I         40,075  09-15-99  8:07p V40s1004.6i
V40S1~20 TXT       542,281  09-15-99 10:15p V40s1004.elem_aqu.txt
V40S1~24 TXT       502,256  09-15-99 10:15p V40s1004.elem_min.txt
V40S1~28 TXT       502,269  09-15-99 10:15p V40s1004.elem_tot.txt
V40S1004 TXT       265,829  09-16-99 12:25a V40S1004.TXT
V40T1002 6I         37,611  09-16-99  6:35p v40t1002.6i
V40T1~36 TXT       105,481  09-16-99  7:38p V40t1002.Elem_aqu.txt
V40T1~38 TXT        97,712  09-16-99  7:38p V40t1002.Elem_min.txt
V40T1~40 TXT        97,725  09-16-99  7:38p V40t1002.Elem_tot.txt
V40T1002 TXT       176,916  09-16-99  7:47p V40T1002.TXT
```

V40T1004	6I	40,514	09-16-99	12:36a	v40t1004.6i
V40T1~48	TXT	542,606	09-16-99	2:47a	V40t1004.elem_aqu.txt
V40T1~52	TXT	502,557	09-16-99	2:47a	V40t1004.elem_min.txt
V40T1~54	TXT	502,570	09-16-99	2:47a	V40t1004.elem_tot.txt
V40T1004	TXT	245,503	09-16-99	6:25a	V40T1004.TXT
V40U1004	6I	40,666	09-16-99	6:21a	v40u1004.6i
V40U1~64	TXT	542,606	09-16-99	7:29a	V40u1004.elem_aqu.txt
V40U1~66	TXT	502,557	09-16-99	7:29a	V40u1004.elem_min.txt
V40U1~70	TXT	502,570	09-16-99	7:29a	V40u1004.elem_tot.txt
V40U1004	TXT	245,503	09-16-99	7:36a	V40U1004.TXT
V41S1002	6I	40,075	09-16-99	2:11p	V41s1002.6i
V41S1~78	TXT	140,581	09-16-99	4:42p	v41s1002.elem_aqu.txt
V41S1~82	TXT	130,220	09-16-99	4:42p	v41s1002.elem_min.txt
V41S1~84	TXT	130,233	09-16-99	4:42p	v41s1002.elem_tot.txt
V41S1002	TXT	306,459	09-19-99	11:51a	V41S1002.TXT
V41S1003	6I	40,075	09-16-99	1:22p	V41s1003.6i
V41S1~90	TXT	537,406	09-16-99	2:48p	v41s1003_Elem_aqu.txt
V41S1~94	TXT	497,741	09-16-99	2:48p	v41s1003_Elem_min.txt
V41S1~98	TXT	497,754	09-16-99	2:48p	v41s1003_Elem_tot.txt
V41S1004	6I	40,001	09-15-99	7:07p	V41s1004.6i
V41S~104	TXT	542,281	09-15-99	8:10p	V41s1004.elem_aqu.txt
V41S~108	TXT	502,256	09-15-99	8:10p	V41s1004.elem_min.txt
V41S~110	TXT	502,269	09-15-99	8:10p	V41s1004.elem_tot.txt
V41S1004	TXT	286,139	09-15-99	11:30p	V41S1004.TXT
V41T1002	6I	37,383	09-17-99	7:14a	v41t1002.6i
V41T~118	TXT	104,506	09-17-99	1:50a	v41t1002.Elem_aqu.txt
V41T~122	TXT	96,809	09-17-99	1:50a	v41t1002.Elem_min.txt
V41T~124	TXT	96,822	09-17-99	1:50a	v41t1002.Elem_tot.txt
V41T1002	TXT	204,057	09-17-99	12:50a	V41T1002.TXT
V41T1003	6I	37,306	09-16-99	3:06p	v41t1003.6i
V41T~130	TXT	460,056	09-16-99	4:30p	v41t1003_Elem_aqu.txt
V41T~134	TXT	426,103	09-16-99	4:30p	v41t1003_Elem_min.txt
V41T~138	TXT	426,116	09-16-99	4:30p	v41t1003_Elem_tot.txt
V41T1004	6I	40,366	09-15-99	11:37p	v41t1004.6i
V41T~142	TXT	542,606	09-16-99	7:42a	V41t1004.elem_aqu.txt
V41T~146	TXT	502,557	09-16-99	7:42a	V41t1004.elem_min.txt
V41T~150	TXT	502,570	09-16-99	7:42a	V41t1004.elem_tot.txt
V41T1004	TXT	133,049	09-16-99	8:08a	V41T1004.TXT
V41U1002	6I	36,039	09-17-99	7:14a	v41u1002.6i
V41U~158	TXT	109,706	09-17-99	9:33a	V41u1002.Elem_aqu.txt
V41U~160	TXT	101,625	09-17-99	9:33a	V41u1002.Elem_min.txt
V41U~162	TXT	101,638	09-17-99	9:33a	V41u1002.Elem_tot.txt
V41U1002	TXT	187,355	09-17-99	10:10a	V41U1002.TXT
V41U1003	6I	35,859	09-16-99	4:42p	v41u1003.6i
V41U~170	TXT	242,306	09-16-99	5:14p	v41u1003_Elem_aqu.txt
V41U~172	TXT	224,433	09-16-99	5:14p	v41u1003_Elem_min.txt
V41U~174	TXT	224,446	09-16-99	5:14p	v41u1003_Elem_tot.txt
V41U1004	6I	40,600	09-16-99	2:05a	v41u1004.6i
V41U~180	TXT	650,831	09-16-99	2:56a	V41u1004.elem_aqu.txt
V41U~184	TXT	602,790	09-16-99	2:56a	V41u1004.elem_min.txt
V41U~188	TXT	602,803	09-16-99	2:56a	V41u1004.elem_tot.txt
V41U1004	TXT	159,569	09-16-99	7:56a	V41U1004.TXT
V41V1004	6I	40,752	09-16-99	1:16p	v41v1004.6i
V41V~196	TXT	650,831	09-16-99	2:26p	v41v1004.Elem_aqu.txt
V41V~200	TXT	602,790	09-16-99	2:26p	v41v1004.Elem_min.txt
V41V~204	TXT	602,803	09-16-99	2:26p	v41v1004.Elem_tot.txt
V41V1004	TXT	122,950	09-16-99	2:31p	V41V1004.TXT

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V41W1004 6I          40,904  09-16-99  2:39p v41w1004.6i
V41W~212 TXT        651,156  09-16-99  3:51p v41w1004.Elem_aqu.txt
V41W~216 TXT        603,091  09-16-99  3:51p v41w1004.Elem_min.txt
V41W~220 TXT        603,104  09-16-99  3:51p v41w1004.Elem_tot.txt
V41W1004 TXT        135,135  09-16-99  5:37p V41W1004.TXT
V41X1004 6I          36,247  09-16-99  5:40p v41x1004.6i
V41X~228 TXT        651,156  09-16-99  6:50p v41x1004.Elem_aqu.txt
V41X~232 TXT        603,091  09-16-99  6:50p v41x1004.Elem_min.txt
V41X~236 TXT        603,104  09-16-99  6:50p v41x1004.Elem_tot.txt
V41X1004 TXT        122,918  09-16-99  6:54p V41X1004.TXT
V41Y1004 6I          36,399  09-16-99  6:57p v41y1004.6i
V41Y~244 TXT        650,831  09-16-99  8:09p V41y1004.Elem_aqu.txt
V41Y~248 TXT        602,790  09-16-99  8:09p V41y1004.Elem_min.txt
V41Y~252 TXT        602,803  09-16-99  8:09p V41y1004.Elem_tot.txt
V41Y1004 TXT        122,918  09-16-99  8:13p V41Y1004.TXT
V49S1002 6I          39,853  09-16-99  2:10p V49s1002.6i
V49S~260 TXT        134,081  09-16-99  3:32p v49s1002.elem_aqu.txt
V49S~262 TXT        124,200  09-16-99  3:32p v49s1002.elem_min.txt
V49S~264 TXT        124,213  09-16-99  3:32p v49s1002.elem_tot.txt
V49S1002 TXT        286,139  09-16-99  8:36p V49S1002.TXT

Directory of D:\excel files

DENSIT~6 XLS        122,368  11-09-99 12:29p density_navy4.xls
NAVYAQ~8 XLS        104,448  10-19-99  4:11p Navy aqueous all elements.xls
NAVY4    XLS        209,408  11-09-99 12:27p navy4.xls
QUARTZ   XLS         21,504  11-09-99  9:56a quartz.xls

Directory of D:\program files

AUTOEXEC BAT            624  09-12-99 12:20p AUTOEXEC.BAT
CONFIG   SYS            463  06-17-98  1:04p CONFIG.SYS
DATA0~10 R8A      2,299,784  11-25-98  3:15p data0.nuc.R8a
DATA1    NUC        791,620  04-22-99  3:22p data1.nuc
DATA1    R8A        791,200  08-18-99  7:20a data1.R8a
DATA1    WEG        792,936  01-19-99 10:34a data1.weg
EQ3NR    EXE      2,169,333  08-18-95  4:47p Eq3nr.exe
EQ6      EXE      1,056,485  12-11-98 12:27p eq6.exe
EQ6NEW   FOR      1,322,545  12-11-98  9:50a eq6new.for
EQLIBNEW FOR        492,613  07-01-98  5:34p eqlibnew.for
EQPT     EXE      2,337,701  08-18-95  4:47p EQPT.EXE
EXTERNAL FNT          9,900  06-29-95  7:27p EXTERNAL.FNT
README   TXT            505  09-12-99 12:51p Readme.txt
RUNEQ3   EXE        388,005  08-18-95  4:46p Runeq3.exe
RUNEQ6   EXE        392,181  08-18-95  4:46p RUNEQ6.EXE
RUNEQPT  EXE        334,517  08-18-95  4:46p RUNEQPT.EXE
```