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EQ6 Calculations for Chemical Degradation of TRIGA Codisposal Waste Packages

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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 Training, Research, Isotopes, General Atomics (TRIGA) reactor (Ref. 1). The TRIGA SNF has been considered for disposal at the potential Yucca Mountain site. Because of the high content of fissile material in the fuel, the waste package design requires special consideration of the amount and placement of neutron absorbers, and of the possible loss of absorbers and fuel materials over geologic time. For some waste packages, the corrosion-allowance material and the corrosion-resistant material may breach (Ref. 3), allowing the influx of water. Water in the waste package moderates neutrons, increasing the likelihood of a criticality event within the waste package; and the water may, in time, gradually leach the fissile components and neutron absorbers out of the waste package, further affecting the neutronics of the system.

This study presents calculations of the long-term geochemical behavior of waste packages containing TRIGA SNF assemblies, and high-level waste (HLW) glass canisters arranged according to the codisposal concept (Ref. 4). The specific study objectives were to determine:

- The extent to which criticality control material, suggested for this waste package design, will remain in the waste package after corrosion/dissolution of the initial waste package configuration (such that it can be effective in preventing criticality)

- The extent to which fissile 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 nominal chemical composition for the criticality evaluations of the waste package design and to suggest the range of parametric variations for additional evaluations.

For this purpose, the chemical compositions (and subsequent criticality evaluations) for some of the simulations are represented for time periods up to 300,000 years. This time frame is shorter than the one-million-year time horizon recently recommended by the National Academy of Sciences to the Environmental Protection Agency for performance assessment related to a nuclear repository (Ref. 5). However, it is important to note that after 100,000 years most of the materials of interest (fissile and absorber materials) will have either been removed from the waste package, reached a steady state, or been transmuted.

The calculation included elements with high neutron-absorption cross sections, notably gadolinium (Gd), as well as the fissile materials. 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 document has been prepared according to Procedure AP-3.12Q/Rev. 0/ICN 0, Calculations, and is subject to the Quality Assurance Requirements and Description (QARD) Document (DOE/RW-0333P, Revision 08) requirements.

2. METHOD

The method used for this calculation involves the following steps:

- Use of basic EQ3/6 (software package, Section 4.1) capability for tracing the progress of reactions with evolution of the chemistry, which includes the estimation of the concentrations remaining in solution and the composition of the precipitated solids. (EQ3 is used to determine a starting fluid composition for 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 "solid-centered flow-through" mode (SCFT) in EQ6; in this mode, an increment of aqueous "feed" solution is added continuously to the waste package system, and a like volume of the existing solution is removed, simulating a continuously stirred tank reactor. This mode is discussed in Section 4.2.

- Determination of fissile material concentrations in solution as a function of time (from the output of EQ6 simulated reaction times up to 300,000 years).

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

- Determination of concentrations of neutron absorbers, such as Gd, in solution as a function of time (from the output of EQ6 over times up to or somewhat greater than 3.0×10^5 years).

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

- Use of 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 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. 6) for ~$3x10^5$ 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 millions of 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 corrosion allowance barrier and corrosion resistant barrier until after that perturbed period. Therefore, the early perturbation is not relevant to the calculations reported in this document.

3.3 The density of J-13 well water is 1.0 g/cm^3. The basis for this assumption is that for dilute solutions, the density differs extremely little from 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 concrete 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. 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. Interaction of water in the fractures with any undegraded concrete between fractures would be minimal owing to the slow rate of diffusion through the concrete matrix compared to rate of flow through fractures.

3.5 The composition of the aqueous solution that will enter the waste package will not be altered by contact with the corrosion allowance material. The basis for this assumption is that the water is expected to move rapidly enough through openings in the waste package materials 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. 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.

3.6 The corrosion-resistant inner barrier 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 corrosion resistant material 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 from the waste package.

3.7 The existing database supplied with the EQ3/6 computer package is sufficiently accurate for the purposes of this calculation. The basis for this assumption 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 (Refs. 7, 8, 9, and 10). These databases are periodically updated and/or new databases added, such as one including extensive data on the lanthanides (Ref. 11). 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. 12). Nevertheless, the quality of data needs to be verified in the future.

3.8 The calculations can satisfactorily be modeled 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 $\geq$ 50 °C (Ref. 13), at times > 25,000 years, the waste package temperatures are likely to be closer to 25 °C.

3.9 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. In general, this assumption is conservative since it provides the greatest acid production, which in turn enhances gadolinium solubility, when gadolinium solubility is controlled by gadolinium carbonates.

3.10 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 and hence on the solubility of uranium, gadolinium, and other elements.

3.11 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 of fissile material inside the waste package.

3.12 The corrosion rates will not be significantly enhanced by microbial induced corrosion due to lack of organic nutrients available to them. The basis for this assumption is that the bacteria are expected to act as catalysts, and are not expected to significantly change the types of solid formed in the waste package.

3.13 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 Ref. 14.

3.14 The reported alkalinity in analyses of J-13 well water corresponds to bicarbonate (HCO_3^-) alkalinity. The basis for this assumption is that contributors to alkalinity in J-13 well 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 well water are 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 in (Ref. 6).

3.15 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.

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

3.17 A number of minor assumptions have been made about the geometry of the TRIGA codisposal waste package. These assumptions are outlined and referenced in the spreadsheet TRIGA_common_items.xls (Ref. 12) and are also discussed in Section 5.1. The basis for this assumption is that the assumptions about waste package geometry are always intended to obtain the greatest accuracy in the representation, and where inadequate information is available to choose among competing models of waste package geometry, the choice that appears to lead to greatest conservatism is always chosen.

3.18 Neutron absorber tubes made of Alloy 22 with 8 atom% gadolinium will be fabricated, and they will be as corrosion resistant as stainless steel. The basis for this assumption is that it is conservative because the corrosion rate of Alloy 22 is much lower than stainless steel.

3.19 The graphite and the zirconium rod in the TRIGA SNF rods are considered inert. The basis for this assumption is that these materials have a low chemical reactivity at low temperatures.

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. 7). Since 1978, 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 models water/rock interaction or fluid mixing in either a reaction progress mode (independent of time) 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 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 make thermodynamic calculations. This is supported by a set of algorithms, which create and optimize starting values. EQ6 uses an ordinary differential equation (ODE) 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 (Refs. 7, 8, 9, and 10).

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. This mode was added to EQ6 per Software Change Request LSCR198 and the Software Qualification Report for Media Number 30084-M04-001 (Ref. 35).

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, was approved for QA work by LLNL. An installation and test report (Ref. 15) was written and submitted to Software Configuration Management (SCM), and the proper installation was verified before the runs described in this calculation were made. The implementation of the SCFT mode is covered by Software Change Request LSCR198 and the Software Qualification Report for Media Number 30084-M04-001. The SCFT addendum was installed on three of the central processing units (CPUs) identified in block 16 of the SCR, and the installation and test reports were filed and returned to SCM before the calculations were run. In this study EQ3/6 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 programs have not been used outside the range of parameters for which they have been verified, except for those years presented in Table 4-1 The results from the EQ3/6 "B-dot" activity model (used in this study) have been verified only for conditions when the ionic strength is less than one. High ionic strengths tend to occur at high HLW glass degradation rates and low J-13 well water drip rates.

Table 4-1. Years for which EQ3/6 Results Are to Be Verified

Case	Run Name	Years When Ionic Strength > 1
6	t!1a1211	281 - 8,058
8	t!1a1222	265 - 1,134
10	t!1a1231	277 - 8,024
12	t!1a2111	1,059 - 6,914
16	t!1a2131	753 - 6,920
18	t!1a2211	98 - 8,628
20	t!1a2222	166 - 1,469
21	t!1a2231	98 - 8,632

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 Pentium series (including "Pentium II") personal computers (PCs). The EQ3/6 package has been verified by its present custodian, LLNL. The source codes were obtained from SCM in accordance with the OCRWM procedure AP-SI.1Q. The code was installed on Pentium PCs according to an M&O-approved Installation and Test procedure (Ref. 15).

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. 12). Spreadsheet TRIGA_common_items.xls contains seven different worksheets that convert various data values into a form suitable for input to EQ6. Table 4-2 lists each worksheet and the calculations performed. Excel spreadsheet density_triga.xls manipulates data from EQ6 output files for presentation in the results tables in Section 5. Table 4-3 lists the calculations performed in spreadsheet density_triga.xls.

The volume and area of the DOE SNF Canister and all its contents were calculated using the software routine eqsetup.c, version 1. A listing of the code and instructions for running the program is provided in Attachment II. A change history is not provided because this is the first version of the routine. The program was written in ANSI C and compiled under Microsoft C++, version 6.0. Besides calculating volumes and areas, the program computes moles of all materials described in the input file "data.in" and constructs an input file for EQ6. Besides "data.in", three files are necessary to run the routine: "template.in," "ratefacs.in," and "atwts.in." These files are provided in Attachment II. The output file "junk.out" provides the volume, area, and mole calculation results. Another file, named as indicated in the "data.in" file, is in the appropriate format for input to EQ6. The accuracy of the volume and area calculations were checked by hand and the results are provided in Attachment II. Also included in Attachment II is the input

data file (triga.txt) that was used to generate the volume and area calculations for the TRIGA SNF and the output file (trigajunk.txt) that contains the "junk.out" results from eqsetup. A test input file (test.txt) and output file (testjunk.txt) that contain shapes that were not included in the TRIGA SNF file are provided in Attachment II. These test files can be used on other CPUs to verify the initial use.

Table 4-2. Calculations Performed in Excel Spreadsheet TRIGA_common_items.xls

Worksheet Name	Calculation Performed	Example Formula (if applicable)
Compositions	Converts weight percent to moles	moles=weight percent/molecular weight
Compositions	For Alloy 22, groups moles of V, Co, and W with other elements since they are weakly represented in EQ3/6 "com" database	moles Fe= moles Fe+ moles V + moles Co
Compositions	Adds 8 atom% Gd to moles of Alloy 22	
Compositions	Calculates density of Alloy 22 with 8 atom% Gd	density Alloy 22 with 8% Gd= (mass alloy with Gd)/((mass Alloy 22 without Gd/density Alloy 22)+(mass Gd/density Gd))
Compositions	Converts weight percent to moles for fuel and combines all isotopes of U	mole U=(mass U-238)/(molecular weight U-238)+(mass U-235)/(molecular weight U-235)
Compositions	From the initial HLW glass composition, decays Pu-238 to U-234 and Pu-241 to Np-237, and removes Cs-133, Cs-135, Th, Zn, and Ag	
Compositions	Calculates average molecular weight of Pu and U based on composition in HLW glass and fuel	average U molecular weight = (mass of all U isotopes)/((mass U234/MW U234) + (mass U235/MW U235)+(mass U236/MW U236) + (mass U238/MW U238))
Vol&Area common items	Calculates the void volume in the waste package	void volume= (volume inside waste package) - (volume glass canisters) - (outer web) - (DOE SNF canister)
Bottom of EQ6 input file	Provides bottom of EQ6 input file	
Atomic weights	Lists atomic weights used in calculations	
Geometries from eqsetup	Sums the volumes and areas calculated by eqsetup	
Rates	Converts rates in g/(m^2·d) to mol/(cm^2·s) assuming 100 g/mol for all materials	mol/(cm^2·s)=g/(m^2·d)/[(100 g/mol)·(s/d)] · (0.0001 m^2/cm^2)
Rates	Converts rates in microns/year to mol/(cm^2·s) assuming 100 g/mol for all materials	mol/(cm^2·s)=microns/year·(0.0001 cm/micron) ·density/[(100 g/mol)·(s/y)]
Densities & Moles_rct	Calculates normalized moles from the volume for all reactants	normalized moles=volume·density/(100 g/mol)/(void volume)
Densities & Moles_rct	Calculates normalized area for all reactants	normalized moles=area/(void volume)
Densities & Moles_rct	Calculates molar volume for each reactant	molar volume=(100 g/mol)/density

Table 4-3. Calculations Performed in Excel Spreadsheet Density_triga.xls

Worksheet Name	Calculation Performed	Example Formula (if applicable)
Aqueous	Creates tables from EQ6 output files *.elem_aqu.txt	
Composition	Converts normalized moles of elements in corrosion product from EQ6 output files *.elem_min.txt to mole percent	mole percent O= (normalized moles O)/(total normalized moles)·100
Tables	Creates tables from worksheets "composition" and "density"	
Density	Calculates density of corrosion product from data in EQ6 output file *.elem_min.txt	density=SUM[(moles of each element) · (molecular weight)]/(volume of corrosion product)

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 TRIGA SNF codisposal waste packages. These quantities are recalculated to the form required for entry into EQ6. For example, weight percentages of elements or component oxides are converted into mole fractions of elements; degradation rates in micrometers/year are converted into moles per square centimeter per second, etc. Spreadsheets (Ref. 12) provide details of these calculations, and the general procedure is also described in detail in Ref. 16. 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 5.1.1.3). The EQ6 output provides the results of simulation of the chemical degradation of the waste package or components thereof. In some calculations the degradation of the waste package is divided into phases, e.g., degradation of HLW glass before breach of the DOE SNF canister and exposure of the fuel assemblies and basket materials 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.

In all tables from this document, the number of digits reported does not necessarly 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.

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 TRIGA SNF codisposal waste packages 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 TRIGA_common_items.xls (Table 4-1) and the software routine eqsetup.c (Attachment II). Additional details of the description may be found in Ref. 1 and Ref. 32, and the references cited therein.

Material nomenclature used throughout this document includes SB-575 N06022, hereafter referred to as Alloy 22; SA-240 S31603, hereafter referred to as 316L; UNS N06625 (SA-240 S30403), hereafter referred to as 304L; and SA-516 ,hereafter referred to as A516.

5.1.1.1 Physical and Chemical Form of TRIGA Waste Packages

It is convenient to consider the TRIGA waste package as several structural components, specifically

- The outer shell, consisting of the corrosion-allowance material and the corrosion resistant material
- The "outer web," a carbon steel (A516) structure designed to hold the HLW glass pour canisters (GPCs) in place
- The GPCs (304L), which contain the solidified HLW glass
- The DOE SNF canister (sometimes called the "18-inch canister"), consisting of the outer shell (316L), the basket (316L), and impact plates (A516)
- Neutron absorber tubes made of Alloy 22 with 8 atom% gadolinium placed within the basket structure and surrounding 45 out of the 111 SNF rods within the DOE SNF canister
- The SNF rods composed of a homogeneous mixture of uranium and zirconium-hydride (Ref. 1 and Ref. 32), graphite reflectors, zirconium rods, and cladding (304L).

The codisposal waste package basket structure (outer web) serves two purposes: it centers and holds in place the DOE SNF canister; and it separates the GPCs and prevents them from transmitting undue stress to the SNF canister in the event of a fall (tip-over) of the entire waste package. At the center of the outer web is a thick (3.175 cm) cylindrical support tube, also constructed of A516. In a breach scenario, the outer web will be exposed to water and corrosion before the rest of the waste package. The outer web is expected to degrade within a few hundred years, based on the surface area and corrosion rates of A516 used in this calculation, or within a few thousand years, if corrosion is inhibited due to the buildup of corrosion products or lack of available oxygen. The resulting transformation of steel's iron, the web's most abundant element, into hematite (Fe_2O_3) can decrease the void space in the waste package by ~13%, and the transformation to goethite (FeOOH) can decrease the void space by ~22% (Ref. 2 and Ref. 28). The differences are due to larger molar volume of goethite and the addition of more mass per atom of iron in goethite compared to hematite. Thus the void space can be significantly reduced, soon after breach of the waste package, by the alteration of the outer web.

The DOE SNF canister fits inside the central support tube of the outer web. The canister is composed primarily of 316L with two internal, thick impact plates of carbon steel (approximated as A516 in the calculations). The basket structure inside the canister will be constructed of 37 stainless steel (316L) tubes welded together at the top and bottom with the bottom tubes welded to a steel base plate. Three such basket assemblies will be stacked in the DOE SNF canister to

provide a total of 111 SNF elements per waste package. Ref. 32 contains a description and a figure of the waste package.

Table 5-1 provides a summary of the compositions of the principal steel alloys used in the calculations. The compositions of the carbon and stainless steel come from Ref. 27. The composition of the Alloy 22 with 8 mole% Gd was calculated in spreadsheet TRIGA_common_items.xls starting with the composition of Alloy 22 in Ref. 27.

Table 5-1. Steel Compositions

	A516 Carbon Steel		304L Stainless Steel		316L Stainless Steel		Alloy 22 with 8 mole% Gadolinium	
Element	wt%	Atom Frac.	wt%	Atom Frac.	wt%	Atom Frac.	wt%	Atom Frac.
C	0.28	0.0138	0.03	0.0014	0.03	0.0014	0.012	0.0007
Mn	1.045	0.0105	2.00	0.0199	2.00	0.0201	0.41	0.0051
P	0.035	0.0006	0.045	0.0008	0.045	0.0008	0.017	0.0004
S	0.035	0.0006	0.03	0.0005	0.03	0.0005	0.017	0.0004
Si	0.29	0.0057	0.75	0.0146	1.00	0.0197	0.066	0.0016
Cr			19.00	0.1997	17.00	0.1806	17.59	0.2301
Ni			10.00	0.0931	12.00	0.1129	45.33	0.5253
Mo					2.50	0.0144	12.47	0.0884
N			0.10	0.0039	0.10	0.0039		
Fe	98.315	0.9698	68.045	0.6660	65.295	0.6457	5.59	0.0681
Gd							18.50	0.08
Total	100.00	1.0000	100.00	1.0000	100.00	1.0000	100.00	1.0000

Table 5-2 gives the atom fraction of the HLW glass used in the calculations. The original HLW glass composition (Ref. 17) was adjusted in worksheet "Compositions" in TRIGA_common_items.xls to remove elements that do not have sufficient data in the EQ3/6 thermodynamic database. The actual HLW glass composition used in the GPCs may vary significantly from these values, since the sources of the HLW glass and melting processes are not currently fixed. For example, compositions proposed for Savannah River HLW glass vary by a factor of ~6 in U_3O_8 content, from 0.53 to 3.16 wt% (Ref. 18). The silica and alkali contents (Na, Li, and K) of the HLW glass have perhaps the most significant bearing on EQ6 calculations. The amount of silica in the HLW glass strongly controls the amount of clay that forms in the waste package, and the silica activity controls the presence of insoluble uranium phases such as soddyite [$(UO_2)_2SiO_4 \cdot 2H_2O$]. The alkali content can induce pH to rise in the early stages of the EQ6 run, as HLW glass degrades. The Si and alkali contents in Table 5-2 are typical for the proposed, DOE glasses (Ref. 17).

Table 5-3 provides the fuel composition of the TRIGA fuel rod type used in the calculation. These are the stainless steel clad Fuel Life Improvement Program (TRIGA-SS FLIP) type rods. The uranium in these fuel rods is enriched to 70 wt% U-235-the highest enrichment of the TRIGA fuel elements (Ref. 1). The calculations used the composition of unirradiated fuel, which is conservative, since most fission products have significant neutron absorption cross sections, and the unirradiated fuel has a higher fissile content than partially spent fuel. The zirconium rods and the graphite reflectors within the fuel elements were assumed to be inert and were not included in the calculations.

Table 5-2. HLW Glass Composition

Element	Weight Percent [a]	Atom Fraction	Element	Weight Percent	Atom Fraction
O	44.93	5.73E-01	Si	21.96	1.60E-01
U	1.88	1.61E-03	Ti	0.60	2.55E-03
Np	0.0010	8.23E-07	B	3.22	6.08E-02
Pu	0.015	1.27E-05	Li	1.48	4.35E-02
Ba	0.11	1.69E-04	F	0.032	3.43E-04
Al	2.34	1.77E-02	Cu	0.15	4.92E-04
S	0.13	8.27E-04	Fe	7.42	2.71E-02
Ca	0.66	3.38E-03	K	3.00	1.57E-02
P	0.014	9.29E-05	Mg	0.83	6.95E-03
Cr	0.083	3.25E-04	Mn	1.56	5.81E-03
Ni	0.74	2.56E-03	Na	8.66	7.68E-02
Pb	0.061	6.02E-05	Cl	0.12	6.69E-04
			Total	100.00	1.00

[a] The HLW glass composition in Ref. 17 was altered as follows: ^{238}Pu decayed to ^{234}U; ^{241}Pu decayed to ^{237}Np; Ag, Cs, Zn, and Th removed because of low quantity, chemical insignificance, and/or lack of reliable thermodynamic data; normalized to 100 percent.

Table 5-3. TRIGA Fuel Composition

Element	Weight Percent	Atom Fraction
U-238	2.57	0.0042
U-235	5.98	0.0098
Zr	89.86	0.3792
H	1.59	0.6068
Total	100.00	1.0000

Table 5-4 provides molar volume, density, initial moles, reaction rate, and surface area for all of the materials in the TRIGA codisposal waste package that were considered in the calculation. The molar volume is the molecular weight divided by the density. The density for all special

reactants are from Ref. 27, except for HLW glass, which came from Ref. 30. The density of Alloy 22 with 8 atom% Gd was calculated in spreadsheet TRIGA_common_items.xls, with the density of Gd taken from Ref. 31. For each EQ6 special reactant, the molecular weight is assumed to be 100 g/mol, which makes the calculation less complicated and has no effect on the results. The initial moles and surface area of the HLW glass and the outer web were calculated in spreadsheet fftf_short.xls (Ref. 12). Spreadsheet fftf_short.xls originated from spreadsheet fftf_fuel_hws.xls (Ref. 28), with changes made to reflect the shorter waste package used in the TRIGA codisposal waste package. These changes are detailed in spreadsheet Changes_to_fftf.xls (Ref. 12). The initial moles and the surface area in Table 5-4 are normalized values based on one liter of water, rather than the total initial void volume of 4,102 liters. The details of the void volume calculation are provided in the excel spreadsheet TRIGA_common_items.xls (Ref. 12).

Table 5-4. Properties of Materials in TRIGA Codisposal Waste Package

		V	ρ	m_i	*rk*			*sk*
					Reaction Rate[b] (mol/cm^2·s)			
Reactant	Type of Reactant	Molar Volume (cm^3/mol)	Density (g/cm^3)	Initial Moles[a]	1	2	3	Surface Area[c] (cm^2)
HLW Glass	Glass	35.09	2.85	21.82	1.16E-15	3.47E-13	Not Applicable (N/A)	1755
Fuel	Fuel	16.82	5.95	0.6204	1.88E-14	1.88E-13	1.88E-12	13.86
304L Cladding	Steel	12.59	7.94	0.0731	2.52E-14	2.52E-13	N/A	36.23
304L Cladding Fittings	Steel	12.59	7.94	0.1443	2.52E-14	2.52E-13	N/A	3.564
304L Glass Pour Canister	Steel	12.59	7.94	5.494	2.52E-14	2.52E-13	N/A	141.5
Outer Web_516	Steel	12.74	7.85	9.269	8.71E-12	2.49E-11	N/A	120.0
A516 Impact Plates	Steel	12.74	7.85	0.2110	8.71E-12	2.49E-11	N/A	1.615
316L DOE SNF Canister	Steel	12.53	7.98	0.8592	2.53E-14	2.53E-13	N/A	22.67
316L Basket Inside DOE SNF Canister	Steel	12.53	7.98	1.876	2.53E-14	2.53E-13	N/A	85.01
Absorber Tubes Alloy22 Gd	Steel	11.72	8.53	0.1185	2.70E-14	2.70E-13	N/A	27.78

[a] m_i equals initial mass (g) divided by 100 g/mol divided by 4102 liters void volume in waste package.
[b] *rk* equals the reaction rate (g/cm^2·s) divided by 100 g/mol.
A516 carbon steel: Ref. 19; Stainless steel: Ref. 29.
[c] *sk* equals total surface area divided by 4102 liters void volume in waste package.

The degradation rates in Table 5-4 are average or high degradation rates (indicated by "1" or "2") for all the reactants except fuel, for which a very high degradation rate (indicated by "3") is provided. The true reaction rate is obtained by multiplying ***rk*** by ***sk*** to get mol/s. Inspection of the rates shows that for a comparable surface area, the A516 carbon steel is expected to degrade much more rapidly than the stainless steels (316L and 304L). Rates for HLW glass degradation were taken from Ref. 19, and normalized in spreadsheet TRIGA_common_items.xls (Ref. 12). The high glass degradation rate corresponds to pH 9 at 70 °C, to pH 3 at 50 °C, and pH 11 at 50 °C. The average HLW glass degradation corresponds to pH 8 at 25 °C.

The degradation rate for the uranium zirconium hydride SNF is similar to stainless steel (Ref. 20) and therefore was set equal to the rate of stainless steel, corrected for the different density. A very high degradation rate for the SNF corresponding to 10 times the highest stainless steel rate (reaction rate=3 in Table 5-4) was also used in the calculation. The degradation rate for the Alloy 22 with 8% Gd was also assumed to be the same as stainless steel (Assumption 3.18).

5.1.1.2 Chemical Composition of J-13 Well Water

It was assumed that the water composition entering the WP would be the same as for water from well J-13 (Assumption 3.2). This water has been analyzed repeatedly over a span of at least two decades (Ref. 6). Table 5-5 contains the EQ3NR input file constraints for J-13 well water composition based on Ref. 6 and based on the assumptions of carbon dioxide fugacity found in Ref. 21. Table 5-5 is in the format required by EQ3NR. For an explanation of terms used in the input file see Ref. 9. Table 5-6 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.

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

It is assumed (Assumption 3.15) 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 (Ref. 22). 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 Ref. 16.

For the present study, the range of allowed drip rates was extended to include an upper value of 0.5 m^3/year and a lower value of 0.0015 m^3/year. The upper value corresponds to the 95 percentile upper limit for a percolation rate of 40 mm/year (Ref. 22), and the lower value is simply 0.1 times the mean value for the percolation rate of 8 mm/year. These extreme values were used, because prior studies (Ref. 23) suggested that when waste forms are codisposed with HLW glass, the greatest chance of Gd removal occurs when: (1) initial high drip rates cause HLW glass leaching and removal of alkali; and (2) subsequent low drip rates allow acid to build from steel degradation.

5.1.1.4 Densities and Molecular Weights of Solids

For input to criticality calculations, one must convert moles of solids to solid volumes. The densities and molar volumes of the solids are found in Ref. 12.

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

Species[a]	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
Ba++		1.000E-16	molality[b]
CrO_4--		1.000E-16	molality[b]
Cu++		1.000E-16	molality[b]
Gd+++		1.000E-16	molality[b]
MoO_4--		1.000E-16	molality[b]
Ni++		1.000E-16	molality[b]
Np++++		1.000E-16	molality[b]
Pb++		1.000E-16	molality[b]
Pu++++		1.000E-16	molality[b]
TcO_4-		1.000E-16	molality[b]
$Ti(OH)_4$(aq)		1.000E-16	molality[b]
UO_2++		1.000E-16	molality[b]
$Zr(OH)_2$++		1.000E-16	molality[b]

[a] Refs. 6 and 21. For definition of terms, see Ref. 9.
[b] The concentration of 1.0E-16 is added as a trace to ensure numerical stability

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

Element	Mole/kg	Element	Mole/kg
O	5.55E+01	Mg	8.27E-05
Al	2.55E-08	Mn	3.05E-16
B	1.24E-05	Mo	1.00E-16
Ba	1.00E-16	N	1.42E-04
Ca	3.24E-04	Na	1.99E-03
Cl	2.01E-04	Ni	1.00E-16
Cr	1.00E-16	Np	1.00E-16
Cu	1.00E-16	Pb	1.00E-16
F	1.15E-04	Pu	1.00E-16
Fe	3.60E-12	S	1.92E-04
Gd	1.00E-16	Si	1.02E-03
H	1.11E+02	Tc	1.00E-16
C	2.09E-03	Ti	1.00E-16
P	1.26E-06	U	1.00E-16
K	1.29E-04	Zr	1.00E-16
Li	6.92E-06		
SOURCE: Refs. 6 and 21			

5.1.1.5 Atomic Weights

Atomic weights were taken from Ref. 24 and Ref. 25 and are listed in Ref. 12 (spreadsheet TRIGA_common_items.xls, sheet "Atom Wts").

5.2 DATA CONVERSION

The data presented in Section 5.1 are largely not in a form suitable for entry into EQ3/6. The transformation to EQ3/6 format consists largely in converting mass fractions to mole fractions; normalizing surface areas, volumes, and moles to 1 liter reactive water in the system; and converting rates from units of micrometers per year to $mol/cm^2 \cdot s$. Most of these conversions are straightforward and are performed in the spreadsheets, which are included in the electronic media for this document (Ref. 12). Ref. 16 describes the conversion process in detail.

5.3 EQ6 CALCULATIONS AND SCENARIOS REPRESENTED

The rationale for selection of scenarios in EQ6 simulations is to provide conservative assessments of solubility and transport of fissile materials (i.e., U compounds) and neutron absorbers species (i.e., Gd) in the waste package. $GdPO_4$ exhibits solubility minimum at pH ranges of 6 to 7, and has enhanced solubility at very low and high pH (Ref. 2). In addition, uranium carbonates complexes at high pH and could cause an increase in solubility of uranium. The *Disposal Criticality Analysis Methodology Topical Report* defined the internal and external

degradation scenarios for disposal criticality analysis (Ref. 26). The internal degradation configurations are based on the assumption that groundwater drips on the upper surface of the waste package and penetrates it. Groundwater accumulates inside the waste package, which could dissolve and flush either neutron absorber or the SNF from the waste package. Following is a summary of three groups of degradation configurations from Ref. 26:

- Waste package internals degrade faster than waste forms.
- Waste package internals degrade at the same rate as the waste form.
- Waste package internals degrade slower than the waste forms.

The waste package internals include all components within the waste package excluding the outer shell and excluding the SNF. The above configurations set the framework in which EQ6 scenarios could be developed. The scenarios are based on sequence of chemical reactions as function of time and could be divided into two general categories: single-stage cases and multiple-stage cases.

Single-Stage Cases–In these calculations all waste package internals, including SNF come in contact with groundwater simultaneously. These cases correspond to an extreme in which the stainless steel cladding is fully breached immediately, thereby exposing all the SNF as soon as the waste package corrosion barriers are breached. These cases simulate the highest concentrations of the radionuclides in solution, and could provide the highest loss estimate of fissile and neutron absorber materials. These cases were designed to maximize exposure of the Gd in the absorber tubes to high pH, and to stress the enhanced solubility of $GdPO_4$ under alkaline conditions.

Multiple-Stage Cases–The first stage of these EQ6 calculations start with the breach of the waste package allowing groundwater to come in contact with waste package internals outside of the DOE SNF canister. During this stage, the DOE SNF canister remains intact. The second stage starts with the breach of the DOE SNF canister and interaction of groundwater with material inside the canister, including waste forms and undegraded reactants left from stage 1. These cases were designed to produce the lowest possible pH during the SNF degradation, by first exposing the HLW glass to infiltrating water to remove alkalinity, prior to exposure of the SNF and absorber tubes in the second stage. Thus, these cases were intended to test the enhanced Gd solubility at low pH.

In total, 27 cases of single and multiple-stage EQ6 simulations, with different degradation rates of steel, SNF, and HLW glass and water fluxes through the waste package were run. Table 5-7 summarizes the total fraction of Gd and U remaining at the end of the EQ6 runs. Cases 1 through 23 are single-stage runs and Cases 24 through 27 are multiple-stage runs. The complete output tables (aqueous, mineral, and total moles) for all the cases are included in the electronic media, as tab-delimited text files. A summary of the files included in the electronic media is given in Attachment III.

Table 5-7. Summary of All Cases

Case	Run Name[b]	Fraction Remaining at the End of the Run		Iron Oxide Formed	Time (years)
		U	Gd		
1[a]	t!1a1111	0.067	0.895	hematite	317,210
2	t@1a1111	0.000	0.893	hematite	317,210
3	t!1a1113	1.000	0.791	hematite	39,187
4[a]	t!1a1122	0.062	0.511	hematite	316,890
5	t!1a1133	1.000	0.819	hematite	39,342
6	t!1a1211	0.137	1.000	hematite	317,290
7	t!1a1213	0.109	0.998	hematite	40,404
8[a]	t!1a1222	0.000	0.999	hematite	316,920
9	t@1a1222	0.000	0.999	hematite	316,920
10	t!1a1231	0.044	1.000	hematite	317,290
11	t!1a1233	0.000	0.998	hematite	39,459
12	t!1a2111	0.067	0.984	hematite	317,210
13[a]	t!1a2113	0.999	0.466	hematite	38,590
14[a]	t@1a2113	0.992	0.463	hematite	38,759
15	t!1a2122	0.062	0.827	hematite	316,890
16	t!1a2131	0.067	0.985	hematite	317,210
17	t!1a2133	0.999	0.593	hematite	38,478
18	t!1a2211	0.000	1.000	hematite	317,090
19	t!1a2213	0.110	0.999	hematite	39,040
20	t!1a2222	0.088	0.998	hematite	316,920
21	t!1a2231	0.000	1.000	hematite	317,090
22	t!1a2233	0.000	0.999	hematite	39,475
23	t!1c1131	0.068	0.927	hematite	317,110
24	t02g1203/t!1g1021	0.997[c]	1.000	goethite	317,410
25	t02g2203/t!1g2021	0.998[c]	1.000	goethite	31,7430
26	t02g2204/t!1g2022	0.973[c]	0.999	goethite	316,910
27[a]	t02a2204/t!1a2022	0.980[c]	0.999	hematite	316,910

[a] For these cases, the elemental composition in the aqueous solution and in the corrosion products are presented in Tables 5-8 through 5-21.

[b] For the runs with "@" as the second character, the UO_2 in the HLW glass is replaced with TiO_2 so that the uranium results would represent only the uranium in the fuel. Case 23 required three separate runs, with file names t!1a1131, t!1b1131, and t!1c1131.

[c] The fraction of U represents the U in the fuel only. All of the U in the HLW glass has been flushed from the waste package by the beginning of the second stage. The first stage of the multiple-stage runs ends at 4,000 years.

The EQ6 input file corresponding to each run is included in the electronic media accompanying this calculation (Ref. 12). Each input file has the form of #.6i, where the "#" represents the name of the run (e.g., t!1a1111.6i is the EQ6 input file name for Case 1). EQ6 (Section 4.2) generates four different types of text output files. Ref. 12 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 electronic media (Ref. 12) includes Excel files listing total molar inventory, including total volume of all minerals (corrosion products) and minerals plus remaining special reactants (uncorroded waste package components) as functions of time.

The run name, in column 2 of Table 5-7, provides most of the important run conditions. The 5th character of the file name indicates the reaction rate of steel (indicated as "1" or "2", with the values listed in Table 5-4). The 6th digit indicates the reaction rate of the HLW glass (indicated as "1" or "2", with the values listed in Table 5-4, or "0" if the HLW glass has been consumed and the run is in stage 2 of a multiple-stage run. The 7th digit indicates the reaction rate of the fuel or fissile material (indicated as "1," "2," or "3" with the values listed in Table 5-4, or "0" if the run is in stage 1 of a two-stage run and no fuel is involved in the reaction. The last character in the file name indicates the choice of J-13 well water flush rate, with 1, 2, 3, and 4 corresponding to 0.0015 m^3/year, 0.015 m^3/year, 0.15 m^3/year, and 0.5 m^3/year, respectively.

Columns 3 and 4 of Table 5-7 contain the fraction of U and Gd remaining at the end of each run. The fifth column of Table 5-7 indicates the iron oxide that was formed. Hematite and goethite are major iron oxide minerals observed to form in rust, though the EQ6 thermodynamic database indicates hematite is thermodynamically more stable, and hematite's stability (relative to goethite) increases with temperature. To see the effect, if any, of goethite formation on the results, hematite formation was suppressed for Cases 24, 25, and 26.

For each run the total moles of unreacted or intact material at any time can be calculated from the EQ6 output files by subtracting the moles in the aqueous phase (file #.elem_aqu.txt) and in the corrosion products (file #.elem_min.txt) from the total moles in the system (file #.elem_tot.txt). The total mass of unreacted material at any time can be calculated from the equation:

$$M_t = 4.102 * V * \rho * (m_i - rk * sk * (t - t_0))$$

where M_t is the mass remaining (kg) at time = t, 4.102 kg/g is a correction factor which converts from a calculation based on one liter to a calculation based on the total void of a waste package, V is the molar volume (cm^3/mole), ρ is the density (g/cm^3) of the reactant, m_i is the initial number of moles, rk is the reaction rate (mol/cm^2·s), sk is the surface area (cm^2), t is the time (s), and t_0 is the starting time for the reactions, which is equal to zero for all reactants for all single stage runs. The values of t_0 for double-stage runs are 4,000 years ($1.26x10^{11}$ s). The rest of the values in the equation are in Table 5-4. As an example, Figure 5-1 shows a plot of M_t versus t for three of the reactants in Case t!1a2113. The line for the degradation of the absorber tubes

with Gd appears near the origin because all of the material has degraded by 500 years at the high degradation rate set for steel for the run.

For six runs (marked by superscript a in Table 5-7), additional results are presented in Tables 5-8 through 5-21. For each of these runs, concentrations of each element in the aqueous phase at selected times are presented in Tables 5-8 through 5-14. The mole percent of each element, the total mass, and the density of the corrosion products are presented at selected times in Tables 5-15 through 5-21. The selected times were based on (1) low pH, (2) high Gd in solution, (3) close to 10,000 years, (4) close to 30,000 years, (5) close to 100,000 years, and (6) end of run.

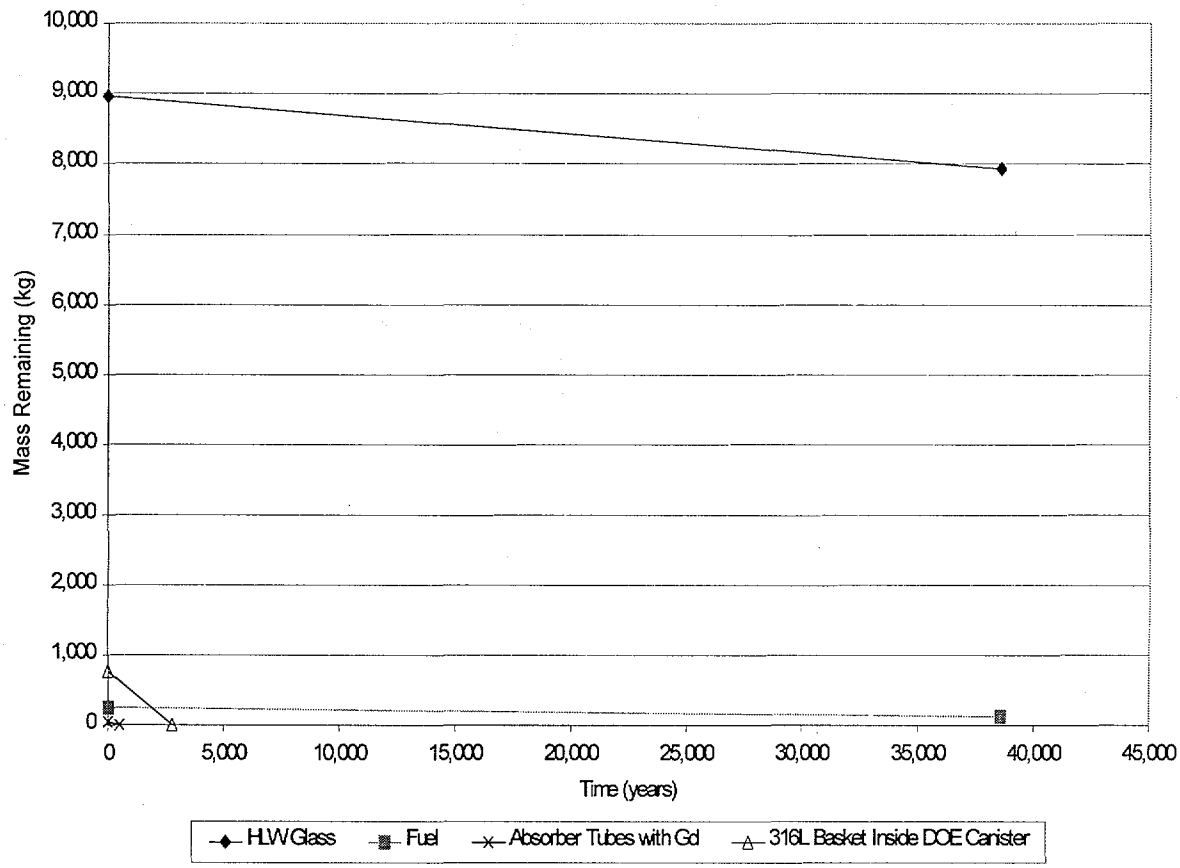

Figure 5-1. Unreacted Mass Remaining vs. Time for Case t!1a2113

Table 5-8. Concentration (moles/liter) in Aqueous Phase and pH at Selected Times for Case 1 (t!1a1111)

	Year					
Element	**281**	**4,997**	**8,448**	**32,301**	**96,173**	**317,210**
Al	7.74E-05	1.08E-05	1.37E-04	1.14E-05	7.33E-08	7.18E-08
B	5.12E-03	4.41E-02	5.01E-02	5.23E-02	5.23E-02	5.23E-02
Ba	9.26E-08	2.11E-07	1.90E-07	1.22E-07	6.34E-11	6.33E-11
Ca	6.13E-04	2.06E-03	2.29E-03	1.27E-03	8.03E-06	8.03E-06
Cl	2.58E-04	6.87E-04	7.53E-04	7.77E-04	7.77E-04	7.77E-04
Cr	2.37E-02	1.88E-01	1.91E-01	1.41E-01	2.79E-04	2.79E-04
Cu	4.13E-05	3.57E-04	4.05E-04	4.23E-04	4.94E-06	4.95E-06
F	1.44E-04	3.43E-04	6.28E-04	1.93E-04	3.83E-04	3.83E-04
Fe	4.88E-07	1.15E-11	1.08E-11	7.14E-12	1.89E-12	1.89E-12
Gd	4.10E-08	2.10E-03	2.29E-09	6.03E-10	1.34E-07	1.34E-07
C	3.34E-05	3.97E-05	3.98E-05	4.51E-05	5.72E-02	5.72E-02
P	2.33E-03	6.94E-12	3.47E-06	3.92E-06	2.25E-06	2.25E-06
K	1.44E-03	7.78E-03	9.28E-03	9.98E-03	4.54E-03	4.61E-03
Li	3.66E-03	3.16E-02	3.59E-02	3.74E-02	3.70E-02	3.75E-02
Mg	6.67E-04	3.14E-03	3.95E-03	4.26E-03	8.72E-06	8.72E-06
Mn	1.42E-06	7.22E-11	6.18E-11	2.34E-11	1.10E-15	1.10E-15
Mo	1.42E-03	1.23E-02	7.77E-03	2.09E-03	7.06E-12	1.00E-16
N	5.80E-04	3.59E-03	3.94E-03	2.96E-03	1.42E-04	1.42E-04
Na	8.45E-03	5.51E-02	6.29E-02	6.59E-02	6.27E-02	6.21E-02
Ni	1.64E-02	6.11E-02	5.29E-02	2.05E-02	1.60E-09	1.60E-09
Np	6.91E-08	5.97E-07	6.77E-07	7.07E-07	7.07E-07	7.07E-07
Pb	7.87E-08	3.73E-10	3.36E-10	2.13E-10	2.73E-11	2.73E-11
Pu	1.07E-06	2.96E-11	8.65E-11	5.32E-11	1.21E-07	1.21E-07
S	1.01E-02	2.97E-03	1.83E-03	1.27E-03	9.02E-04	9.02E-04
Si	1.87E-04	5.66E-05	5.56E-05	5.33E-05	5.83E-05	5.83E-05
Ti	2.26E-10	2.24E-10	2.24E-10	2.24E-10	2.24E-10	2.24E-10
U	3.03E-05	4.32E-08	1.10E-07	5.21E-08	1.39E-03	1.39E-03
Zr	6.79E-10	6.70E-10	6.70E-10	6.71E-10	6.73E-10	6.73E-10
pH	3.35	5.55	5.58	5.77	9.33	9.33

Table 5-9. Concentration (moles/liter) in Aqueous Phase and pH at Selected Times for Case 4 (t!1a1122)

	Year					
Element	**281**	**4,999**	**12,674**	**31,870**	**103,830**	**316,890**
Al	6.88E-05	1.72E-12	2.02E-06	6.09E-07	1.13E-07	1.16E-07
B	3.38E-03	5.24E-03	5.24E-03	5.24E-03	5.24E-03	5.24E-03
Ba	1.05E-07	1.66E-07	1.27E-07	9.88E-08	4.03E-10	3.84E-10
Ca	5.38E-04	3.85E-04	3.06E-04	3.25E-04	2.37E-05	2.28E-05
Cl	2.38E-04	2.59E-04	2.59E-04	2.59E-04	2.59E-04	2.59E-04
Cr	1.57E-02	2.14E-02	1.92E-02	1.31E-02	2.79E-05	2.79E-05
Cu	2.73E-05	4.23E-05	4.23E-05	4.23E-05	4.63E-07	4.69E-07
F	1.38E-04	1.44E-04	1.17E-04	1.24E-04	1.41E-04	1.41E-04
Fe	4.18E-07	6.04E-12	4.62E-12	3.20E-12	1.31E-12	1.31E-12
Gd	2.20E-08	6.70E-04	4.00E-11	4.74E-11	3.57E-08	3.62E-08
C	3.36E-05	4.73E-05	4.94E-05	5.91E-05	1.02E-02	1.02E-02
P	2.55E-03	2.61E-12	7.12E-06	2.09E-06	6.15E-08	6.46E-08
K	9.98E-04	1.22E-03	1.26E-03	1.29E-03	1.01E-03	1.03E-03
Li	2.42E-03	3.75E-03	3.75E-03	3.75E-03	3.75E-03	3.75E-03
Mg	4.72E-04	3.60E-04	4.05E-04	4.25E-04	3.27E-05	3.13E-05
Mn	9.80E-07	1.30E-11	6.51E-12	2.24E-12	2.91E-16	2.95E-16
Mo	9.38E-04	1.45E-03	6.12E-04	1.29E-04	1.00E-16	1.00E-16
N	4.31E-04	5.34E-04	5.34E-04	4.02E-04	1.42E-04	1.42E-04
Na	6.25E-03	8.43E-03	8.46E-03	8.48E-03	8.28E-03	8.27E-03
Ni	1.08E-02	6.09E-03	5.47E-03	1.93E-03	1.47E-08	1.39E-08
Np	4.56E-08	7.07E-08	7.07E-08	7.07E-08	7.07E-08	7.07E-08
Pb	7.74E-08	2.79E-10	2.12E-10	1.65E-10	2.37E-10	2.25E-10
Pu	7.06E-07	1.17E-11	6.64E-11	7.39E-12	4.60E-11	4.94E-11
S	6.70E-03	3.17E-04	3.14E-04	2.97E-04	2.63E-04	2.63E-04
Si	1.87E-04	1.87E-04	5.76E-05	5.48E-05	3.76E-05	3.76E-05
Ti	2.26E-10	2.26E-10	2.26E-10	2.26E-10	2.26E-10	2.26E-10
U	2.85E-05	9.77E-09	4.99E-08	2.11E-08	2.04E-04	1.39E-04
Zr	6.79E-10	6.77E-10	6.77E-10	6.77E-10	6.77E-10	6.77E-10
pH	3.40	5.79	5.93	6.14	8.72	8.73

Table 5-10. Concentration (moles/liter) in Aqueous Phase and pH at Selected Times for Case 8 (t!1a1222)

	Year					
Element	**1,135**	**11,117**	**26,670**	**30,610**	**103,780**	**316,920**
Al	1.85E-09	3.15E-08	1.58E-05	6.44E-06	2.48E-08	2.47E-08
B	2.13E-01	1.25E-05	1.24E-05	1.24E-05	1.24E-05	1.24E-05
Ba	2.25E-11	8.83E-09	1.73E-07	1.70E-07	5.81E-09	5.88E-09
Ca	4.51E-06	3.89E-04	1.65E-04	1.16E-04	8.94E-05	2.18E-04
Cl	1.72E-02	2.01E-04	2.01E-04	2.01E-04	2.01E-04	2.01E-04
Cr	3.21E-02	1.92E-02	1.92E-02	1.31E-02	1.00E-16	1.00E-16
Cu	3.36E-04	3.37E-07	2.50E-04	1.66E-04	3.26E-07	3.26E-07
F	8.22E-03	8.77E-05	2.15E-04	1.61E-04	1.14E-04	1.14E-04
Fe	4.31E-12	1.20E-12	6.05E-12	5.19E-12	1.19E-12	1.19E-12
Gd	1.13E-06	1.77E-08	2.08E-11	1.08E-11	2.72E-09	1.18E-08
C	1.21E+00	2.66E-03	4.53E-05	4.71E-05	2.03E-03	2.02E-03
P	1.68E-04	5.43E-09	3.42E-05	3.91E-05	1.18E-08	2.80E-09
K	1.65E-01	9.11E-03	1.31E-03	1.02E-03	4.08E-04	1.74E-04
Li	9.91E-01	6.92E-06	6.92E-06	6.92E-06	6.92E-06	6.92E-06
Mg	3.45E-06	5.57E-04	5.26E-04	3.39E-04	1.28E-04	1.20E-04
Mn	7.49E-15	4.17E-16	1.25E-11	8.25E-12	3.13E-16	3.15E-16
Mo	1.43E-03	6.12E-04	6.12E-04	1.29E-04	1.00E-16	1.00E-16
N	5.84E-04	5.34E-04	5.34E-04	4.02E-04	1.42E-04	1.42E-04
Na	1.19E+00	3.23E-02	1.00E-03	1.28E-03	2.00E-03	1.99E-03
Ni	1.24E-10	3.28E-07	1.03E-02	6.79E-03	2.12E-07	2.15E-07
Np	2.09E-05	1.00E-16	1.00E-16	1.00E-16	1.00E-16	1.00E-16
Pb	2.61E-12	5.82E-11	2.89E-10	2.83E-10	2.02E-09	3.61E-09
Pu	3.23E-04	1.43E-12	2.50E-08	3.04E-08	4.92E-13	4.92E-13
S	2.15E-02	2.43E-04	2.43E-04	2.26E-04	1.92E-04	1.92E-04
Si	1.09E-03	3.50E-05	5.99E-05	5.99E-05	3.93E-05	3.90E-05
Ti	1.81E-10	2.26E-10	2.26E-10	2.26E-10	2.26E-10	2.26E-10
U	4.18E-02	1.01E-09	1.00E-16	1.00E-16	1.00E-16	1.00E-16
Zr	5.41E-10	6.76E-10	6.78E-10	6.78E-10	6.78E-10	6.78E-10
pH	10.00	8.13	5.79	5.86	8.08	8.08

Table 5-11. Concentration (moles/liter) in Aqueous Phase and pH at Selected Times for Case 13 (tl1a2113)

	Year				
Element	**98**	**500**	**10,151**	**30,211**	**38,590**
Al	4.07E-08	5.89E-12	6.61E-16	6.61E-16	6.61E-16
B	5.22E-04	5.35E-04	5.35E-04	5.35E-04	5.35E-04
Ba	2.70E-07	2.22E-07	3.05E-09	3.05E-09	3.05E-09
Ca	1.77E-04	3.16E-04	2.08E-04	2.08E-04	2.08E-04
Cl	2.07E-04	2.07E-04	2.07E-04	2.07E-04	2.07E-04
Cr	2.37E-02	2.14E-02	2.79E-06	2.79E-06	2.79E-06
Cu	4.12E-06	4.23E-06	3.25E-07	3.25E-07	3.25E-07
F	8.90E-05	1.18E-04	1.17E-04	1.17E-04	1.17E-04
Fe	3.42E-10	7.74E-12	1.20E-12	1.20E-12	1.20E-12
Gd	2.68E-11	6.77E-04	3.35E-08	3.35E-08	3.35E-08
C	3.51E-05	4.34E-05	2.87E-03	2.87E-03	2.87E-03
P	2.16E-03	3.49E-12	2.25E-09	2.25E-09	2.25E-09
K	2.50E-04	2.54E-04	2.52E-04	2.52E-04	2.52E-04
Li	3.72E-04	3.81E-04	3.81E-04	3.81E-04	3.81E-04
Mg	1.09E-04	1.12E-04	5.07E-05	5.07E-05	5.07E-05
Mn	7.55E-10	2.35E-11	2.33E-16	2.33E-16	2.33E-16
Mo	1.42E-03	1.45E-03	1.00E-16	1.00E-16	1.00E-16
N	5.79E-04	5.34E-04	1.42E-04	1.42E-04	1.42E-04
Na	2.63E-03	2.64E-03	2.64E-03	2.64E-03	2.64E-03
Ni	1.62E-02	1.10E-02	5.05E-08	5.05E-08	5.05E-08
Np	6.89E-09	7.07E-09	7.07E-09	7.07E-09	7.07E-09
Pb	1.10E-09	3.73E-10	1.87E-09	1.87E-09	1.87E-09
Pu	1.07E-07	1.59E-11	7.93E-13	7.93E-13	7.93E-13
S	3.04E-03	2.53E-04	1.99E-04	1.99E-04	1.99E-04
Si	1.87E-04	1.87E-04	1.91E-04	1.91E-04	1.91E-04
Ti	2.26E-10	2.26E-10	2.26E-10	2.26E-10	2.26E-10
U	3.18E-06	1.15E-08	1.13E-07	1.13E-07	1.13E-07
Zr	6.77E-10	6.77E-10	6.78E-10	6.78E-10	6.78E-10
pH	4.94	5.66	8.23	8.23	8.23

Table 5-12. Concentration (moles/liter) in Aqueous Phase and pH at Selected Times for Case 14 (t@1a2113)

	Year				
Element	**98**	**500**	**10,151**	**30,211**	**38,759**
Al	4.12E-08	5.89E-12	6.61E-16	6.61E-16	6.61E-16
B	5.22E-04	5.35E-04	5.35E-04	5.35E-04	5.35E-04
Ba	2.70E-07	2.22E-07	3.05E-09	3.05E-09	3.05E-09
Ca	1.77E-04	3.16E-04	2.08E-04	2.08E-04	2.08E-04
Cl	2.07E-04	2.07E-04	2.07E-04	2.07E-04	2.07E-04
Cr	2.37E-02	2.14E-02	2.79E-06	2.79E-06	2.79E-06
Cu	4.12E-06	4.23E-06	3.25E-07	3.25E-07	3.25E-07
F	8.90E-05	1.18E-04	1.17E-04	1.17E-04	1.17E-04
Fe	3.46E-10	7.74E-12	1.20E-12	1.20E-12	1.20E-12
Gd	2.68E-11	6.77E-04	3.35E-08	3.35E-08	3.35E-08
C	3.51E-05	4.34E-05	2.87E-03	2.87E-03	2.87E-03
P	2.17E-03	3.49E-12	2.25E-09	2.25E-09	2.25E-09
K	2.50E-04	2.54E-04	2.52E-04	2.52E-04	2.52E-04
Li	3.72E-04	3.81E-04	3.81E-04	3.81E-04	3.81E-04
Mg	1.09E-04	1.12E-04	5.07E-05	5.07E-05	5.07E-05
Mn	7.60E-10	2.35E-11	2.33E-16	2.33E-16	2.33E-16
Mo	1.42E-03	1.45E-03	1.00E-16	1.00E-16	1.00E-16
N	5.79E-04	5.34E-04	1.42E-04	1.42E-04	1.42E-04
Na	2.63E-03	2.64E-03	2.64E-03	2.64E-03	2.64E-03
Ni	1.62E-02	1.10E-02	5.05E-08	5.05E-08	5.05E-08
Np	6.89E-09	7.07E-09	7.07E-09	7.07E-09	7.07E-09
Pb	1.10E-09	3.73E-10	1.87E-09	1.87E-09	1.87E-09
Pu	1.07E-07	1.59E-11	7.93E-13	7.93E-13	7.93E-13
S	3.04E-03	2.53E-04	1.99E-04	1.99E-04	1.99E-04
Si	1.87E-04	1.87E-04	1.91E-04	1.91E-04	1.91E-04
Ti	2.26E-10	2.26E-10	2.26E-10	2.26E-10	2.26E-10
U	3.19E-06	1.15E-08	1.13E-07	1.13E-07	1.13E-07
Zr	6.77E-10	6.77E-10	6.78E-10	6.78E-10	6.78E-10
pH	4.94	5.66	8.23	8.23	8.23

Table 5-13. Concentration (moles/liter) in Aqueous Phase and pH at Selected Times for Case 17 (t!1a2133)

	Year				
Element	98	500	10,137	30,201	38,478
Al	1.71E-08	5.90E-12	6.61E-16	6.61E-16	6.61E-16
B	5.22E-04	5.35E-04	5.35E-04	5.35E-04	5.35E-04
Ba	2.67E-07	2.22E-07	3.05E-09	3.05E-09	3.05E-09
Ca	1.74E-04	3.18E-04	2.08E-04	2.08E-04	2.08E-04
Cl	2.07E-04	2.07E-04	2.07E-04	2.07E-04	2.07E-04
Cr	2.37E-02	2.14E-02	2.79E-06	2.79E-06	2.79E-06
Cu	4.12E-06	4.23E-06	3.25E-07	3.25E-07	3.25E-07
F	8.84E-05	1.18E-04	1.17E-04	1.17E-04	1.17E-04
Fe	1.61E-10	7.75E-12	1.20E-12	1.20E-12	1.20E-12
Gd	2.41E-11	6.77E-04	3.35E-08	3.35E-08	3.35E-08
C	3.55E-05	4.34E-05	2.87E-03	2.87E-03	2.87E-03
P	1.44E-03	3.49E-12	2.25E-09	2.25E-09	2.25E-09
K	2.50E-04	2.54E-04	2.52E-04	2.52E-04	2.52E-04
Li	3.72E-04	3.81E-04	3.81E-04	3.81E-04	3.81E-04
Mg	1.09E-04	1.11E-04	5.07E-05	5.07E-05	5.07E-05
Mn	4.84E-10	2.35E-11	2.33E-16	2.33E-16	2.33E-16
Mo	1.42E-03	1.45E-03	1.00E-16	1.00E-16	1.00E-16
N	5.79E-04	5.34E-04	1.42E-04	1.42E-04	1.42E-04
Na	2.63E-03	2.64E-03	2.64E-03	2.64E-03	2.64E-03
Ni	1.59E-02	1.10E-02	5.05E-08	5.05E-08	5.05E-08
Np	6.89E-09	7.07E-09	7.07E-09	7.07E-09	7.07E-09
Pb	1.08E-09	3.73E-10	1.87E-09	1.87E-09	1.87E-09
Pu	1.07E-07	1.59E-11	7.93E-13	7.93E-13	7.93E-13
S	3.04E-03	2.53E-04	1.99E-04	1.99E-04	1.99E-04
Si	1.87E-04	1.87E-04	1.91E-04	1.91E-04	1.91E-04
Ti	2.26E-10	2.26E-10	2.26E-10	2.26E-10	2.26E-10
U	2.57E-06	1.15E-08	1.13E-07	1.13E-07	1.13E-07
Zr	6.78E-10	6.78E-10	6.78E-10	6.78E-10	6.78E-10
pH	5.04	5.66	8.23	8.23	8.23

Table 5-14. Concentration (moles/liter) in Aqueous Phase and pH at Selected Times for Case 27 (t02a2204/t!1a2022)

	Year					
Element	**4,000[a]**	**4,681**	**10,044**	**31,855**	**101,590**	**316,910**
Al	4.91E-07	2.78E-04	2.02E-09	2.44E-08	2.42E-08	2.47E-08
B	1.24E-05	1.24E-05	1.24E-05	1.24E-05	1.24E-05	1.24E-05
Ba	2.10E-07	2.85E-07	1.15E-06	6.10E-09	6.12E-09	5.90E-09
Ca	1.58E-04	1.41E-03	8.07E-05	1.59E-04	1.68E-04	2.47E-04
Cl	2.01E-04	2.01E-04	2.01E-04	1.86E-04	2.06E-04	2.01E-04
Cr	3.61E-03	1.90E-01	2.31E-04	8.83E-05	1.00E-16	1.00E-16
Cu	3.60E-05	2.51E-03	6.05E-06	3.26E-07	3.26E-07	3.26E-07
F	1.11E-04	9.51E-04	5.34E-13	1.29E-04	1.10E-04	1.14E-04
Fe	3.05E-12	1.54E-11	1.55E-12	1.19E-12	1.19E-12	1.19E-12
Gd	1.00E-16	9.48E-10	1.09E-12	6.85E-09	7.07E-09	1.44E-08
C	5.81E-05	3.69E-05	1.37E-04	2.00E-03	1.98E-03	2.02E-03
P	4.45E-06	1.86E-05	5.85E-04	4.81E-09	4.44E-09	2.30E-09
K	3.76E-04	9.08E-04	2.33E-04	2.83E-04	1.91E-04	1.35E-04
Li	6.92E-06	6.92E-06	6.92E-06	6.92E-06	6.92E-06	6.92E-06
Mg	2.83E-04	1.79E-03	1.18E-04	2.05E-04	1.48E-04	1.14E-04
Mn	1.75E-12	1.28E-10	9.80E-14	3.23E-16	3.23E-16	3.16E-16
Mo	1.93E-05	9.28E-03	1.67E-08	1.00E-16	1.00E-16	1.00E-16
N	2.13E-04	3.84E-03	1.43E-04	1.42E-04	1.42E-04	1.42E-04
Na	1.54E-03	3.12E-03	1.10E-03	1.98E-03	1.98E-03	1.99E-03
Ni	1.48E-03	1.04E-01	6.70E-05	2.24E-07	2.24E-07	2.16E-07
Pb	3.47E-10	5.04E-10	1.20E-11	3.75E-09	3.76E-09	3.62E-09
Pu	1.16E-11	4.01E-08	4.07E-05	4.88E-13	4.81E-13	4.91E-13
S	2.01E-04	3.94E-04	1.54E-04	1.92E-04	1.92E-04	1.92E-04
Si	5.66E-05	6.25E-05	5.11E-05	3.87E-05	3.91E-05	3.90E-05
Ti	2.26E-10	2.25E-10	2.26E-10	2.26E-10	2.26E-10	2.26E-10
U	1.00E-16	2.93E-07	6.11E-07	4.02E-07	3.82E-07	4.08E-07
Zr	1.00E-16	6.74E-10	6.78E-10	6.78E-10	6.78E-10	6.78E-10
pH	6.15	5.43	6.80	8.07	8.07	8.08

[a] This is the year that run t02a2204 ended and run t!1a2022 began.

Table 5-15. Element Composition in Corrosion Products (mole%) and Density at Selected Times for Case 1 (t!1a1111)

	Year					
Element	**281**	**4,997**	**8,448**	**32,301**	**96,173**	**317,210**
O	6.01E+01	6.00E+01	6.00E+01	6.00E+01	6.00E+01	5.97E+01
Al	3.48E-03	5.80E-02	9.15E-02	2.46E-01	5.49E-01	1.15E+00
Ba	3.48E-05	5.52E-04	8.73E-04	2.34E-03	5.23E-03	1.09E-02
Ca	0.00E+00	5.36E-03	7.10E-03	2.88E-02	8.99E-02	2.27E-01
Cl	0.00E+00	0.00E+00	0.00E+00	6.73E-14	1.30E-15	2.26E-18
Cr	1.23E-05	7.49E-04	1.19E-03	3.18E-03	8.61E-17	1.76E-19
Cu	0.00E+00	0.00E+00	0.00E+00	6.04E-14	8.27E-03	2.72E-02
F	0.00E+00	4.61E-04	1.01E-08	3.26E-03	4.17E-03	4.03E-03
Fe	3.91E+01	3.77E+01	3.70E+01	3.36E+01	2.84E+01	1.92E+01
Gd	1.84E-03	2.39E-02	2.44E-02	1.71E-02	1.28E-02	8.12E-03
H	4.66E-02	4.16E-01	5.84E-01	1.33E+00	2.32E+00	5.06E+00
C	1.36E-13	1.94E-14	1.60E-13	3.21E-13	1.10E-01	3.27E-01
P	1.92E-02	2.38E-02	2.44E-02	2.69E-02	2.53E-02	2.02E-02
K	0.00E+00	1.66E-02	2.48E-02	6.27E-02	2.41E-01	6.25E-01
Li	0.00E+00	0.00E+00	0.00E+00	9.27E-13	9.24E-02	5.38E-02
Mg	0.00E+00	9.49E-03	1.34E-02	3.24E-02	1.42E-01	4.08E-01
Mn	4.27E-01	4.80E-01	5.11E-01	6.42E-01	6.82E-01	6.95E-01
N	0.00E+00	1.81E-18	0.00E+00	7.61E-13	2.78E-19	3.53E-20
Na	0.00E+00	1.17E-02	1.67E-02	4.06E-02	2.01E-01	4.38E-01
Ni	0.00E+00	3.05E-01	4.19E-01	9.32E-01	1.06E+00	7.91E-01
Np	0.00E+00	8.19E-21	0.00E+00	3.99E-14	0.00E+00	0.00E+00
Pb	1.23E-05	1.98E-04	3.13E-04	8.39E-04	1.87E-03	3.91E-03
Pu	0.00E+00	2.91E-05	5.42E-05	1.69E-04	3.88E-04	8.15E-04
S	3.48E-05	4.53E-18	2.54E-18	1.20E-11	8.40E-14	1.55E-16
Si	2.68E-01	8.02E-01	1.13E+00	2.63E+00	5.35E+00	1.07E+01
Ti	5.30E-04	8.37E-03	1.32E-02	3.55E-02	7.92E-02	1.66E-01
U	4.57E-04	8.41E-03	1.33E-02	3.57E-02	0.00E+00	0.00E+00
Zr	5.37E-03	8.48E-02	1.34E-01	3.60E-01	6.28E-01	3.98E-01
Total (%)	100	100	100	100	100	100
Total (kg)	5540	6183	6575	9147	11594	16114
Density (g/cm^3)	5.2627	5.2009	5.1667	5.0101	4.6570	3.9830

Table 5-16. Element Composition in Corrosion Products (mole%) and Density at Selected Times for Case 4 (t!1a1122)

	Year					
Element	**281**	**4,999**	**12,674**	**31,870**	**103,830**	**316,890**
O	6.01E+01	6.02E+01	6.02E+01	6.01E+01	5.99E+01	5.96E+01
Al	3.40E-03	5.65E-02	1.24E-01	2.39E-01	5.70E-01	1.11E+00
Ba	3.44E-05	5.33E-04	1.17E-03	2.26E-03	5.41E-03	1.05E-02
Ca	0.00E+00	8.95E-03	2.19E-02	4.61E-02	1.68E-01	3.97E-01
Cr	1.22E-05	7.26E-04	1.59E-03	3.08E-03	2.99E-16	1.44E-17
Cu	0.00E+00	2.74E-15	2.35E-16	0.00E+00	8.39E-03	2.58E-02
F	0.00E+00	9.84E-13	1.25E-03	3.41E-03	4.33E-03	4.26E-03
Fe	3.90E+01	3.68E+01	3.51E+01	3.30E+01	2.74E+01	1.86E+01
Gd	1.84E-03	1.42E-02	1.26E-02	9.67E-03	7.06E-03	4.47E-03
H	4.41E-02	4.42E-01	8.08E-01	1.38E+00	3.09E+00	5.92E+00
C	1.29E-13	0.00E+00	0.00E+00	0.00E+00	1.73E-01	4.79E-01
P	1.39E-02	1.42E-02	1.63E-02	1.99E-02	2.00E-02	1.72E-02
K	0.00E+00	9.30E-03	1.88E-02	3.41E-02	1.55E-01	3.14E-01
Mg	0.00E+00	1.16E-02	2.40E-02	4.40E-02	1.76E-01	4.29E-01
Mn	4.27E-01	4.68E-01	5.27E-01	6.29E-01	6.70E-01	6.71E-01
N	0.00E+00	3.14E-14	1.07E-15	0.00E+00	1.90E-17	8.69E-19
Na	0.00E+00	6.14E-03	1.20E-02	2.13E-02	1.19E-01	2.35E-01
Ni	0.00E+00	3.08E-01	5.08E-01	8.53E-01	9.55E-01	7.16E-01
Pb	1.22E-05	1.93E-04	4.21E-04	8.15E-04	1.94E-03	3.77E-03
Pu	0.00E+00	2.92E-05	7.91E-05	1.65E-04	4.05E-04	7.94E-04
S	3.44E-05	1.30E-12	3.29E-14	0.00E+00	4.00E-14	1.97E-15
Si	2.70E-01	8.10E-01	1.50E+00	2.70E+00	5.85E+00	1.09E+01
Ti	5.30E-04	8.17E-03	1.79E-02	3.46E-02	8.22E-02	1.60E-01
U	2.19E-03	3.56E-02	5.08E-02	5.22E-02	3.73E-02	0.00E+00
Zr	5.36E-02	8.28E-01	1.07E+00	8.26E-01	6.04E-01	3.84E-01
Total (%)	100	100	100	100	100	100
Total (kg)	5551	6385	7335	9311	11865	16381
Density (g/cm^3)	5.2624	5.2106	5.1405	5.0090	4.6039	3.9594

Table 5-17. Element Composition in Corrosion Products (mole%) and Density at Selected Times for Case 8 (t!1a1222)

	Year					
Element	**1,135**	**11,117**	**26,670**	**30,610**	**103,780**	**316,920**
O	5.34E+01	5.95E+01	5.97E+01	5.97E+01	5.97E+01	5.98E+01
Al	1.01E+00	1.36E+00	1.29E+00	1.27E+00	1.20E+00	1.18E+00
B	2.89E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Ba	9.61E-03	1.30E-02	1.23E-02	1.21E-02	1.14E-02	1.12E-02
Ca	1.94E-01	2.67E-01	1.32E-01	1.33E-01	1.67E-01	2.45E-01
Cl	1.85E-18	4.47E-18	1.10E-15	7.63E-16	8.18E-04	6.76E-20
Cr	0.00E+00	4.64E-03	1.67E-02	1.64E-02	2.63E-30	2.58E-30
Cu	2.73E-02	3.69E-02	3.31E-02	3.08E-02	2.20E-02	2.15E-02
F	3.05E-03	2.28E-03	2.56E-03	1.97E-03	1.30E-03	2.29E-03
Fe	1.06E+01	1.61E+01	1.78E+01	1.80E+01	1.89E+01	1.86E+01
Gd	1.68E-03	1.00E-02	9.49E-03	9.36E-03	8.85E-03	8.69E-03
H	1.88E+01	6.85E+00	6.51E+00	6.43E+00	6.18E+00	6.29E+00
C	2.91E-01	3.04E-01	1.28E-13	8.92E-14	1.14E-02	1.52E-02
P	1.08E-02	1.69E-02	1.89E-02	1.89E-02	1.52E-02	1.55E-02
K	5.25E-01	5.66E-01	2.03E-01	1.91E-01	1.08E-01	4.28E-02
Li	2.44E-01	3.78E-20	1.91E-17	1.87E-17	4.84E-21	8.45E-21
Mg	3.96E-01	5.33E-01	2.85E-01	2.79E-01	2.51E-01	2.25E-01
Mn	4.32E-01	6.38E-01	6.81E-01	6.86E-01	7.05E-01	6.92E-01
N	0.00E+00	4.13E-18	3.41E-14	1.70E-14	3.44E-20	1.01E-19
Na	1.68E+00	1.84E-01	1.48E-02	2.28E-02	4.97E-02	4.61E-02
Ni	1.83E-01	5.70E-01	8.58E-01	8.43E-01	7.77E-01	7.63E-01
Pb	3.43E-03	4.64E-03	4.39E-03	4.33E-03	4.09E-03	4.02E-03
Pu	2.44E-17	3.95E-05	3.72E-05	3.64E-05	3.98E-09	3.67E-09
S	0.00E+00	4.14E-16	6.75E-13	4.83E-13	1.43E-17	1.83E-17
Si	9.15E+00	1.24E+01	1.19E+01	1.17E+01	1.13E+01	1.16E+01
Ti	1.45E-01	1.96E-01	1.86E-01	1.83E-01	1.73E-01	1.70E-01
U	0.00E+00	0.00E+00	1.00E-24	9.07E-25	0.00E+00	0.00E+00
Zr	4.91E-02	4.40E-01	4.16E-01	4.11E-01	3.88E-01	3.81E-01
Total (%)	100	100	100	100	100	100
Total (kg)	14719	13807	14970	15216	16268	16474
Density (g/cm^3)	3.1263	3.7859	3.9332	3.9480	3.9972	3.9729

Table 5-18. Element Composition in Corrosion Products (mole%) and Density at Selected Times for Case 13 (tl1a2113)

	Year				
Element	**98**	**500**	**10,151**	**30,211**	**38,590**
O	6.01E+01	6.01E+01	6.02E+01	6.02E+01	6.02E+01
Al	1.27E-03	5.99E-03	7.64E-02	2.05E-01	2.52E-01
Ba	9.18E-06	4.72E-05	6.74E-04	1.90E-03	2.34E-03
Ca	2.13E-03	1.47E-03	6.30E-02	1.87E-01	2.31E-01
Cl	0.00E+00	4.53E-17	0.00E+00	3.31E-20	3.18E-20
Cr	0.00E+00	6.75E-05	1.15E-21	3.10E-21	0.00E+00
Cu	0.00E+00	5.40E-18	1.01E-03	4.40E-03	5.63E-03
F	3.73E-04	2.19E-14	3.21E-03	3.52E-03	3.63E-03
Fe	3.91E+01	3.88E+01	3.65E+01	3.31E+01	3.19E+01
Gd	6.38E-03	1.37E-02	8.83E-03	7.93E-03	7.61E-03
H	2.09E-02	6.54E-02	5.47E-01	1.45E+00	1.78E+00
C	5.93E-14	1.48E-14	2.44E-02	1.12E-01	1.44E-01
P	8.10E-03	1.37E-02	1.85E-02	1.85E-02	1.85E-02
K	8.72E-05	3.52E-04	5.52E-03	1.48E-02	1.82E-02
Mg	2.79E-04	1.18E-03	3.12E-02	1.10E-01	1.39E-01
Mn	4.36E-01	4.77E-01	6.87E-01	6.64E-01	6.55E-01
N	0.00E+00	1.33E-15	0.00E+00	0.00E+00	0.00E+00
Na	8.78E-05	3.49E-04	5.43E-03	1.46E-02	1.79E-02
Ni	7.41E-04	1.25E-01	1.15E-01	1.23E-01	1.26E-01
Pb	4.32E-06	2.04E-05	2.60E-04	6.96E-04	8.53E-04
Pu	0.00E+00	3.11E-06	5.05E-05	1.43E-04	1.77E-04
S	9.18E-06	3.26E-14	7.34E-20	9.92E-20	9.53E-20
Si	2.62E-01	3.70E-01	1.58E+00	3.39E+00	4.04E+00
Ti	1.84E-04	8.64E-04	1.10E-02	2.96E-02	3.63E-02
U	1.57E-04	8.45E-04	1.10E-02	2.96E-02	3.63E-02
Zr	1.86E-03	8.75E-03	1.12E-01	2.99E-01	3.67E-01
Total (%)	100	100	100	100	100
Total (kg)	5605	6045	9428	10111	10397
Density (g/cm^3)	5.2496	5.2450	5.1036	4.8829	4.8042

Table 5-19. Element Composition in Corrosion Products (mole%) and Density at Selected Times for Case 14 (t@1a2113)

	Year				
Element	**98**	**500**	**10,151**	**30,211**	**38,759**
O	6.01E+01	6.01E+01	6.02E+01	6.03E+01	6.03E+01
Al	1.27E-03	5.99E-03	7.65E-02	2.05E-01	2.53E-01
Ba	9.17E-06	4.72E-05	6.74E-04	1.90E-03	2.36E-03
Ca	2.13E-03	1.47E-03	6.18E-02	1.86E-01	2.32E-01
Cr	0.00E+00	6.75E-05	0.00E+00	3.11E-21	2.98E-21
Cu	0.00E+00	3.20E-17	1.01E-03	4.41E-03	5.66E-03
F	3.73E-04	1.29E-13	3.21E-03	3.52E-03	3.64E-03
Fe	3.91E+01	3.88E+01	3.65E+01	3.31E+01	3.19E+01
Gd	6.38E-03	1.36E-02	8.79E-03	7.90E-03	7.58E-03
H	2.06E-02	6.42E-02	5.12E-01	1.36E+00	1.67E+00
C	1.65E-15	1.02E-13	2.69E-02	1.22E-01	1.57E-01
P	8.00E-03	1.36E-02	1.84E-02	1.85E-02	1.85E-02
K	8.72E-05	3.52E-04	5.52E-03	1.48E-02	1.83E-02
Mg	2.79E-04	1.18E-03	3.11E-02	1.10E-01	1.39E-01
Mn	4.36E-01	4.77E-01	6.87E-01	6.65E-01	6.56E-01
N	0.00E+00	7.83E-15	7.34E-20	0.00E+00	0.00E+00
Na	8.78E-05	3.49E-04	5.43E-03	1.46E-02	1.80E-02
Ni	6.98E-04	1.25E-01	1.15E-01	1.23E-01	1.26E-01
Pb	4.32E-06	2.04E-05	2.60E-04	6.97E-04	8.58E-04
Pu	0.00E+00	3.12E-06	5.05E-05	1.44E-04	1.78E-04
S	9.17E-06	1.93E-13	0.00E+00	3.31E-20	3.18E-20
Si	2.62E-01	3.70E-01	1.58E+00	3.39E+00	4.06E+00
Ti	3.00E-04	1.41E-03	1.80E-02	4.83E-02	5.95E-02
U	4.07E-05	2.98E-04	4.04E-03	1.09E-02	1.34E-02
Zr	1.86E-03	8.75E-03	1.12E-01	3.00E-01	3.69E-01
Total (%)	100	100	100	100	100
Total (kg)	5605	6045	9423	10097	10384
Density (g/cm^3)	5.2495	5.2450	5.1044	4.8843	4.8043

Table 5-20. Element Composition in Corrosion Products (mole%) and Density at Selected Times for Case 17 (t!1a2133)

	Year				
Element	**98**	**500**	**10,137**	**30,201**	**38,478**
O	6.02E+01	6.03E+01	6.03E+01	6.03E+01	6.03E+01
Al	1.27E-03	5.83E-03	7.45E-02	2.02E-01	2.48E-01
Ba	9.15E-06	4.58E-05	6.57E-04	1.87E-03	2.31E-03
Ca	2.14E-03	1.43E-03	7.03E-02	1.92E-01	2.36E-01
Cr	0.00E+00	6.56E-05	0.00E+00	3.56E-21	2.45E-21
Cu	0.00E+00	1.55E-17	9.83E-04	4.33E-03	5.55E-03
F	3.75E-04	6.28E-14	3.13E-03	3.46E-03	3.58E-03
Fe	3.89E+01	3.77E+01	3.56E+01	3.26E+01	3.15E+01
Gd	6.34E-03	1.70E-02	1.10E-02	9.95E-03	9.58E-03
H	3.87E-02	1.33E-01	6.67E-01	1.51E+00	1.82E+00
C	5.81E-14	1.67E-13	1.95E-02	1.11E-01	1.44E-01
P	1.40E-02	1.70E-02	2.04E-02	2.03E-02	2.03E-02
K	8.70E-05	3.43E-04	5.38E-03	1.46E-02	1.79E-02
Mg	2.78E-04	1.14E-03	3.11E-02	1.09E-01	1.37E-01
Mn	4.33E-01	4.64E-01	6.70E-01	6.54E-01	6.48E-01
N	0.00E+00	3.81E-15	0.00E+00	0.00E+00	0.00E+00
Na	8.75E-05	3.40E-04	5.29E-03	1.43E-02	1.76E-02
Ni	2.92E-03	1.17E-01	1.09E-01	1.19E-01	1.22E-01
Pb	4.30E-06	1.98E-05	2.53E-04	6.85E-04	8.41E-04
Pu	0.00E+00	2.49E-06	4.88E-05	1.41E-04	1.74E-04
S	9.15E-06	9.36E-14	0.00E+00	0.00E+00	0.00E+00
Si	2.60E-01	3.60E-01	1.54E+00	3.33E+00	3.98E+00
Ti	1.82E-04	8.40E-04	1.07E-02	2.91E-02	3.57E-02
U	6.89E-03	3.18E-02	3.64E-02	4.53E-02	4.85E-02
Zr	1.85E-01	8.51E-01	8.07E-01	7.34E-01	7.08E-01
Total (%)	100	100	100	100	100
Total (kg)	5649	6268	9723	10317	10562
Density (g/cm^3)	5.2571	5.2623	5.1160	4.8944	4.8152

Table 5-21. Element Composition in Corrosion Products (mole%) and Density at Selected Times for Case 27 (t02a2204/t!1a2022)

	Year					
Element	**4,000[a]**	**4,681**	**10,044**	**31,855**	**101,590**	**316,910**
O	5.96E+01	5.97E+01	5.97E+01	5.98E+01	5.98E+01	5.98E+01
Al	1.32E+00	1.27E+00	1.20E+00	1.19E+00	1.19E+00	1.17E+00
Ba	1.26E-02	1.21E-02	1.14E-02	1.14E-02	1.13E-02	1.11E-02
Ca	2.08E-01	1.96E-01	1.85E-01	1.94E-01	2.19E-01	2.69E-01
Cl	2.12E-15	1.82E-20	1.36E-16	6.14E-04	6.23E-04	1.67E-20
Cr	1.71E-02	1.64E-02	1.14E-02	8.84E-04	0.00E+00	3.80E-31
Cu	3.56E-02	2.94E-02	2.15E-02	2.13E-02	2.12E-02	2.06E-02
F	6.45E-03	3.61E-03	2.33E-03	3.13E-03	3.16E-03	3.92E-03
Fe	1.75E+01	1.82E+01	1.89E+01	1.88E+01	1.87E+01	1.84E+01
Gd	2.78E-24	9.33E-03	8.84E-03	8.81E-03	8.75E-03	8.59E-03
H	6.79E+00	6.55E+00	6.25E+00	6.24E+00	6.28E+00	6.38E+00
C	3.74E-13	4.47E-14	0.00E+00	1.15E-02	1.22E-02	1.51E-02
P	1.93E-02	2.02E-02	1.99E-02	2.00E-02	2.01E-02	2.04E-02
K	8.28E-02	7.75E-02	7.01E-02	6.24E-02	4.65E-02	3.33E-02
Mg	3.07E-01	2.90E-01	2.70E-01	2.64E-01	2.49E-01	2.21E-01
Mn	6.79E-01	6.91E-01	7.04E-01	7.01E-01	6.97E-01	6.84E-01
Na	3.21E-02	2.65E-02	3.13E-02	4.12E-02	4.54E-02	4.63E-02
Ni	7.48E-01	7.61E-01	7.29E-01	7.25E-01	7.21E-01	7.08E-01
Pb	4.49E-03	4.31E-03	4.09E-03	4.07E-03	4.05E-03	3.97E-03
Pu	9.44E-04	9.07E-04	8.17E-04	8.35E-04	8.30E-04	8.15E-04
S	1.20E-12	5.87E-04	2.84E-05	0.00E+00	0.00E+00	3.81E-18
Si	1.24E+01	1.19E+01	1.14E+01	1.14E+01	1.15E+01	1.17E+01
Ti	1.90E-01	1.83E-01	1.73E-01	1.72E-01	1.71E-01	1.68E-01
U	3.33E-24	1.36E-03	1.15E-02	1.42E-02	1.40E-02	1.36E-02
Zr	1.58E-24	3.70E-02	3.11E-01	3.86E-01	3.84E-01	3.77E-01
Total (%)	100	100	100	100	100	100
Total (kg)	14348	15127	16246	16331	16398	16612
Density (g/cm^3)	3.8678	3.9219	3.9905	3.9930	3.9842	3.9576

[a] This is the year that run t02a2204 ended and run t!1a2022 began.

For Cases 2, 9, and 14, listed in Table 5-7, the second character is "@". In these runs, the UO_2 (depleted U) in the HLW glass was replaced with TiO_2 so that the uranium results would represent only the uranium in the fuel (70% U-235). EQ6 does not distinguish between various isotopes of the same element. For criticality calculations, it is important to know what portion of the uranium is fissile. Figures 5-2 and 5-3 are plots of total moles of uranium versus time for

two of the cases. Figure 5-2 shows the results for average degradation rates for Cases 1 and 2, whereas Figure 5-3 shows the results for high degradation rates of HLW glass and SNF for Cases 8 and 9. Also note that only the first 25,000 years of the run are shown in Figure 5-3.

Figure 5-4 can help explain the change in total moles of uranium versus time observed in Figure 5-2. From the start of the run until about 50,000 year, the total moles of uranium in the waste package remain constant in Figure 5-2. As the HLW glass and SNF (both containing uranium) degrade, the uranium-bearing mineral soddyite is formed (Figure 5-4) and none of the U is flushed from the waste package. The pH is about 6 during this time period due to the degradation of the steel in the waste package. Once the steel is all degraded at about 50,000 year, the pH rises; the uranium in the soddyite dissolves into the water; a spike of higher U concentration in the water is observed (65,000 year in Figure 5-4); a sharp decline in the total U in the waste package is observed ((60,000 year in Figure 5-2); and from about 75,000 year and later, the total U in the waste package slowly decreases (Case 1 in Figure 5-2) as the HLW glass degrades and the U is flushed out with the water.

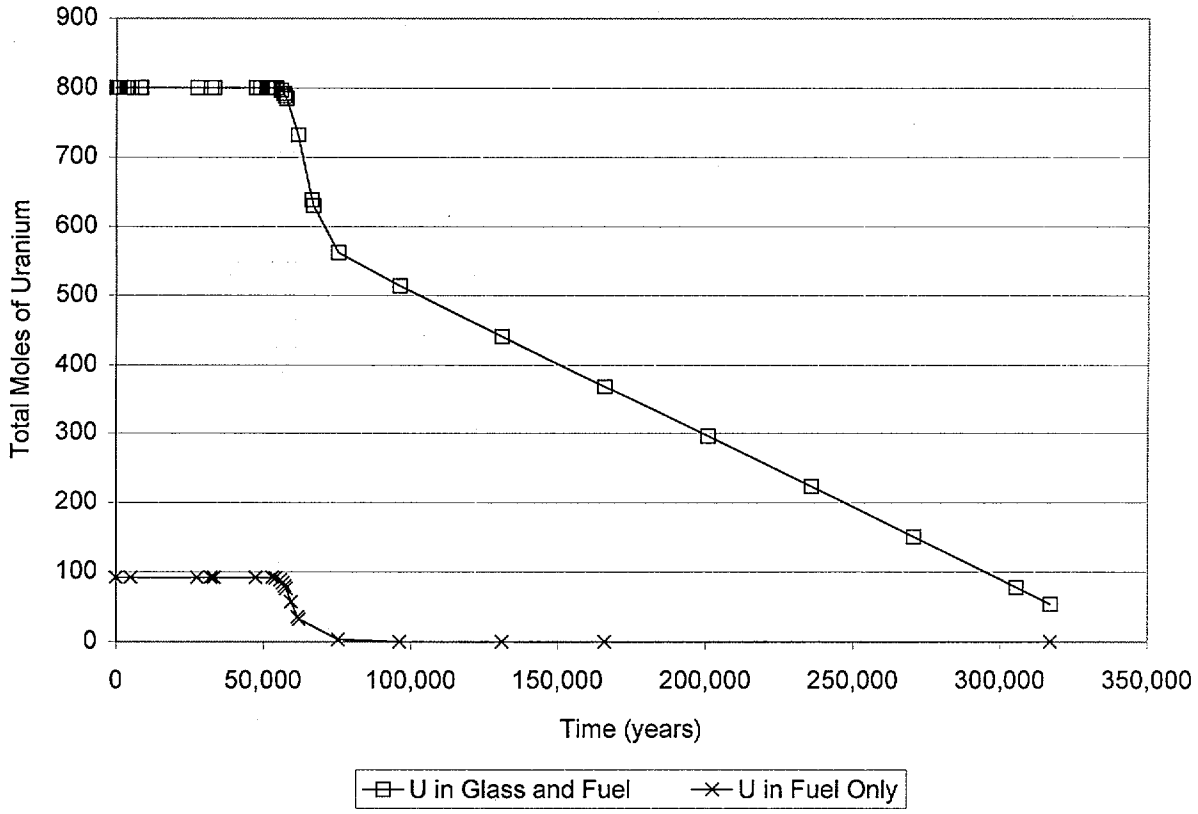

Figure 5-2. Moles of Uranium in All Phases, Cases 1 and 2 (t!1a1111 and t@1a1111)

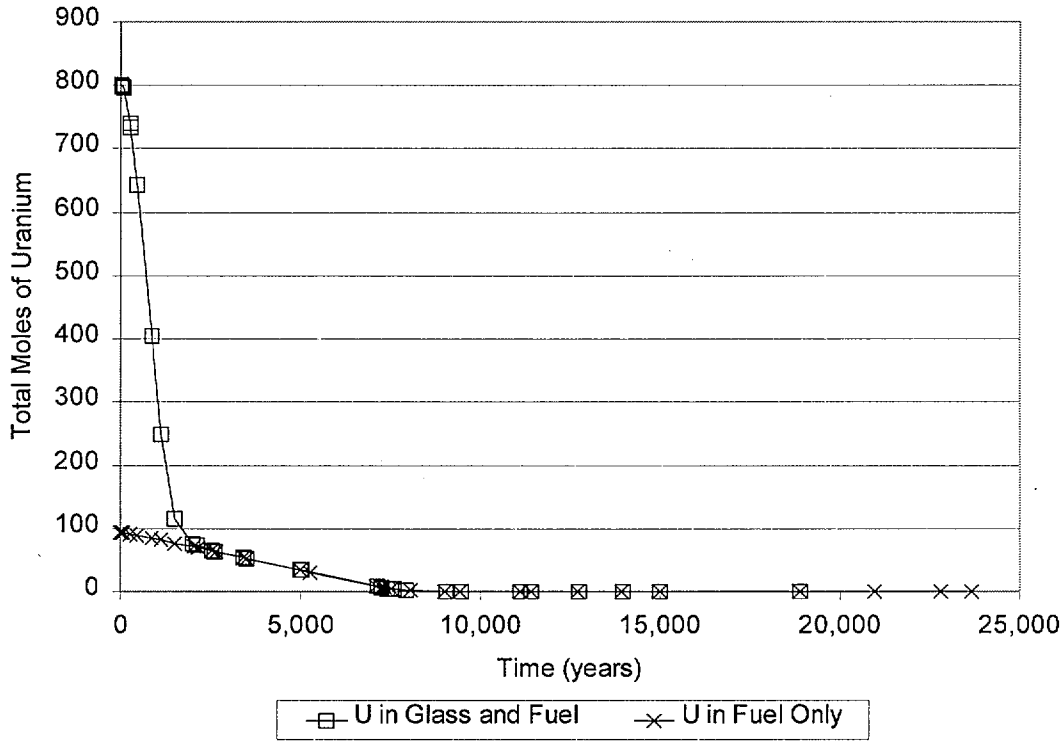

Figure 5-3. Moles of Uranium in All Phases, Cases 8 and 9 (t!1a1222 and t@1a1222)

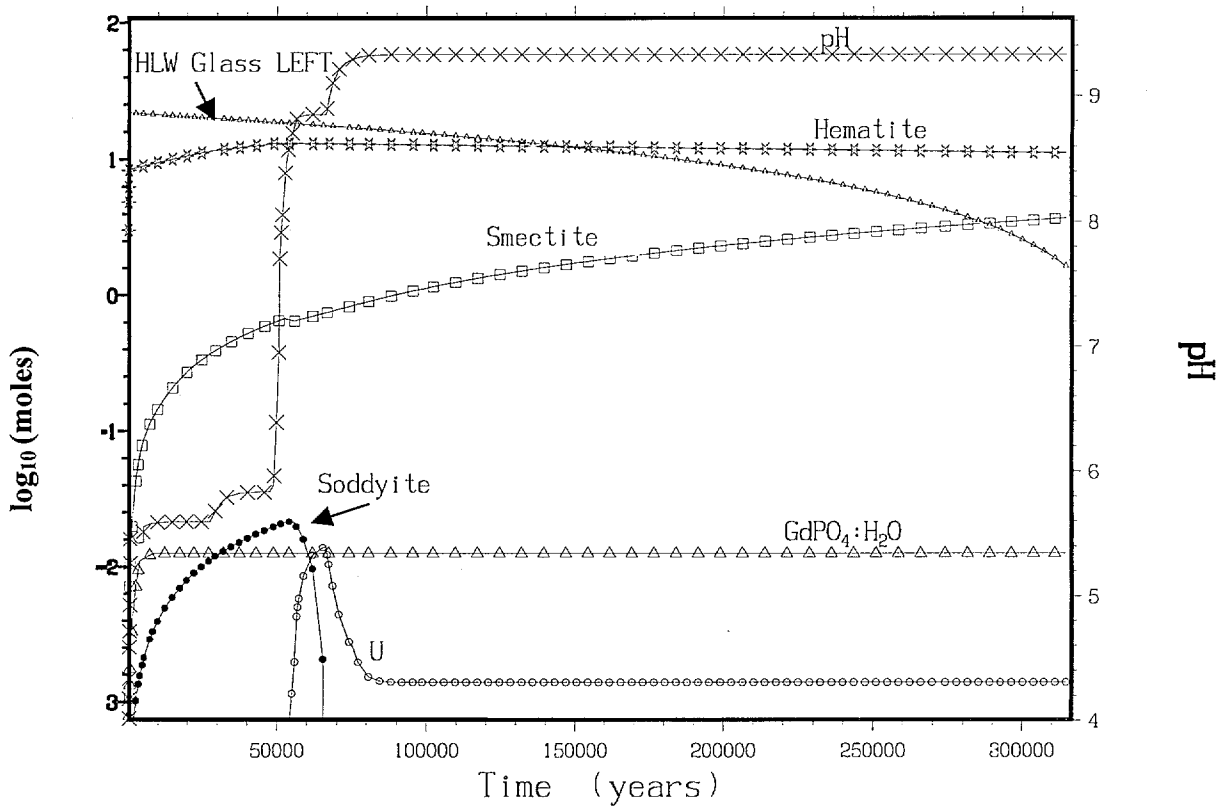

Figure 5-4. Moles of HLW Glass Remaining, Moles of Major Minerals Formed (hematite [Fe_2O_3], smectite, soddyite [$(UO_2)_2(SiO_4)\cdot 2H_2O$], and $GdPO_4\cdot H_2O$), pH of solution, and moles per liter of U in solution as a function of time for Case 1 (t!1a1111)

Case 27 is a double-stage case. In the first stage, the outer web (A516), the HLW glass, the HLW glass pour canisters (304L), and the outer surface of the DOE SNF canister (316L) are the only reactants included. The first stage ended at 4,000 years, which was the beginning of the low-pH plateau in the first stage. At the end of run t02a2204 and the beginning of run t!1a2022, all of the outer web and HLW glass have totally degraded; whereas, 81.8 mole% of the HLW glass pour canisters and 42.1 mole% of the DOE SNF canister have degraded.

6. RESULTS

Unqualified data were used in the development of the results presented in this calculation.

A principal objective of this calculation was to assess the chemical circumstances that could lead to removal of neutron absorbers (Gd) from the waste package, while fissile materials (U) remain behind. Such circumstances could increase the probability of a nuclear criticality occurrence within the waste package. Gadolinium is assumed to be present in absorber tubes made of Alloy 22 with 8 mole% Gd located within the basket structure that is located within the DOE SNF 18-inch canister. Water with 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 twenty-seven EQ6 cases and examined the results to identify the reasons for the chemical changes during degradation of waste package materials and flushing by J-13 well water. The scenarios and conditions of EQ6 were chosen to emphasize conditions that could create either acid or alkaline conditions, and to determine if these conditions are of sufficient duration to induce Gd loss.

Twenty-seven EQ6 reaction-path cases were constructed to bound the range of possible Gd and SNF degradation (Table 5-7). Two general EQ6 scenarios were selected: single- and double-stages. Cases 1 through 23 were single-stage cases where high pH was achieved by simultaneous exposure of SNF to degrading HLW glass. In the longer run cases (> 300,000 year), most of the uranium was lost, with 0 to 14% of U remaining at the end of the run. In the shorter run cases (~40,000 year) with the high rates of HLW glass degradation, the U remaining at the end of the runs ranged from 0 to 11%. In the shorter run cases with average HLW glass degradation rates, nearly all of the U was retained in the waste package. Cases 13 (t!1a2113) and 17 (t!1a2133) resulted in the highest U remaining (99.9%) and the lowest Gd remaining (47% and 59%, respectively) at the end of the run (~40,000 year). Both of these cases had high rates of steel degradation, average rate for HLW glass degradation, and high rates of water drip rate.

Multiple-stage cases were Cases 24 through 27 of Table 5-7. These cases tested the effect of exposing the Gd and U to long-lived acidic conditions (pH ~5 to 6). The highest level of acidity was achieved during first-stage EQ6 simulations, where it is assumed that the DOE SNF canister to be intact, and only the outside of the DOE SNF canister, the HLW glass and its container, and the A516 outer web structure were allowed to interact with the water dripping into the waste package. With a sufficiently high drip rate, the alkaline components of the HLW glass are removed (as well as all the U in the HLW glass) during this stage. In the second stage, the absorber tubes containing Gd, SNF, and other components within the DOE SNF canister are exposed to J-13 well water at a much lower drip rate, allowing pH to drop. Cases 24 through 27 resulted in essentially no loss of Gd, and a few percent loss of U from the SNF (Table 5-7). In all cases the predicted major corrosion products are an iron-rich smectite clay (nontronite) and hematite or goethite. The smectite and iron oxide typically comprise over 90% of the corrosion

product volume. The Gd enters into rhabdophane (hydrated $GdPO_4$) as the absorber tubes corrode, and the dominant U solid is soddyite $[(UO_2)_2(SiO_4)\cdot 2H_2O]$.

7. ATTACHMENTS

Attachment I. Document Input Reference Sheet (9 pages)

Attachment II. Documentation for Software Routine: eqsetup (48 pages)

Attachment III. Listing of Files on Electronic Media (5 pages)

8. REFERENCES

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OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT
DOCUMENT INPUT REFERENCE SHEET

1. Document Identifier No./Rev.:	Change:	Title:
CAL-EDC-MD-000001 REV 00	N/A	EQ6 Calculations for Chemical Degradation of TRIGA Codisposal Waste Packages

Input Document							8. TBV Due To		
	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
2a 1	DOE (U.S. Department of Energy) 1999. *TRIGA (UZrH) Fuel Characteristics for Disposal Criticality Analysis.* DOE/SNF/REP-048 Revision 0. Washington, D.C.: DOE, Office of Environmental Management. TIC: 244162. *INITIAL USE*	3	TBV-3524	1, 5	Fuel rod composition and dimensions.	3	x	N/A	N/A
2	CRWMS M&O (Civilian Radioactive Waste Management System Management and Operating Contractor) 1998. *EQ6 Calculation for Chemical Degradation of Fast Flux Test Facility (FFTF) Waste Packages.* BBA000000-01717-0210-00028 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19981229.0081.	5.1.1.1, p. 20 5.3.1, p. 23	N/A	1, 5	Void space discussion. Solubility of gadolinium. Not an input, reference only.	N/A	N/A	N/A	N/A
3	CRWMS M&O 1998. *Total System Performance Assessment - Viability Assessment (TSPA-VA) Analyses Technical Basis Document.* Chapter 10, Disruptive Events. B00000000-01717-4301-00010 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19980724.0399.	10.5.1.2	N/A	1	Discussion of degradation scenarios. Not an input, reference only.	N/A	N/A	N/A	N/A

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	2. Technical Product Input Source Title and Identifier(s) with Version	3. Section					Unqual.	From Uncontrolled Source	Un-confirmed
4	CRWMS M&O 1998. *Evaluation of Codisposal Viability for Aluminum-Clad DOE-Owned Spent Fuel: Phase II. Degraded Codisposal Waste Package Internal Criticality.* BBA000000-01717-5705-00017 REV 01. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19980616.0098.	Entire	N/A	1	Description of codisposal concept. Not an input, reference only.	N/A	N/A	N/A	N/A
5	National Research Council of the National Academy of Sciences 1995. *Technical Bases for Yucca Mountain Standards.* Washington, D.C.: National Academy Press. TIC: 104273.	pp. 54-55, 71-72, 119	N/A	1	Discussion of time frame for calculations. Not an input, reference only.	N/A	N/A	N/A	N/A
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Input Document			4. Input Status	5. Section Used in	6. Input Description	7. TBV/TBD Priority	8. TBV Due To		
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Input Document							8. TBV Due To		
	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
12	CRWMS M&O 1998. *Electronic Media for EQ6 Calculations for Chemical Degradation of TRIGA Codisposal Waste Packages (CAL-EDC-MD-000001 REV 00).* ACC: MOL.19991028.0108.	Entire	N/A	3, 4, 5	EQ6 database files, geometry calculations for fuel, software routines. Excel files cite other references as indicated in these DIRS.	N/A	N/A	N/A	N/A
13	DOE 1998. *Viability Assessment of a Repository at Yucca Mountain, Volume 3: Total System Performance Assessment.* DOE/RW-0508. Washington, D.C.: DOE, Office of Civilian Radioactive Waste Management. ACC: MOL.19981007.0030.	Figs. 3-20 to 3-22, pp. 3-34 to 3-37	N/A	3	Discussion of temperature at which initial breach of waste package will occur. Not an input, reference only.	N/A	N/A	N/A	N/A
14	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.	Sec. 7.3.3 Att. 6	N/A	3	Basis for assumption of convective circulation and mixing of water inside waste package. Not an input, reference only.	N/A	N/A	N/A	N/A
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CAL-EDC-MD-000001 REV 00	N/A	EQ6 Calculations for Chemical Degradation of TRIGA Codisposal Waste Packages

	Input Document: 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	8. TBV Due To: Unqual.	From Uncontrolled Source	Un-confirmed
17	CRWMS M&O 1999. *DOE SRS HLW Glass Chemical Composition.* BBA000000-01717-0210-00038 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19990215.0397.	Att I, p. I-7	TBV-3022	5	Molar composition of the glass. Wide range tested for study; effects of variation were trivial, so TBV can be lifted if approved composition is within tested range.	3	N/A	x	N/A
18	DOE 1992. *Characteristics of Potential Repository Wastes.* DOE/RW-0184-R1 Vol. 1. Oak Ridge, Tennessee: Oak Ridge National Laboratory. TIC: 242019.	p. 3.3-15, Table 3.3.8 Fig. 3.3.1 Table 3.3.1 p. 3.3-6	TBV-3150	5	Glass composition for comparison. Length and thickness of glass pour canisters. Fill fraction of glass pour canisters.	N/A 3 3	N/A x x	N/A N/A N/A	N/A N/A N/A
19	CRWMS M&O 1995. *Total System Performance Assessment – 1995: An Evaluation of the Potential Yucca Mountain Repository.* B00000000-01717-2200-00136 REV 01. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19960724.0188.	p. 6-5, Fig. 6.2-5 Figs. 5.4-3 , -4, -5	TBV-3443	5	Glass degradation rate. Degradation rate of A516 carbon steel. To lift TBV, AMOPE must approve approximate range of rates, or must approve rates within the three-orders-of-magnitude variation used in this study.	3	N/A	x	N/A
20	TRIGA Group 1999. *TRIGA Research Reactors.* San Diego, California: TRIGA Group. TIC: 243984.	Entire	N/A	5	Degradation rate of fuel is equal to stainless steel. Used only to suggest broad range; rate varied three orders of magnitude in calculations.	N/A	N/A	N/A	N/A

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DOCUMENT INPUT REFERENCE SHEET

1. Document Identifier No./Rev.:	Change:	Title:
CAL-EDC-MD-000001 REV 00	N/A	EQ6 Calculations for Chemical Degradation of TRIGA Codisposal Waste Packages

Input Document							8. TBV Due To		
	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
21	CRWMS M&O 1998. *Total System Performance Assessment – Viability Assessment (TSPA-VA) Analyses Technical Basis Document. Chapter 4: Near-Field Geochemical Environment.* B00000000-01717-4301-00004 REV 01. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19981008.0004.	Fig. 4-27	TBV-3412	5	Carbon dioxide fugacity in water.	3	x	N/A	N/A
22	CRWMS M&O 1998. *Complete Draft VA UZ Abstraction/Test Document. Unsaturated-Zone Flow: Preliminary Draft Section 2.3 of TSPA-VA Document.* B00000000-01717-2200-00201. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19980428.0202. *INITIAL USE*	Fig. 2.3-110 & Table 2.3-49 & 2.3-50	TBV-3525	5	Correlation between percolation rate and drip rate. To lift TBV, AMOPE must approve approximate range of drip rates, or must approve rates within the three-orders-of-magnitude variation used in this study.	3	N/A	x	N/A
23	CRWMS M&O 1997. *Degraded Mode Criticality Analysis of Immobilized Plutonium Waste Forms in a Geologic Repository.* A00000000-01717-5705-00014 REV 01. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19980422.0911.	5.3	N/A	5	Discussion of conditions for highest Gd removal from waste package. Not an input, reference only.	N/A	N/A	N/A	N/A
24	CRWMS M&O 1996. *Material Compositions and Number Densities For Neutronics Calculations.* BBA000000-01717-0200-00002 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19960624.0023.	pp. 29-31	TBV-3384	5	Isotopic weights. Values from handbooks.	3	N/A	x	N/A

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Input Document							8. TBV Due To		
	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
25	Walker, E.W.; Parrington, J.R.; and Feiner, F. 1989. *Nuclides and Isotopes, Fourteenth Edition, Chart of the Nuclides.* San Jose, California: General Electric Co. TIC: 201637.	List of Elements p. 50	N/A	5	Atomic weights. Handbook data.	N/A	N/A	N/A	N/A
26	CRWMS M&O 1998. *Disposal Criticality Analysis Methodology Topical Report.* B00000000-01717-5705-00095 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19980918.0005.	pp. 3-9 to 3-12	N/A	5	Degradation scenario for disposal criticality analysis. Not input, reference only.	N/A	N/A	N/A	N/A
27	CRWMS M&O 1999. *Waste Package Materials Properties.* BBA000000-01717-0210-00017 REV 00, Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19990407.0172.	5.2, 5.3, 5.4, 5.7	TBV-3149	5	Composition and density of A 516 Carbon Steel Grade 70, 316L and 304L Stainless Steel, and Alloy C-22. These data are accepted but require concurrence from DOE AMOPE.	3	N/A	x	N/A
28	CRWMS M&O 1998. *Electronic Media for EQ6 Calculations for Chemical Degradation of Fast Flux Facility (FFTF) Waste Packages (BBA000000-01717-0210-00028 REV 00).* ACC: MOL.19981229.0082.	Excel spreadsheet fftf_fuel_hws.xls Sheets glass_canisters & outerweb	N/A	5	Spreadsheet used to calculate volume and area of HLW glass canisters and outer web.	3	x	N/A	N/A

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Input Document			4. Input Status	5. Section Used in	6. Input Description	7. TBV/TBD Priority	8. TBV Due To		
	2. Technical Product Input Source Title and Identifier(s) with Version	3. Section					Unqual.	From Uncontrolled Source	Un-confirmed
29	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-3442	5	Degradation rate for 304L and 316L Stainless Steel. To lift TBV, AMOPE must approve approximate range of rates, or must approve rates within the three-orders-of-magnitude variation used in this study.	3	N/A	x	N/A
30	Baxter, R.G. 1988. *Defense Waste Processing Facility Wasteform and Canister Description.* DP-1606 Rev. 2. Aiken, South Carolina: Savannah River Plant. TIC: 8704. *INITIAL USE*	p. 26 Fig. 2 and pp. 54-57	TBV-3526	5	Glass density.	3	x	N/A	N/A
31	Weast, R.C., ed. 1984. *CRC Handbook of Chemistry and Physics, 65th Edition 1984-1985.* Boca Raton, Florida: CRC Press, Inc. TIC: 206666.	p. B-96	N/A	5	Density of Gadolinium. Data from a handbook, therefore accepted data.	N/A	N/A	N/A	N/A
32	CRWMS M&O 1999. *Volume/Mass of DOE Canister and TRIGA SNF.* BBA000000-01717-0210-00046 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19990713.0238.	6 Sketch SK-0124	TBV-3148	5	Void volume of canister Dimensions of TRIGA waste package	3	x	N/A	N/A

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	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
33	Beyer, W.H., ed. 1987. *CRC Standard Mathematical Tables, 28th Edition.* Boca Raton, Florida: CRC Press, Inc. TIC: 240507.	Section IV	N/A	Att. II	Equations of volumes and areas for different geometric shapes used to check software routine. Not an input, reference only.	N/A	N/A	N/A	N/A
34	Bauccio, M., ed. 1993. *ASM Metals Reference Book, Third Edition.* Materials Park, Ohio: ASM International. TIC: 240701.	pp. 567-572	N/A	Att. II	Equations of volumes and areas for different geometric shapes used to check software routine. Not an input, reference only	N/A	N/A	N/A	N/A
35	CRWMS M&O 1999. *Software Change Request (SCR) LSCR198; Addendum to EQ6 Computer Program for Theoretical Manual, Users Guide, and Related Documentation.* UCRL-MA-110662 PT IV. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19990920.0169.	Entire	N/A	4	Software Qualification. Not an input, reference only.	N/A	N/A	N/A	N/A

Attachment II Documentation for Software Routine: Eqsetup

1. Listing of eqsetup code (pages II-2 through II-19)
2. Documentation of correct results (pages II-20 through II-22)
3. Sample input files for eqsetup: triga.txt, test.txt (pages II-23 through II-31)
4. Sample output files for eqsetup: trigajunk.txt, testjunk.txt (pages II-32 through II-34)
5. Files (atwts.in, template.in, ratefacs.in) necessary to run eqsetup (pages II-35 through II-48)

1. Listing of eqsetup

```
/*eqsetup.c Program that parses namelist style parameter input for EQ3/6. In
  particular, it calculates areas and volumes of shapes of materials.  In
  calculating the areas of prism and cylinder shells, the small area at the
two
  ends, between the principal surfaces is not included. The program also
  calculates the moles of these shapes, according to composition and
  atomic weights (which are called components, instead of elements).
  All the input is checked for consistency, except the number of components
  (elements) in each material.  For checking purposes, the program also
  accumulates mass and area for all of the instances of each shape and puts
them
  in a debug file, junk.out.  Although this information is not needed for
EQ3/6
  input, it is usefull for producing the waste form description document
  (volumes and masses).

  The atomic weights are read in from the file atwts.in, using the subroutine
  bldatwts().  The elements use their international chemical symbols, with
the
  first letter capitalized.  The individual element weight values are for the
  natural isotopic mixture, except for Pu, which uses only the Pu-239 value,
and
  U, for which the principal isotopes of interest, (233, 235, 238, etc)
  can be entered individually (e.g. U-233, etc).  These isotopic designations
  cannot be used in the present version of EQ3/6, so they are combined into
  a single element with symbol "U" having an average atomic weight calculated
  from the isotopic composition for that material.  Two, or more, materials
  having different U isotope compositions will give slightly different
  molecular weights, but that doesn't matter because EQ3/6 uses its own value
  for atomic weight.  The only parameters fed to EQ3/6 are moles remaining
  and molar volume, and this procedure ensures that they will be calculated
  in a consistent manner.  For this system to work, all of the
  uranium isotopes must appear at the end of the material component list, but
  they may appear in any order.  If they are not confined to the end of the
  list, the program will quit with an appropriate error message.

  The input, data.in, is read into an array of lines. This array is processed
as
  blocks of shapes, materials, and structures.  The structures are built from
  shapes. Total mass and area are accumulated by traceing the shapes through
  their occurrences in the hierarchy of structures.  Since each shape is
  associated with a single material (mtrl[i]) the mass and area of each
material
  can be accumulated along with accumulation for shapes.  The principal
results
  of this process are the surface areas and moles for each material (the
latter
  being computed from the total mass for the material and its molecular
weight),
  since this is the primary input to EQ3/6.  The shape components of a
  structure have one line each.  Each shape component line starts with the
keyword component,
```

```
  followed by an equal sign and two fields.  The first field is the name
  of the shape; the second field is the number of times the shape occurs in
  the structure.  If this number is negative, the area and volume of the
shape
  will be subtracted instead of added.  This capability is used to remove
  surfaces that are double counted when a solid structure is built of
  elementary shapes (such as a cone on top of a cylinder).

  Areas for each material are accumulated in the routine bldmoles() for
  convenience.  The area calculation incorporates a fracture factor, which
can
  account for additional area due to internal fracturing, or for reduced
exposed
  area due to protection such as intact cladding.  Bookkeeping for these
  factor values is by shape.  The designator in the file data.in is
  fracture_factor; for internal fracturing fracture_factor > 1; for
simulating
  the protection by partly intact cladding fracture_factor < 1, and the value
  is inversely proportional to the amount of cladding protection left (which
  decreases with time).

  There are two different forms for comments: (1) Anything after the
obligatory
  fields in a keyword statement;  (2) Any line that begins below with an '*'.
  The former are copied into the input array of lines, but not read because
  each keyword keys a read of only a limited number of fields.  The latter
  are simply diverted into the debugging file, "junk.out".

  The input file, "data.in" also has a capability like the FORTRAN namelist,
  provided that the variable name is preceded by a character less than
  ASCII 48 (decimal) and then a code line for reading that variable is
  inserted at an appropriate place in the program.  This capability is
  presently implemented for the global variable literswater, for which a
  nominal value is assigned in the program, but which may be overridden
  by reading in the function bldmoles().  The overriding value will be read
  if it occurs on any line of "data.in" provided the variable name
  (literswater) is prefixed by '$'.

  The following keywords are used for the spherical segment: sphereseg,
  altitude, largerad, smallrad.

  The degradation rates are specified by a four field statement.  The first
  field is the keyword degrate; the second field is '='; the third field is
  value; the fourth field is the keyword grams or moles, depending on
  whether the degradation rate is in grams/cm2/day or moles/cm2/day.  In both
  cases, the input is converted to the output in pseudomoles/cm2/day, where
  pseudomoles have a molecular weight of 100.  The moles keyword case is the
  only use of the molecular weight calculation (in the function bldmolwt()),
  performed by this code.
  */

#include <stdio.h>
#include <float.h>
#include <string.h>
#include <stdlib.h>
#include <math.h>
#define PI (float)acos(-1)
```

```
#define MAXLOOP 100//max steps in trace of a shape through structure
hierarchy

//In the following array definitions i refers to the first index; j to the
second
FILE *fin,*fout,*ferr,*ftemp,*fratefacs;
float findfloat(char*,int,int);//gets a float number from an array of strings
int findatwtindx(char*);//finds the index of an element in the atomic wt
table
float areas[100], //areas of individual shapes
     volumes[100],//volumes of individual shapes
      densities[100],//densities of individual materials
      degrates[100],//degradation rates of individual materials
      gramvals[30][30],//wt fraction of element j in material i
      compvals[30][30];//mole fraction of element j in material i
float mass[100]={0},//accumulates mass of material i
      mareas[20]={0},//accumulates area of material i
       literswater=3937,//water in bathtub, may be overridden in bldmoles().
       atwts[100],//array of atomic weights (read from atwts.in)
       nmoles[100]={0};//moles of material i
float bldmolwt(int),//builds molecular weight for each material
      mvolumes[20],//volume of a gram mole of material i
       fudgefac[20],//simply goes into EQ3/6 input; not now used for anything
       temperature=25,//selects thermo libriary for EQ3/6
       fracfac=1;//fracture factor for glass; should be an array for
additional mtrl
void etrim(char*),//trims blanks from end of a string
      ftrim(char*),//trims blanks from the beginning of a string
       errproc(char*,char*),//outputs two strings describing the error and
exits
       bldmoles(),//builds total masses and volumes for each material and
shape
      bldratefacarry(char*,float*,int,int),//builds a ratefactor array
       getstr(char*,char*,int),//gets the string following a keystring= in
lines[]
      bldratefacs(int),//builds the rate factors for this case
       outline(int),//prints separator line
       bldatwts();//builds the atomic weights array from atwts.in
char filenames[50][10],//*.6i filenames for cases to be run
     casedescs[50][100],//comment lines to be transferred to *.6i files
     lines[800][100],  //array of input lines
      rlines[20][100];//array for ratelines
char Uxnames[5][3]={"Ua","Ub","Uc","Ud","Ue"};//dummy names for U
combinations
         //used internally; EQ3/6 reads only U for uranium.
float mwtUxvals[5]={0};//Average atomic wt for all the U isotopes in this
mtrl
int  goethflag,// =1 if goethite is to be enhanced by surpressing hematite
     stageflag,// =1 if first stage of a 2 stage run (so no fuel degradation)
      glassflag,//=0 if glass is not present (stage 2)
      fuelflag,//=0 if fuel not present (stage  1)
     numUwts=0;//Counts the number of materials with multiple U isotopes
char mtrl[100][20],//name of material for shape i
     compnames[30][30][20],//name (symbol) of element j of material i
      matnames[100][20],//name of material i
      shapenames[100][20];//name of shape i
int buildvals(int,int),//builds array of lines from the input file, data.in
```

```
      numshapes=0,//number of shape blocks read from the lines array
       nummaterials=0,//number of material  blocks read
       numstructures=0,//accumulates number of structures read from data.in
      get1of3(char*,char*,char*,int);//identify 3 basic input block types
(data.in)
int mindex=0,//tracks index for material block currently being read
   sindex=0,//tracks index for shape block currently being read
    findint(char*,int,int),//returns integer parameter when keyword is found
    findstr(char*,char*,int,int),//copies string parameter when keyword is
found
   stype[100],//shapetype for shape i
    ttype[100],//solid or shell for shape i
    occrrncs[100]={0},//lowest level occurrences for shape i (from data.in)
    compnums[100],//number of elements in material i
    numlines,//number of lines read from data.in
    get2(char*,char*,char),//splits a string at the third argument
    numelements,//number of elements read from atwts.in
    dislaw=3,//dissolution law index; simply passed to EQ3/6
    plaw=0,//precipitation law index; simply passed to EQ3/6
    loopcount;//counts steps in traceing a shape through the structure
hierarchy
char atnames[120][7]; //to be read from atwts.in, large to permit isotopes
char stnames[25][20],        //array of structure names
     subnames[25][20][20];   //array of substructure names within structure
int nstoccrrncs[25]={0},  //number of occurrences for this structure
    nsuboccrrncs[25][20]={{0}}, //number of this substructure occurrences
     numsubs[25];          //number of substructures in this structure
int getcomps(int,char*); //returns num occurrences of this component in
structure
float atwts[100],//array of atomic weights
    afcone(float,float,float),//calculates area of the frustrum of a cone
     vfcone(float,float,float);//calculates volume of the frustrum of a cone
float matvolume[100]={0},//accumulates total volume of material i
    smass[100]={0},//accumulates total mass for all occurrences of shape i
     sarea[100]={0},//accumulates total area for all occurrences of shape i
     svolume[100]={0};//accumulates total volume for all occurrences of shape
i
int calcoccrrncs(char*),//calc number of occurrences of a shape or structure
    ctoi(char),//converts a character to an integer, which is a single digit
     numcases,//number of cases to be run
    foundc; //used as BOOL for occurrence of a shape

void main()
{int i=0,j,k,key,ii,found,nratelines;
float steelratefac[6],//factors for steel rates, from fratefracs
     glassratefac[6],//factors for glass rates, from fratefracs
      fuelratefac[6],//factors for fuel rates, from fratefracs
      dripratefac[6],//factors for drip rates, from fratefracs
     fuelfac,glassfac,dripfac,steelfac;//case specific factors
char dummy[100],creatstr[50],datestr[15],filestr[15],*p;
for(i=0;i<20;i++)fudgefac[i]=1;//nominal value for unused parameter
bldatwts();//read table of atomic weights
if((fin=fopen("data.in","r"))==NULL)
  {printf("couldn't open data input\n");
  exit(0);}
if((fratefacs=fopen("ratefacs.in","r"))==NULL)
  {printf("couldn't open ratefactor file\n");
```

```
  exit(0);}
ferr=fopen("junk.out","w");
i=0;
while((fgets(dummy,90,fratefacs)!=NULL)&&(i<10))//copy ratefac lines into
array
  strcpy(rlines[i++],dummy);
nratelines=i;//now build the ratefac arrays
bldratefacarry("glassratefac",glassratefac,0,nratelines);
bldratefacarry("steelratefac",steelratefac,0,nratelines);
bldratefacarry("fuelratefac",fuelratefac,0,nratelines);
bldratefacarry("dripratefac",dripratefac,0,nratelines);
fclose(fratefacs);//now we'll re-use the array lines[]
printf("rate arrays built\n");
i=0;   //the following lines copy non-comment lines of data.in into lines[]
while((fgets(dummy,90,fin)!=NULL)&&(i<700))
  {if(dummy[0]=='*') fprintf(ferr,"%s",dummy);//divert comment to "junk.out"
  else strcpy(lines[i++],dummy);}
numlines=i;
printf("data.in copied\n");
getstr("creator",creatstr,0);//build the header and the arrays of case
parameters
getstr("date",datestr,1);
i=2;
while((lines[i][0]>48)&&(i<50))i++;//read to end of first block
numcases= i/2 - 1;
for(i=0;i<numcases;i++)
  {getstr("filename",filenames[i],2*i+2);
  strcpy(casedescs[i],lines[2*i+3]);}
i=2*numcases+2;//The following loop builds a data array for each shape,
material, structure
printf("header built\n");
while (i<=numlines)
  {while((lines[i][0]<48)&&(i<numlines))i++;//readthrough blank lines and any
                                          //namelist items
  if(i>=numlines)break;
  if((key=get1of3("shape","material","structure",i))==0)//type of block
     errproc("shape or material or structure",lines[i]);
  i+=buildvals(key,i);}//build array for this block
bldmoles();//comprehensive calculations of areas and volumes
printf("BY SHAPE\n");//diagnostic print to screen and file
fprintf(ferr,"BY SHAPE\n");
for(i=0;i<numshapes;i++)
  {printf("%s Area=%f Volume=%f Material=%s\n",
              shapenames[i],sarea[i],svolume[i],mtrl[i]);
  fprintf(ferr,"%s Area=%f Volume=%f Material=%s\n",
              shapenames[i],sarea[i],svolume[i],mtrl[i]);}
printf("\nBY MATERIAL\n");
fprintf(ferr,"\nBY MATERIAL\n");
for(i=0;i<nummaterials;i++)
  {printf("%s Density=%f Moles=%f Area=%g Volume=%g\n",
        matnames[i],densities[i],nmoles[i],mareas[i],matvolume[i]);
  fprintf(ferr,"%s Density=%f Moles=%f Area=%g Volume=%g\n",
        matnames[i],densities[i],nmoles[i],mareas[i],matvolume[i]);}
printf("%d input lines read\n",numlines);
for(ii=0;ii<numcases;ii++)//main loop to generate each case
  {steelfac=steelratefac[ctoi(filenames[ii][4])];//build rate factors
  glassfac=glassratefac[ctoi(filenames[ii][5])]; //for this case
```

```
fuelfac=fuelratefac[ctoi(filenames[ii][6])];
dripfac=dripratefac[ctoi(filenames[ii][7])];
if((ftemp=fopen("template.in","r"))==NULL)
  {printf("couldn't open template file\n");
  exit(0);}
if(filenames[ii][3]=='g')goethflag=1;
else goethflag=0;
if(ctoi(filenames[ii][5])==0)glassflag=0;
else glassflag=1;
if(ctoi(filenames[ii][6])==0)fuelflag=0;
else fuelflag=1;
strcpy(filestr,filenames[ii]);
strcat(filestr,".6i");
if((fout=fopen(filestr,"w"))==NULL)errproc("cant open",filestr);
outline(70);//print output file header
fprintf(fout,"|EQ6 input file name= %-12s",filestr);
for(i=0;i<37;i++)fprintf(fout,"%c",' ');
fprintf(fout,"%c\n",'|');
etrim(casedescs[ii]);
fprintf(fout,"%c%-70s%c\n",'|',casedescs[ii],'|');
fprintf(fout,"|Created %-13sCreator= %-40s%c\n",datestr,creatstr,'|');
found=0;
i=5;//starting line for a simple transfer
while((found==0)&&(i<120))
  {fgets(dummy,90,ftemp);
   if((p=strstr(dummy,"HLW_Glass"))!=NULL)found=1;
   etrim(dummy);
   if((found==0)||(glassflag!=0))fprintf(fout,"%s\n",dummy);
   i++;}
if(found==0)errproc("Missing HLW_Glass in first 120 lines","");
found=0;
if(glassflag!=0)
 {while((found==0)&&(i<120))
  {fgets(dummy,90,ftemp);
   if((p=strstr(dummy,"rk1"))!=NULL)
     {found=1;
      p=strchr(p,'|');
      k=(int)(p-dummy);
      fprintf(fout,"| rate constant rk1| %-20e|csigma1  |              |\n",
             (float)atof(p+1)*glassfac);}
   else
        {etrim(dummy);
         fprintf(fout,"%s\n",dummy);}}
 if(found==0)errproc("Missing glass rk1 in first 120 lines","");}
else //skip glass reactant data if glassfac=0
  {i=0;
   while((found==0)||(i<50))
     {fgets(dummy,90,ftemp);
      if(dummy[0]='c')found=1;
      i++;}
  if(found==0)errproc("template file out of sync???","");}
for(j=0;j<2;j++)//now do blocks for OutWeb and GPC steel
  {i=0;
  found=0;
  while((found==0)&&(i<30))
    {fgets(dummy,90,ftemp);
     if((p=strstr(dummy,"rk1"))!=NULL)
```

```
        {found=1;
         p=strchr(p,'|');
         k=(int)(p-dummy);
         fprintf(fout,"| rate constant rk1| %-20e|csigma1   |
|\n",
               (float)atof(p+1)*steelfac);}
       else
          {etrim(dummy);
          fprintf(fout,"%s\n",dummy);}}
    if(found==0)errproc("Missing an rk1 in a steel block","");}
  i=0;
  found=0;      //now do canister steel block
  while((found==0)&&(i<30))
    {fgets(dummy,90,ftemp);
     etrim(dummy);
    if((p=strstr(dummy,"reactant type"))==NULL)fprintf(fout,"%s\n",dummy);
     else found=1;}
  if(found==0)errproc("no reactant type for canister","");
  etrim(dummy);
  if(fuelflag!=0)fprintf(fout,"%s\n",dummy);
  else
   {for(i=0;i<3;i++)p=strchr(p+1,'|');
    fprintf(fout,"| reactant type    |  special             |sk       |");
    fprintf(fout,"%-14f|\n",atof(p+1)/2);}   //half area if no fuel
   i=0;
   found=0;
   while((found==0)&&(i<30))
      {fgets(dummy,90,ftemp);
       if((p=strstr(dummy,"rk1"))!=NULL)
         {found=1;
          p=strchr(p,'|');
          k=(int)(p-dummy);
          fprintf(fout,"| rate constant rk1| %-20e|csigma1   |
|\n",
               (float)atof(p+1)*steelfac);}
       else
          {etrim(dummy);
          fprintf(fout,"%s\n",dummy);}}
    if(found==0)errproc("Missing an rk1 in canister steel block","");
 for(i=0;i<2;i++)//last 2 lines of the SNF canister block but not the c---
line
  {fgets(dummy,90,ftemp);
  etrim(dummy);
  fprintf(fout,"%s\n",dummy);}
 if(fuelflag!=0)           //solids blocks for canister components
   for(i=0;i<nummaterials;i++)
    {strcpy(dummy,"c");
    for(j=2;j<72;j++)strcat(dummy,"-");
    strcat(dummy,"|");
    fprintf(fout,"%s\n",dummy);
    sprintf(dummy,"| %-17s| %-25s|status    | %-
13d|","REACTANT",matnames[i],0);
    fprintf(fout,"%s\n",dummy);
    sprintf(dummy,"| %-17s| %-25.6f|destroyed| %-13.5f|",
            "moles remaining",nmoles[i],0);//gm moles
    fprintf(fout,"%s\n",dummy);
    sprintf(dummy,"| %-17s| %-25s|sk        | %-13.5f|",
```

```
            "reactant type","special",mareas[i]);
      fprintf(fout,"%s\n",dummy);
      sprintf(dummy,"| %-17s| %-25d|fk        | %-13.5f|",
            "surface type",0,fudgefac[i]);
      fprintf(fout,"%s\n",dummy);
      sprintf(dummy,"| %-17s| %-25s|mole fr   | %-13s|",
            "end member","","");
      fprintf(fout,"%s\n",dummy);
      sprintf(dummy,"| %-17s| %-25.6f|          | %-13s|",
            "volume",mvolumes[i],"");
      fprintf(fout,"%s\n",dummy);
      for(j=0;j<compnums[i];j++)
        {if(compnames[i][j][0]=='U')strcpy(compnames[i][j],"U");//combine names
now
         sprintf(dummy,"| %-17s| %-25s|moles     | %-13.6e|","element",
            compnames[i][j],compvals[i][j]*100);//per 100 gm
        fprintf(fout,"%s\n",dummy);}
      sprintf(dummy,"| %-17s| %-25d|          | %-13s|","dissolution
law",dislaw,"");
      fprintf(fout,"%s\n",dummy);
      sprintf(dummy,"| %-17s| %-25.6g|csignal   | %-13s|",
            "rate constant rk1",degrates[i],"");
      fprintf(fout,"%s\n",dummy);
      sprintf(dummy,"| %-17s| %-25.2f|          | %-13s|",
            "temperature (C)",temperature,"");
      fprintf(fout,"%s\n",dummy);
      sprintf(dummy,"| %-17s| %-25d|          | %-13s|",
            "precipitation law",plaw,"");
      fprintf(fout,"%s\n",dummy);} //end of canister components
 i=0;
 found=0;
 while((found==0)&&(i<30)) //now do J-13 block
       {fgets(dummy,90,ftemp);
        if((p=strstr(dummy,"rk1"))!=NULL)
          {found=1;
           p=strchr(p,'|');
           k=(int)(p-dummy);
           fprintf(fout,"| rate constant rk1| %-20e|csigma1   |
|\n",
                (float)atof(p+1)*dripfac);}
        else
           {etrim(dummy);
           fprintf(fout,"%s\n",dummy);}}
 if(found==0)errproc("Missing an rk1 in a J-13 block","");
 found=0;
 while((found==0)&&(fgets(dummy,90,ftemp)!=NULL))//now copy to suppressed
species
  {if((p=strstr(dummy,"suppressed species"))!=NULL) found=1;
  etrim(dummy);
  fprintf(fout,"%s\n",dummy);}
 if(p==NULL)errproc("missing suppressed species in template\n","");
 fgets(dummy,90,ftemp);       //copy next line (block separator)
 etrim(dummy);
 fprintf(fout,"%s\n",dummy);
 i=0;
 found=0;
 while((i<30)&&(found==0))
```

```
  {fgets(dummy,90,ftemp);
  if(strncmp(dummy,"|------",4)==0)found=1;//find next block separator
  else
    {etrim(dummy);
     fprintf(fout,"%s\n",dummy);}}        //otherwise copy to output
 if(found==0)errproc("no end of suppressed species block","");
 if(goethflag==1)        //add hematite suppression
  fprintf(fout,"| Hematite                    | mineral        | suppress |
.00000E+00  |\n");
 etrim(dummy);
 fprintf(fout,"%s\n",dummy);//write separator and copy the rest of
template.in
 while((fgets(dummy,90,ftemp))!=NULL)
   {etrim(dummy);
    fprintf(fout,"%s\n",dummy);}
 fclose(ftemp);}//end this case
}//end main

//Determines  if line i starts a block of one of the 3 types
int get1of3(char *s1,char *s2,char *s3,int i)
{int j;
char *p,stag[20];
if((p=strchr(lines[i],'='))==NULL) return 0;
j=(int)(p-lines[i]);
strncpy(stag,lines[i],j);
stag[j]='\0';
etrim(stag);
if(strcmp(s1,stag)==0) return 1;
else if (strcmp(s2,stag)==0) return 2;
else if (strcmp(s3,stag)==0) return 3;
else return 0;}

//Builds data array for each block of data.in, including calculation of
//volume and surface area for each shape.
int buildvals(int type,int row)
{int i=1,j,numgrp,k;//number of lines in this block/group
char tempstr[100],stag[20];//to hold substrings for further processing
float x,y,z,r,t,t1,t2,f,a,turns,dr,r1,r2;//for shape dimensions
while((get1of3("shape","material","structure",row+i)==0)&&(lines[row+i][0]>=4
8)&&
    (row+i<=numlines))i++;   //find number of lines in this block
numgrp=i;//number of lines in this group/block
strcpy(tempstr,lines[row]);
if(type==2) //build array for this material block
  {get2(stag,tempstr,'=');
  strcpy(matnames[mindex],tempstr);
  if((densities[mindex]=findfloat("density",row,numgrp))==0)
            errproc("no density for ",tempstr);
  if((j=findstr(stag,"degrate",row,numgrp))==0)
            errproc("no degradation rate for ",tempstr);
  strcpy(tempstr,lines[row+j]);
  i=get2(stag,tempstr,'=');
  strcpy(tempstr,lines[row+j]+i+1);
  if((k=get2(stag,tempstr,' '))==-1)
          errproc("missing degrate units for ",matnames[mindex]);
  degrates[mindex]=(float)atof(stag);
  if(strcmp(tempstr,"moles")==0)degrates[mindex]*= -1;//flag for alternate
```

```
units
  else if (strcmp(tempstr,"grams")!=0)                    //used in bldmoles
    errproc("invalid name for degradation rate units for ",matnames[mindex]);
  if((compnums[mindex]=findint("numelements",row,numgrp))==0)
            errproc("no component number for ",tempstr);
  if(compnums[mindex]+3>numgrp)
    {printf("compnums=%d  numgrp=%d  nummtrls=%d\n",
                    compnums[mindex],numgrp,nummaterials);
     errproc("too many lines",tempstr);}
  for(j=0;j<compnums[mindex];j++)  //elements must be last
    {strcpy(tempstr,lines[row+4+j]);  //four lines for the previous items
    get2(stag,tempstr,'=');
    strcpy(compnames[mindex][j],stag);
   gramvals[mindex][j]=(float)atof(tempstr)/100;
    compvals[mindex][j]=
        gramvals[mindex][j]/atwts[findatwtindx(compnames[mindex][j])];}
  mindex++; //processing for this material completed
  nummaterials++;}
else if(type==1)//processing for a shape block
  {get2(stag,tempstr,'=');
  strcpy(shapenames[sindex],tempstr);
  if((j=findstr(stag,"type",row,numgrp))==0) errproc("no type for
shape",tempstr);
  strcpy(tempstr,lines[row+j]);
  i=get2(stag,tempstr,'=');
  strcpy(tempstr,lines[row+j]+i+1);
  get2(stag,tempstr,' ');
  if(strcmp(stag,"cube")==0) stype[sindex]=0;
  else if(strcmp(stag,"box")==0) stype[sindex]=1;
  else if(strcmp(stag,"cylinder")==0) stype[sindex]=2;
  else if(strcmp(stag,"sphere")==0) stype[sindex]=3;
  else if(strcmp(stag,"rtprism")==0) stype[sindex]=4;
  else if(strcmp(stag,"etprism")==0) stype[sindex]=5;
  else if(strcmp(stag,"hprism")==0) stype[sindex]=6;
  else if(strcmp(stag,"helix")==0) stype[sindex]=7;
  else if(strcmp(stag,"conefrustrum")==0) stype[sindex]=8;
  else if(strcmp(stag,"sphereseg")==0) stype[sindex]=9;
  else errproc("No shape type ",stag);
  if(strcmp(tempstr,"shell")==0) ttype[sindex]=0;
  else ttype[sindex]=1;
  occrrncs[sindex]=findint("occurrences",row,numgrp);//returns zero if the
                                                     //shape occurs in a structure
  if(findstr(stag,"matname",row,numgrp)==0) //material for this shape
     errproc("no material for shape",shapenames[sindex]);
  strcpy(mtrl[sindex],stag);
  if((x=findfloat("fracture_factor",row,numgrp))>0) fracfac=x;
  else fracfac=1;
  switch(stype[sindex])//get the appropriate dimensions for this shape
                       //and calculate its area and volume
  {case 0:                                           //cube
      if((x=findfloat("side",row,numgrp))==0)errproc("no side for ",stag);
       if(ttype[sindex]==1)  //for solid
         {areas[sindex]=6*(float)pow(x,2);
         areas[sindex]*=fracfac;
         volumes[sindex]=(float)pow(x,3);}
       else                  //for shell
         {if((t=findfloat("thickness",row,numgrp))==0)
```

```
            errproc("no thickness for cube shell","");
          areas[sindex]=6*(float)((pow(x,2)+pow(x-2*t,2)));
          areas[sindex]*=fracfac;
          volumes[sindex]=(float)((pow(x,3)-pow(x-2*t,3)));}
        break;
    case 1:                                          //rectangular box
      if((x=findfloat("side1",row,numgrp))==0)errproc("no side1 for ",stag);
      if((y=findfloat("side2",row,numgrp))==0)errproc("no side2 for ",stag);
      if((z=findfloat("side3",row,numgrp))==0)errproc("no side3 for ",stag);
       if(ttype[sindex]==1)
         {areas[sindex]=2*(x*y+y*z+x*z);
         areas[sindex]*=fracfac;
         volumes[sindex]=x*y*z;}
       else
         {if((t=findfloat("thickness",row,numgrp))==0)
             errproc("no thickness for box shell","");
         areas[sindex]=2*(x*y+y*z+x*z)
             +2*(float)((x-2*t)*(y-2*t)+(y-2*t)*(z-2*t)+(z-2*t)*(x-2*t));
         areas[sindex]*=fracfac;
        volumes[sindex]=x*y*z-(x-2*t)*(y-2*t)*(z-2*t);}
       break;
    case 2:                                         //cylinder
      if((r=findfloat("radius",row,numgrp))==0)errproc("no radius for
",stag);
      if((z=findfloat("length",row,numgrp))==0)errproc("no length for
",stag);
       if(ttype[sindex]==1)
         {areas[sindex]=2*PI*r*z+2*PI*r*r;
         areas[sindex]*=fracfac;
         volumes[sindex]=PI*r*r*z;}
       else
         {if((t=findfloat("thickness",row,numgrp))==0)
             errproc("no thickness for cylinder shell","");
         areas[sindex]=2*PI*r*z+2*PI*(r-t)*z;
         areas[sindex]*=fracfac;
        volumes[sindex]=PI*r*r*z-PI*(r-t)*(r-t)*z;}
       break;
   case 3:                              //sphere
      if((r=findfloat("radius",row,numgrp))==0)errproc("no radius for
",stag);
       if(ttype[sindex]==1)
         {areas[sindex]= 4*PI*r*r;
         areas[sindex]*=fracfac;
         volumes[sindex]=4*PI*r*r*r/3;}
       else
         {if((t=findfloat("thickness",row,numgrp))==0)
             errproc("no thickness for spherical shell","");
         areas[sindex]=4*PI*(r*r+(r-t)*(r-t));
         areas[sindex]*=fracfac;
        volumes[sindex]=4*PI*r*r*r/3-4*PI*(r-t)*(r-t)*(r-t)/3;}
       break;
    case 4:                              //isoceles right triangle prism
      if((x=findfloat("side",row,numgrp))==0)errproc("no side for ",stag);
      if((z=findfloat("length",row,numgrp))==0)errproc("no length for
",stag);
      f=2+(float)sqrt(2);      // also 1+cot(22.5deg)
       if(ttype[sindex]==1)
```

```
        {areas[sindex]=x*f*z+x*x; //area of sides and ends
        areas[sindex]*=fracfac;
        volumes[sindex]=x*x*z/2;}
      else
        {if((t=findfloat("thickness",row,numgrp))==0)
            errproc("no thickness for right triangle prism shell","");
        areas[sindex]=x*f*z+(x-f*t)*f*z;
        areas[sindex]*=fracfac;
       volumes[sindex]=(x*x-(x-f*t)*(x-f*t))*z/2;}
      break;
   case 5:                              //equilateral triangle prism
     if((x=findfloat("side",row,numgrp))==0)errproc("no side for ",stag);
     if((z=findfloat("length",row,numgrp))==0)errproc("no length for
",stag);
       if(ttype[sindex]==1)
        {areas[sindex]=3*x*z+x*x*(float)sqrt(3)/2; //area of sides and ends
        areas[sindex]*=fracfac;
        volumes[sindex]=x*x*z*(float)sqrt(3)/4;}
      else
        {if((t=findfloat("thickness",row,numgrp))==0)
            errproc("no thickness for equilateral triangle prism shell","");
        f=2*(float)sqrt(3);      // also 2cot(30deg)
        areas[sindex]=3*x*z+3*(x-f*t)*z;
        areas[sindex]*=fracfac;
       volumes[sindex]=x*x*z*(float)sqrt(3)/4-(x-f*t)*(x-
f*t)*z*(float)sqrt(3)/4;}
      break;
   case 6:                              //hexagon based prism
     if((x=findfloat("side",row,numgrp))==0)errproc("no side for ",stag);
     if((z=findfloat("length",row,numgrp))==0)errproc("no length for
",stag);
       if(ttype[sindex]==1)
        {areas[sindex]=6*x*z+3*x*x*(float)sqrt(3); //area of sides and ends
        areas[sindex]*=fracfac;
        volumes[sindex]=6*x*x*z*(float)sqrt(3)/4;}
      else
        {if((t=findfloat("thickness",row,numgrp))==0)
            errproc("no thickness for hexagonal prism shell","");
        f=2/(float)sqrt(3);      // also 2tan(30deg)
        areas[sindex]=6*x*z+6*(x-f*t)*z;
        areas[sindex]*=fracfac;
       volumes[sindex]=6*x*x*z*(float)sqrt(3)/4
                       -6*(x-f*t)*(x-f*t)*z*(float)sqrt(3)/4;}
      break;
   case 7:                              //helix
     if((turns=findfloat("turns",row,numgrp))==0)
                     errproc("no turns for ",stag);
     if((a=findfloat("smallradius",row,numgrp))==0)
                     errproc("no smallradius for ",stag);
     if((r=findfloat("largeradius",row,numgrp))==0)
                     errproc("no largeradius for ",stag);
     if((z=findfloat("altitude",row,numgrp))==0)errproc("no altitude for
",stag);
       if(ttype[sindex]==1)
        {areas[sindex]=2*PI*a*(float)sqrt(z*z+pow(2*PI*r*turns,2));
        volumes[sindex]=areas[sindex]*a/2;
        areas[sindex]*=fracfac;}  //now adjust area for fractures
```

```
      else errproc("no helical shell","");
       break;
/* Alternative area=PI*a*z/sin(alph), where alph is the dihedral angle
between
   the horizontal and any tangent plane of the helix.  This formulation would
    require only 3 input parameters.*/

    case 8:                              //frustum of cone
      if((z=findfloat("altitude",row,numgrp))==0)errproc("no altitude for
",stag);
      if((r1=findfloat("bottomrad",row,numgrp))==0)
                           errproc("no bottom radius for ",stag);
      if((r2=findfloat("toprad",row,numgrp))==0)
                           errproc("no top radius for ",stag);
       if(ttype[sindex]==1)
         {areas[sindex]=afcone(r1,r2,z);
         areas[sindex]*=fracfac;
         volumes[sindex]=vfcone(r1,r2,z);}
      else
         {if((t=findfloat("thickness",row,numgrp))==0)
             errproc("no thickness for cone frustrum shell","");
        dr=t*(float)sqrt(1+pow(r1-r2,2)/z/z);
         areas[sindex]=afcone(r1,r2,z)+afcone(r1-dr,r2-dr,z);
        areas[sindex]-=PI*(r2*r2+r1*r1);//remove top and bottom from outer
        areas[sindex]-=PI*(pow(r2-dr,2)+pow(r1-dr,2));//and from inner
         areas[sindex]*=fracfac;
        volumes[sindex]=vfcone(r1,r2,z)-vfcone(r1-dr,r2-dr,z);}
       break;
   case 9://segment of a sphere; large and small radii of the segment (r1,r2)
          //are meassured from an axis of the sphere; the radius of the
           //actual sphere is derived from r1,r2, and the altitude, z. For a
           //shell, the thickness, t, is for the material itself.  The
           //projections of this thickness onto the large and small segment
           //planes are derived as the variables t1,t2.
      if((z=findfloat("altitude",row,numgrp))==0)//distance between top *
bottom
                           errproc("no altitude for ",stag);
       if((r1=findfloat("largerad",row,numgrp))==0)//
                           errproc("no largerad for ",stag);
      if((r2=findfloat("smallrad",row,numgrp))==0)
                           errproc("no smallrad for ",stag);
      r=(float)sqrt(r2*r2+pow(r1*r1-r2*r2+z*z,2)/(4*z*z));//radius of sphere
       if(ttype[sindex]==1)
         {areas[sindex]=PI*(2*r*z+r1*r1+r2*r2); //area of upper and lower too
         areas[sindex]*=fracfac;
         volumes[sindex]=PI*z*(z*z+3*(r1*r1+r2*r2))/6;}
      else
         {if((t=findfloat("thickness",row,numgrp))==0)
             errproc("no thickness for sphere segment shell","");
         t1=t*r/r1;//project thickness onto large plane of segment
         t2=t*r/r2;//onto the small plane of segment
         areas[sindex]=2*PI*(r*z+(r-t)*(z-t));
         areas[sindex]*=fracfac;
        volumes[sindex]=PI*z*(z*z+3*(r1*r1+r2*r2))/6
                     -PI*(z-t)*((z-t)*(z-t)+3*((r1-t1)*(r1-t1)+
                       (r2>t2?(r2-t2)*(r2-t2):0)))/6;}//If the small segement
radius
```

```
                        //is less than the projected thickness, it is omitted
from
                        //the volume calculation.  This is the usual
condition,
                        //since the segment is usually a cap.
       break;}
    sindex++;  //processing for this shape complete
    numshapes++;}
else if (type==3)//build array for this structure
  {get2(stag,tempstr,'=');
  strcpy(stnames[numstructures],tempstr);
  for(i=1;i<numgrp;i++)
    if((j=getcomps(row+i,stag))!=0)
       {nsuboccrrncs[numstructures][numsubs[numstructures]]=j;
        strcpy(subnames[numstructures][numsubs[numstructures]],stag);
      numsubs[numstructures]++;}
  nstoccrrncs[numstructures]=findint("occurrences",row,numgrp);
  numstructures++;}
return numgrp;}

//for a component line of a structure block, returns occurrences
int getcomps(int rw,char* retstr)
{int i;
char *p,stag[20],tempstr[100];
if(strncmp(lines[rw],"component",9)!=0) return 0;
strcpy(tempstr,lines[rw]);
p=strchr(lines[rw],'=');
i=(int)(p-lines[rw]);
strcpy(tempstr,lines[rw]+i+1);
get2(stag,tempstr,' ');
strcpy(retstr,stag);
return atoi(tempstr);}

float afcone(float rl,float ru,float h) //area of the frustum of a cone
{float area;
area=PI*(rl*rl+ru*ru);//top and bottom disks
area+= PI*h*(rl+ru)*(float)sqrt(1+pow(rl-ru,2)/h/h);
return area;}

float vfcone(float rl,float ru,float h) //volume of the frustum of a cone
{return PI*h*(rl*rl+rl*ru+ru*ru)/3;}

//Find the float numerical value in a statement that begins with the
specified
//keyword (keystr).
float findfloat(char* keystr,int startrow,int numrows)
{int i=0;
char stag[20],tempstr[100];
while ((strncmp(keystr,lines[startrow+i],strlen(keystr))!=0)&&(i<=numrows))
    i++;
if (i==numrows+1) return 0;
strcpy(tempstr,lines[startrow+i]);
get2(stag,tempstr,'=');
return (float)atof(tempstr);}

//Find the int numerical value in a statement that begins with the specified
//keyword (keystr).
```

```
int findint(char* keystr,int startrow,int numrows)
{int i=0;
char stag[20],tempstr[100];
while
((strncmp(keystr,lines[startrow+i],strlen(keystr))!=0)&&(i<=numrows))i++;
if (i>=numrows) return 0;
strcpy(tempstr,lines[startrow+i]);
get2(stag,tempstr,'=');
return atoi(tempstr);}

//This function searches for a key at the start of the line and copies the
//string (containing no blanks) following the equal sign into retstr.
//It returns zero if the keystring is not found, otherwise the row in which
found.
//It is analogous to findfloat and findint, but does not return the
//information, since C cannot assign to a character string.
int findstr(char *retstr,char *keystr,int startrow,int numrows)
{int i=0;
char stag[20],tempstr[100];
while
((strncmp(keystr,lines[startrow+i],strlen(keystr))!=0)&&(i<=numrows))i++;
if (i==numrows) return 0;
strcpy(tempstr,lines[startrow+i]);
get2(stag,tempstr,'=');
strcpy(retstr,tempstr);
return i;}

//copies the strings occurring before and after the separator c ('=' or ' ')
int get2(char *stag,char *sdummy,char c)
{int i,index,len;
char *p;
len=strlen(sdummy);
p=strchr(sdummy,c);
i=(int)(p-sdummy);
index=i;
strncpy(stag,sdummy,i);
stag[i]='\0';
etrim(stag);
strcpy(sdummy,p+1);
i=0;
while((sdummy[i]==' ')&&(i<len))i++;
if((i==len)||(sdummy[i]=='\n')) return -1;//can't find a second word on rt
side
strcpy(sdummy,sdummy+i);
while((sdummy[i]!=' ')&&(sdummy[i]!='\0')&&(sdummy[i]!='\n'))i++;
sdummy[i]='\0';
ftrim(sdummy);
return index;}

void etrim(char *dummy)//trims trailing blanks
{int i;
i=strlen(dummy)-1;
while(dummy[i]<=32)i--;
dummy[i+1]='\0';}

//trims leading blanks
void ftrim(char *dummy)     //use in get2 so that fdummy starts with a non-
```

```
blank
{int i=0;
while(dummy[i]<=32)i++;
strcpy(dummy,dummy+i);}

//prints a two string error message
void errproc(char *str1,char *str2)
{printf("%s %s\n",str1,str2);
exit(0);}

//accumulate total mass, area, and volume for shapes[j] and mtrls[i]
void bldmoles()
{int i,j,k;
float x,molwt,checkvol;
if((x=findfloat("$literswater",0,numlines))>0) literswater=x;
for(i=0;i<nummaterials;i++)
  {checkvol=0;
  for(j=0;j<numshapes;j++)
    if(strcmp(matnames[i],mtrl[j])==0)
          {if((k=occrrncs[j])==0)
             {foundc=0;
            loopcount=0;
              k=calcoccrrncs(shapenames[j]);
            if((foundc==0)||(k==0))errproc("no occurrences for
",shapenames[j]);}
           mass[i]+=volumes[j]*k*densities[i];
           mareas[i]+=areas[j]*k;
           checkvol+=volumes[j]*k;
           smass[j]+=volumes[j]*k*densities[i];
           sarea[j]+=areas[j]*k;
           svolume[j]+=volumes[j]*k;}
  fprintf(ferr,"composition of %s in grams, check vol=%f\n",
                          matnames[i],checkvol);
  for(j=0;j<compnums[i];j++)
    fprintf(ferr,"%s  %f\n",compnames[i][j],mass[i]*gramvals[i][j]);
  molwt=bldmolwt(i);
  degrates[i]/=100;
  if (degrates[i]<0) degrates[i]*= -molwt;//only use for molwt now
  mareas[i]/=literswater;
  mvolumes[i]=100/densities[i]; //used to be molwt/densities[i];
  matvolume[i]=mass[i]/densities[i];
  nmoles[i]=mass[i]/100/literswater;}} //used to be mass[i]/molwt/literswater

int calcoccrrncs(char* sstr)//num occurrences of sstr in this level or above
  //additive counter chains beginning at this level; multiplicative counter
  //for propagating a chain up the structure hierarchy
{int i,j,k,no,//multiplicative counter
    acount=0,//additive counter
     kk;
for(i=0;i<numstructures;i++)
  {j=0;
  while((j<numsubs[i])&&(kk=strcmp(subnames[i][j],sstr))!=0)j++;
  if(kk==0)
       {no=nsuboccrrncs[i][j];
       if((k=nstoccrrncs[i])>0)
         {no*=k;
          foundc=1;}      //found the end of the structure chain for this shape
```

```
       else
         {no*=calcoccrrncs(stnames[i]);
         loopcount++;
          if(loopcount>MAXLOOP) errproc("Idiot, you have an occurrence
loop","");}
      acount+=no;}}
return acount;}

//builds the molecular weight (from the atwts table) for each material block
//of the input; if the material contains more than one isotope of U, these
//are averaged together, and the individual isotope entries in the material
//components are collapsed into one atomic weight and one symbol using the
//variable Uxnames={"Ua",...}
float bldmolwt(int ndx)
{int j,k,kk,numUs,hasIso=0;
char *p;
float mwt=0;
j=0;
while ((j<compnums[ndx])&&((p=strchr(compnames[ndx][j],'-'))==NULL))j++;
if(p!=NULL)
  {hasIso=1;
  while ((j<compnums[ndx])&&((p=strchr(compnames[ndx][j],'-'))!=NULL))j++;
  if(j!=compnums[ndx]) errproc("","all isotopes must come last");}
if(hasIso==1)
 {j=compnums[ndx]-1;
 while((p=strchr(compnames[ndx][j],'-'))!=NULL)
  {if(((p-compnames[ndx][j])!=1)||(compnames[ndx][j][0]!='U'))
      errproc(compnames[ndx][j],"is a strange isotope");
    j--;}
 if(j<compnums[ndx]-1)
  {numUs=compnums[ndx]-j-1;
  for (k=0;k<numUs;k++)
    {kk=compnums[ndx]-k-1;
    mwtUxvals[numUwts]+=
        atwts[findatwtindx(compnames[ndx][kk])]*gramvals[ndx][kk];}
  compnums[ndx]-=numUs-1;
  strcpy(compnames[ndx][compnums[ndx]-1],Uxnames[numUwts]);
  atwts[numelements]=mwtUxvals[numUwts];
  strcpy(atnames[numelements],Uxnames[numUwts]);
  numelements++;
  numUwts++;}}
for(j=0;j<compnums[ndx];j++)//cycle through the elements of this material
  mwt+=atwts[findatwtindx(compnames[ndx][j])]*gramvals[ndx][j];
return mwt;}

void bldatwts()//builds the table of atomic weights from the file atwts.in
{int i=0;
if((fin=fopen("atwts.in","r"))==NULL)
  {printf("couldn't open atomic wts input\n");
  exit(0);}
while(fscanf(fin,"%s %f",atnames[i],&atwts[i])!=EOF)i++;
numelements=i;
fclose(fin);}

int findatwtindx(char elname[7]) //finds the atomic wt for the named element
{int i=0;
while((i<numelements)&&(strcmp(elname,atnames[i])!=0))i++;
```

```
if (i==numelements)
  errproc(elname," is not in the table of atomic weights");
return i;}

int ctoi(char c)
{char s[2];
s[0]=c;
s[1]='\0';
return atoi(s);}

void bldratefacarry(char* keystr,float *vals,int startrow,int numrows)
{int i,j,k=1,lnum,len,vcount,found=0;
char *p,dummy[100],dummy2[50];
i=startrow;
while(((k=strncmp(keystr,rlines[i],strlen(keystr)))!=0)
      &&(i<numrows+startrow))i++;
if(k!=0)errproc("no rates for ",keystr);
lnum=i;
p=strchr(rlines[lnum],'=');
strcpy(dummy,p+1);
ftrim(dummy);
len=strlen(dummy);
i=0;
vcount=1;//skip element 0 for consistency with flags in filename
while(i<len)
  {p=strchr(dummy,' ');
  if(p==NULL)
    {p=strchr(dummy,'\0');
     if(p==NULL)errproc("ill formed ratefac line for ",keystr);
     else found=1;}
  j=(int)(p-dummy);
  if(j>0)
    {strncpy(dummy2,dummy,j);
    dummy2[j]='\0';
    vals[vcount++]=(float)atof(dummy2);
    strcpy(dummy,p+1);
    ftrim(dummy);
    i+=j;}}}

void getstr(char* keystr,char* retstr,int lnum)
{char *p;
if(strncmp(keystr,lines[lnum],strlen(keystr))!=0)
    errproc("Not in proper place, ",keystr);
p=strchr(lines[lnum],'=');
strcpy(retstr,p+1);
ftrim(retstr);
etrim(retstr);}

void outline(int n)
{int i;
fprintf(fout,"%c",'|');
for(i=0;i<n;i++)fprintf(fout,"%c",'-');
fprintf(fout,"%c\n",'|');}
```

2. Documentation of correct results

Table II-1 presents the volume and area of various shapes calculated by eqsetup using input files "triga.txt" and "test.txt," with the results presented in output files "trigajunk.out" and "testjunk.txt." The hand calculations differed slightly from the eqsetup results for the volume of the spherical segment shell. This is because the hand calculations used a horizontal cut at the base of the spherical segment; whereas, eqsetup used a cut perpendicular to the radius of curvature. The hand calculations confirmed that the eqsetup results are correct.

Table II-1. Comparison of Eqsetup and Hand Calculation Results to Confirm Eqsetup Software Routine

Item Name	Shape with Number of Items in Parentheses	Volume (cm^3)				Area (cm^2)			
		Eqsetup Result		Hand Calculated		Eqsetup Result		Calculated	
		Volume All Items	Volume 1 Item	Volume Equation[a]	Volume	Area All Items	Area 1 Item	Area Equation[a]	Area
sstubes	cylinder shell (111)	88401	796	volume=PI*rout^2*L-PI*(rout-thickness)^2*L	796	319297	2877	area=2*PI*rout*L+2*Pi*(rout-thickness)*L	2877
baseplate	cyldinder solid (3)	4062	1354	volume=PI*r^2*L	1354	8933	2978	area=2*PI*r*L+2*PI*r^2	2978
bracket	box solid (36)	3970	110	volume=L1*L2*L3	110	11400	317	area=2*L1*L2+2*L1*L3+2*L2*L3	317
fitting	conefrustrum solid (222)	7453	34	volume=1/3*(areabase+areatop+(areabase*areatop)^(1/2))*alt	34	14619	66	area=PI*rbase^2+PI*rtop^2+1/2*(2*PI*rbase+2*PI*rtop)*(alt^2+(rbase-rtop)^2)^(1/2)	66
impactplates 2	sphereseg solid (2)	8426	4213	volume=1/6*PI*alt*(3*rtop^2+3*rbottom^2+alt^2)	4213	6382	3191	R (radius of circle)=sqrt(1/(4*alt^2)*(rbot^2-rtop^2+alt^2)^2+rtop^2) area=2*PI*R*alt+PI*(rbot^2+rtop^2)	5 3191
dishheadsph	sphereseg shell (2) (like a cap)	2995	1498	Rout(radius of outer circle)=sqrt(1/(4*alt^2)*(rbot^2-rtop^2+alt^2)^2+rtop^2) volume=1/3*PI*alt^2*(3*Rout-alt)-1/3*PI*(alt-t)^2*(3*(Rout-t)-(alt-t))	47 1520	6389	3194	area=2*PI*Rout*alt+2*PI*(Rout-t)*(alt-t)	3194
shape1	cube solid (10)	80	8	volume=side^3	8	240	24	area=6*side^2	24
shape2	cube shell (10)	22	2	volume=side^3-(side-2*t)^3	2	434	43	area=6*side^2+6*(side-2*t)^2	43
shape3	box shell (10)	48	5	volume=L1*L2*L3-(L1-2*t)*(L2-2*t)*(L3-2*t)	5	970	97	area=2*(L1*L2+L1*L3+L2*L3+(L1-2*t)*(L2-2*t)+(L1-2*t)*(L3-2*t)+(L2-2*t)*(L3-2*t))	97
shape4	sphere solid (10)	335	34	volume=4/3*PI*r3	34	503	50	area=4*PI*r^2	50
shape5	sphere shell (10)	48	5	volume=4/3*PI*(r^3-(r-t)^3)	5	956	96	area=4*PI*(r^2+(r-t)^2	96
shape6	rtprism solid (10)	400	40	volume=1/2*side^2*length	40	1406	141	area=2*(1/2*side^2)+(side+side+hypotenuse)*length	141

Table II-1. Comparison of Eqsetup and Hand Calculation Results to Confirm Eqsetup Software Routine (continued)

Item Name	Shape with Number of Items in Parentheses	Volume (cm^3)				Area (cm^2)			
		Eqsetup Result		Hand Calculated		Eqsetup Result		Calculated	
		Volume All Items	Volume 1 Item	Volume Equation[a]	Volume	Area All Items	Area 1 Item	Area Equation[a]	Area
shape7	rtprism shell (10)	125	12	volume=1/2*length*(side^2-(side-t-t/tan(22.5*PI/180))^2)	12	2498	250	hypotenuseinside=sqrt(2*(side-t-t/tan(22.5*PI/180))^2) area=(side+side+hypotenuse)*length+(side-t-t/tan(22.5)+side-t-t/tan(22.5)+hypotenuseinside)*length	2 250
shape8	etprism solid (10)	346	35	volume=1/4*side^2*(3^(1/2))*length	35	1234	123	area=3*side*length+2*1/4*side^2*(3^(1/2))	123
shape9	etprism shell (10)	110	11	volume=3^(1/2)/4*length*(side^2-(side-2*t*3^(1/2))^2)	11	2192	219	area=3*length*(side+side-2*t*3^(1/2))	219
shape10	hprism solid (10)	2079	208	volume=3/2*side^2*(3^(1/2))*length	208	2607	261	area=3*side^2*(3^(1/2))+6*side*length	261
shape11	hprism shell (10)	233	23	volume=3/2*3^(1/2)*length*(side^2-(side-2*t/3^(1/2))^2)	23	4661	466	area=6*length*(side+side-2*t/(3^(1/2)))	466
shape12	helix solid (10)	124	12	volume=#turns*2*PI^2*larger*smallr^2	12	2472	247	area=#turns*4*pi^2*larger*smallr	247
shape13	conefrustum shell (10)	154	15	a (horizontal thickness)=t/sin(invtan(h/(rbot-rtop))) volume=1/3*PI*H*((rbot^2+rtop^2+rbot*rtop)-((rbot-a)^2+(rtop-a)^2+(rtop-a)*(rbot-a))	0.20 15	1537	154	s (slant height) =(alt^2+(rbase-rtop)^2)^(1/2) area=1/2*s*(2*PI*rbase+2*PI*rtop+2*PI*(rbase-a)+2*PI*(rtop-a))	5 154

SOURCE: [a] References 33 and 34.

3. Sample input file: triga.txt

```
creator=Susan LeStrange
date=July 7, 1999
filename=abcx1111
this is the hematite case
filename=abbg1102
this is the goethite case

structure=fuelrods
component=trigaIA 111
occurrences=1

structure=trigaIA
component=fuel 1
component=centerrod 1
component=upperreflector 1
component=lowerreflector 1
component=cladding 1
component=fitting 2


$literswater=4100

*   We are assuming all the rods are the standard-streamline fuel types
*   of the TRIGA-SS FLIP type. The absorber is Alloy 22 with 8 mole% Gd.

shape=fuel
type=cylinder shell
length=38.1
radius=1.82245
thickness=1.50495
matname=UZrHFLIP

shape=centerrod
type=cylinder solid
length=38.1
radius=0.28575
matname=zirc

shape=upperreflector
type=cylinder solid
length=6.5024
radius=1.82245
matname=graphite

shape=lowerreflector
type=cylinder solid
length=9.4488
radius=1.82245
matname=graphite

shape=cladding
```

type=cylinder shell
length=57.531
radius=1.87706
thickness=0.0508
matname=304LSSC

shape=fitting
type=conefrustrum solid
bottomrad=1.87706
toprad=0.01
altitude=9.05
matname=304LSSD

* DOE Canister

shape=outer18pipe
type=cylinder shell
length=299.9
radius=22.86
thickness=0.9525
matname=316LSSE
occurrences=1

shape=dishheadsph
type=sphereseg shell
altitude=5.94
largerad=22.86
smallrad=0.001
thickness=0.9525
matname=316LSSE
occurrences=2

shape=plugplates
type=cylinder solid
length=0.64
radius=3.34
matname=316LSSE
occurrences=2

shape=plugs
type=cylinder solid
length=1.27
radius=1.27
matname=316LSSE
occurrences=2

shape=liftingrings
type=cylinder shell
length=1.27
radius=21.755
thickness=2.5399
matname=316LSSE
occurrences=2

shape=backingring
type=cylinder shell

length=5.08
radius=21.905
thickness=0.47752
matname=316LSSE
occurrences=1

structure=impactplate
component=impactplates1 1
component=impactplates2 1
component=impactplatemeet -1
occurrences=2

shape=impactplates1
type=cylinder solid
length=0.9144
radius=21.275
matname=A516Grade70

shape=impactplates2
type=sphereseg solid
altitude=4.17
largerad=22.19
smallrad=12.04
matname=A516Grade70

shape=impactplatemeet
type=cylinder solid
length=0.001
radius=21.275
matname=A516Grade70

* Basket Structure

shape=sstubes
type=cylinder shell
length=83.6
radius=3.015
thickness=0.55372
matname=316LSSG
occurrences=111

shape=baseplate
type=cylinder solid
length=0.95
radius=21.3
matname=316LSSG
occurrences=3

shape=abstubes
type=cylinder shell
length=83.6
radius=2.46
thickness=0.1
matname=alloy22Gd

occurrences=45

shape=bracket
type=box solid
side1=10.798
side2=0.79
side3=12.928
matname=316LSSG
occurrences=36

* Material Descriptions

material=alloy22Gd
density=8.534171
degrate=2.7043E-12 grams
numelements=10
C=0.012415727
P=0.016554303
S=0.016554303
Si=0.066217212
Cr=17.58894707
Mn=0.413857578
Fe=5.589382029
Ni=45.32982052
Mo=12.4699554
Gd=18.49629586

material=UZrHFLIP
density=5.947
degrate=1.8928E-12 grams
numelements=4
H=1.588616303
Zr=89.86145852
U-238=2.5737
U-235=5.9762

material=zirc
density=6.49
degrate=4.0E-14 grams
numelements=1
Zr=100

*assume nuclear grade graphite bulk density

material=graphite
density=2.25
degrate=4.0E-14 grams
numelements=1
C=100

material=A516Grade70
density=7.850
degrate=8.7063E-10 grams
numelements=6
C=0.28
Mn=1.045

P=0.035
S=0.035
Si=0.29
Fe=98.315

material=316LSSE
density=7.980
degrate=2.52871E-12 grams
numelements=10
C=0.03
Mn=2.0
P=0.045
S=0.03
Si=1.0
Cr=17.0
Ni=12.0
Mo=2.5
N=0.1
Fe=65.295

material=316LSSG
density=7.980
degrate=2.52871E-12 grams
numelements=10
C=0.03
Mn=2.0
P=0.045
S=0.03
Si=1.0
Cr=17.0
Ni=12.0
Mo=2.5
N=0.1
Fe=65.295

material=304LSSC
density=7.940
degrate=2.51603E-12 grams
numelements=9
C=0.03
Mn=2.0
P=0.045
S=0.03
Si=0.75
Cr=19.0
Ni=10.0
N=0.1
Fe=68.045

material=304LSSD
density=7.940
degrate=2.51603E-12 grams
numelements=9
C=0.03
Mn=2.0
P=0.045

S=0.03
Si=0.75
Cr=19.0
Ni=10.0
N=0.1
Fe=68.045

Sample input file: test.txt

```
creator=Susan LeStrange
date=July 7, 1999
filename=abcx1111
this is the hematite case

structure=assembly
component=shape1 10
component=shape2 10
component=shape3 10
component=shape4 10
component=shape5 10
component=shape6 10
component=shape7 10
component=shape8 10
component=shape9 10
component=shape10 10
component=shape11 10
component=shape12 10
component=shape13 10
occurrences=1

shape=shape1
type=cube solid
side=2.0
matname=316LSS

shape=shape2
type=cube shell
side=2.0
thickness=0.1
matname=316LSS

shape=shape3
type=box shell
side1=2.0
side2=3.0
side3=4.0
thickness=0.1
matname=316LSS

shape=shape4
type=sphere solid
radius=2.0
matname=316LSS

shape=shape5
type=sphere shell
radius=2.0
thickness=0.1
matname=316LSS

shape=shape6
type=rtprism solid
```

side=2.0
length=20.0
matname=316LSS

shape=shape7
type=rtprism shell
side=2.0
length=20.0
thickness=0.1
matname=316LSS

shape=shape8
type=etprism solid
side=2.0
length=20.0
matname=316LSS

shape=shape9
type=etprism shell
side=2.0
length=20.0
thickness=0.1
matname=316LSS

shape=shape10
type=hprism solid
side=2.0
length=20.0
matname=316LSS

shape=shape11
type=hprism shell
side=2.0
length=20.0
thickness=0.1
matname=316LSS

shape=shape12
type=helix solid
altitude=25.0
smallradius=0.1
largeradius=0.5
turns=125
matname=316LSS

shape=shape13
type=conefrustrum shell
altitude=5.0
bottomrad=3.0
toprad=2.0
thickness=0.2
matname=316LSS

material=316LSS
density=7.980
degrate=2.516E-12 grams

numelements=10
C=0.03
Mn=2.0
P=0.045
S=0.03
Si=1.0
Cr=17.0
Ni=12.0
Mo=2.5
N=0.1
Fe=65.295

4. Sample output file: trigajunk.out

```
*    We are assuming all the rods are the standard-streamline fuel types
*    of the TRIGA-SS FLIP type. The absorber is Alloy 22 with 8 mole% Gd.
*   DOE Canister
*   Basket Structure
*   Material Descriptions
*assume nuclear grade graphite bulk density
composition of alloy22Gd in grams, check vol=5696.601074
C 6.036001
P 8.048001
S 8.048001
Si 32.192003
Cr 8551.001596
Mn 201.200034
Fe 2717.320842
Ni 22037.439589
Mo 6062.364356
Gd 8992.115820
composition of UZrHFLIP in grams, check vol=42788.152344
H 4042.411243
Zr 228662.492383
U-238 6549.066536
U-235 15207.106950
composition of zirc in grams, check vol=1084.851440
Zr 7040.685547
composition of graphite in grams, check vol=18474.703125
C 41568.082031
composition of A516Grade70 in grams, check vol=11023.248047
C 242.290969
Mn 904.264538
P 30.286371
S 30.286371
Si 250.944224
Fe 85074.420156
composition of 316LSSE in grams, check vol=44388.121094
C 106.265171
Mn 7084.344217
P 159.397746
S 106.265171
Si 3542.172108
Cr 60216.927821
Ni 42506.065300
Mo 8855.430601
N 354.217236
Fe 231286.129030
composition of 316LSSG in grams, check vol=96432.812500
C 230.860173
Mn 15390.677156
P 346.290238
S 230.860173
Si 7695.338578
Cr 130820.760126
Ni 92344.062936
Mo 19238.347162
```

N 769.533912
Fe 502467.135095
composition of 304LSSC in grams, check vol=3774.243164
C 8.990247
Mn 599.349791
P 13.485370
S 8.990247
Si 224.756172
Cr 5693.823073
Ni 2996.749068
N 29.967492
Fe 20391.379396
composition of 304LSSD in grams, check vol=7452.574707
C 17.752033
Mn 1183.468802
P 26.628048
S 17.752033
Si 443.800801
Cr 11242.953726
Ni 5917.344229
N 59.173444
Fe 40264.569520
BY SHAPE
fuel Area=56863.218750 Volume=42788.152344 Material=UZrHFLIP
centerrod Area=7649.958984 Volume=1084.851440 Material=zirc
upperreflector Area=10581.199219 Volume=7531.088867 Material=graphite
lowerreflector Area=14326.184570 Volume=10943.614258 Material=graphite
cladding Area=148592.203125 Volume=3774.243164 Material=304LSSC
fitting Area=14618.901367 Volume=7452.574707 Material=304LSSD
outer18pipe Area=84356.625000 Volume=40174.828125 Material=316LSSE
dishheadsph Area=6388.553711 Volume=2994.970459 Material=316LSSE
plugplates Area=167.047272 Volume=44.859325 Material=316LSSE
plugs Area=40.536598 Volume=12.870369 Material=316LSSE
liftingrings Area=653.853699 Volume=830.361572 Material=316LSSE
backingring Area=1383.111328 Volume=330.231842 Material=316LSSE
impactplates1 Area=5932.325684 Volume=2600.489990 Material=A516Grade70
impactplates2 Area=6382.131348 Volume=8425.601563 Material=A516Grade70
impactplatemeet Area=-5688.128418 Volume=-2.843931 Material=A516Grade70
sstubes Area=319296.937500 Volume=88400.554688 Material=316LSSG
baseplate Area=8933.275391 Volume=4062.130859 Material=316LSSG
abstubes Area=113931.992188 Volume=5696.601074 Material=alloy22Gd
bracket Area=11400.486328 Volume=3970.125977 Material=316LSSG

BY MATERIAL
alloy22Gd Density=8.534171 Moles=0.118575 Area=27.7883 Volume=5696.6
UZrHFLIP Density=5.947000 Moles=0.620637 Area=13.8691 Volume=42788.2
zirc Density=6.490000 Moles=0.017172 Area=1.86584 Volume=1084.85
graphite Density=2.250000 Moles=0.101386 Area=6.07497 Volume=18474.7
A516Grade70 Density=7.850000 Moles=0.211055 Area=1.61618 Volume=11023.2
316LSSE Density=7.980000 Moles=0.863944 Area=22.6804 Volume=44388.1
316LSSG Density=7.980000 Moles=1.876912 Area=82.8368 Volume=96432.8
304LSSC Density=7.940000 Moles=0.073091 Area=36.242 Volume=3774.24
304LSSD Density=7.940000 Moles=0.144325 Area=3.56559 Volume=7452.57

Sample output file: testjunk.txt

composition of 316LSS in grams, check vol=4102.795410
C 9.822092
Mn 654.806118
P 14.733138
S 9.822092
Si 327.403059
Cr 5565.852187
Ni 3928.836709
Mo 818.507678
N 32.740308
Fe 21377.782856
BY SHAPE
shape1 Area=240.000000 Volume=80.000000 Material=316LSS
shape2 Area=434.399994 Volume=21.680000 Material=316LSS
shape3 Area=970.400024 Volume=48.480000 Material=316LSS
shape4 Area=502.654846 Volume=335.103210 Material=316LSS
shape5 Area=956.300781 Volume=47.794109 Material=316LSS
shape6 Area=1405.685425 Volume=400.000000 Material=316LSS
shape7 Area=2498.233887 Volume=124.911690 Material=316LSS
shape8 Area=1234.640991 Volume=346.410187 Material=316LSS
shape9 Area=2192.153809 Volume=109.607712 Material=316LSS
shape10 Area=2607.846191 Volume=2078.460938 Material=316LSS
shape11 Area=4661.436035 Volume=233.071808 Material=316LSS
shape12 Area=2472.395996 Volume=123.619804 Material=316LSS
shape13 Area=1536.559082 Volume=153.655930 Material=316LSS

BY MATERIAL
316LSS Density=7.980000 Moles=0.083161 Area=5.51504 Volume=4102.8

File: atwts.in

```
H         1.00794
He         4.0026
Li          6.941
B          10.811
C          12.011
N        14.00674
O         15.9994
F         18.9984
Na       22.98977
Mg         24.305
Al       26.98154
Si        28.0855
P        30.97376
S           32.066
Cl        35.4527
K         39.0983
Ca         40.078
Ti          47.88
V         50.9415
Cr        51.9961
Mn       54.93805
Fe         55.847
Co        58.9332
Ni          58.69
Cu         63.546
Zn          65.39
As       74.92159
Sr            87.62
Zr          91.224
Nb       92.90638
Mo            95.94
Tc       98.90628
Ru          101.07
Rh       102.9055
Ag       107.8682
Cd        112.411
In          114.82
Sn          118.71
Cs       132.9054
Ba        137.327
La       138.9055
Ce        140.115
Nd          144.24
Sm          150.36
Eu        151.965
Gd          157.25
Hf          178.49
Ta       180.9480
W           183.85
Pb           207.2
Th       232.0381
U        238.0289
U-233    233.0395
```

U-234	234.0409
U-235	235.0439
U-236	236.0456
U-238	238.0508
Np	237.048
Pu	239.0521
Er	167.26

File: template.in

```
|Revised              Revisor=                                                |
|========== Change History ==========================================|
| 5/22/99 this is set t01, revised from set t00 to NOT use EDA-2.      |
|Derived from r4noc30.6i (No Calcite control in 3i, log10 fO2= -3.0 in |
|  J13noc30.3i).                                                       |
|========== End Change History ========================================|
|Reference spreadsheet for rates, compositions, moles and surface area:|
| CPU# 116720; Sandia CPU# S803293 TRIGA_common_items.xls              |
|NOTE on file name format: pRRxSGFJ.6i :                               |
| -First char always 't' for TRIGA;                                    |
| -Second, 3rd and 4th chars give revision #s, special constraints     |
|   (up to originator);                                                |
| -5th, 6th, 7th and 8th chars give rate info, per codes in sheet      |
|   'Rates' of pu-ceram.xls:                                           |
|   S indicates Steel rates, and gives number 1 to ns;                 |
|   G indicates Glass rates; 0 when glass not present;                 |
|   F indicates Fissile rates; 0 when fissile (e.g. UZrH) not present; |
|   J indicates J-13 drip rates, 1 to 4, viz:                          |
|     1 = 0.0015 m^3/year                                              |
|     2 = 0.015  m^3/year                                              |
|     3 = 0.15   m^3/year                                              |
|     4 = 0.5    m^3/year.                                             |
|NOTE: All special reactants (except J-13) forced to 100 g/mol in orig.|
|NOTE: suppress dolomites, micas, zircon, Celadonite because they are  |
|  extremely unlikely to form at low T.  Suppress BaZrO3 because of    |
|  suspicions about data quality.  Suppress more stable Quartz         |
|  because J-13 water is supersaturated with respect to these.         |
|----------------------------------------------------------------------|
| calculational mode   |*normal     | economy           | super economy|
|----------------------------------------------------------------------|
| model type           |*titration  | closed            | open         |
|----------------------------------------------------------------------|
| temperature model    |*power      | fluid mixing                     |
|----------------------------------------------------------------------|
c power model  -->   temp = tstart + tk1*zi + tk2*zi**2 + tk3*zi**3    |
c mixing model -->   temp = (tstart * tk1 + zi*tk2) / (zi + tk1)       |
c---------------------------------------------------------------------|
| tstart(c)|  25.00    |tk1| 0.0000    |tk2| 0.0000    |tk3| 0.0000    |
|----------------------------------------------------------------------|
| starting value of zi | 0.0           |max. value of zi| 1.00000E+38  |
|----------------------------------------------------------------------|
| starting time (sec)  | 0.0           |max. time (sec) | 1.00000E+13  |
|----------------------------------------------------------------------|
| max. steps           |     10000     |max. steps w/o print|     150  |
|----------------------------------------------------------------------|
| linear print interval|  15.000       |log print interval  | 2.00000E+09 |
|----------------------------------------------------------------------|
| suppress mineral phases                                              |
|----------------------------------------------------------------------|
| phases w/ elements|                          |                        |n
| phases except     |                          |                        |n
| phases except     |                          |                        |n
```

```
|-----------------------------------------------------------------------|
| fixed fugacity phases- species, moles(per kg h2o), log fugacity(bars) |
| CO2(g)                              |200.00000      | -3.0000        |n
| O2(g)                               |200.00000      | -0.7000        |n
|-----------------------------------------------------------------------|
|-----------------------------------------------------------------------|
c                  R A T E     L A W S
c 1 = relative                   rate = rk1 + rk2*zi + (1/2)rk3*zi*zi
c 2 = transition state theory    rate = CHECK DOCUMENTATION
c 3 = specified rate
c 4 = activity term rate         rate = CHECK DOCUMENTATION
c
c                  R E A C T A N T     T Y P E S
c mineral     solid solution     special    aqueous    gas
c
c                  S U R F A C E     T Y P E
c 0 = fixed surface area     1 = fixed specific surface area
c
c                  N O T E S
c status and jreac are normally not set by the user
|-----------------------------------------------------------------------|
| reactants   (ss) solid solution only     (sp) special reactant only   |
|-----------------------------------------------------------------------|
| REACTANT          | HLW_Glass           |status    | 0              |
| moles remaining   | 21.8194             |destroyed | 0.00000        |
| reactant type     |  special            |sk        | 1755.2346      |
| surface type      |   0                 |fk        | 1.00000        |
| end-member        |                     |moles     |                |ss,n
| volume            | 35.0877             |          |                |sp
| element           | Si                  |moles     |7.820395E-01    |sp,n
| element           | Ti                  |moles     |1.250704E-02    |sp,n
| element           | Ba                  |moles     |8.258300E-04    |sp,n
| element           | B                   |moles     |2.980151E-01    |sp,n
| element           | Al                  |moles     |8.672353E-02    |sp,n
| element           | Li                  |moles     |2.134365E-01    |sp,n
| element           | Na                  |moles     |3.766185E-01    |sp,n
| element           | K                   |moles     |7.670634E-02    |sp,n
| element           | Cl                  |moles     |3.280770E-03    |sp,n
| element           | O                   |moles     |2.807943E+00    |sp,n
| element           | Fe                  |moles     |1.327982E-01    |sp,n
| element           | Ca                  |moles     |1.657235E-02    |sp,n
| element           | F                   |moles     |1.682371E-03    |sp,n
| element           | P                   |moles     |4.554802E-04    |sp,n
| element           | Cr                  |moles     |1.593477E-03    |sp,n
| element           | Cu                  |moles     |2.410401E-03    |sp,n
| element           | Mg                  |moles     |3.405157E-02    |sp,n
| element           | Mn                  |moles     |2.845150E-02    |sp,n
| element           | Ni                  |moles     |1.256535E-02    |sp,n
| element           | Pb                  |moles     |2.952349E-04    |sp,n
| element           | S                   |moles     |4.051165E-03    |sp,n
| element           | U                   |moles     |7.914684E-03    |sp,n
| element           | Pu                  |moles     |6.241702E-05    |sp,n
| element           | Np                  |moles     |4.031999E-06    |sp,n
| DISSOLUTION LAW   |    3                |          |                |
| rate constant rk1 | 1.157400e-015       |csigma1   |                |
| TEMPERATURE (C)   |  25.0               |          |                |234
| PRECIPITATION LAW |    0                |          |                |
```

REACTANT	OutWeb_516	status	0	
moles remaining	9.2689	destroyed	0.00000	
reactant type	special	sk	120.0201	
surface type	0	fk	1.00000	
end-member		moles		ss,n
volume	12.7389			sp
element	C	moles	2.331196E-02	sp,n
element	Si	moles	1.032561E-02	sp,n
element	P	moles	1.129989E-03	sp,n
element	S	moles	1.091499E-03	sp,n
element	Fe	moles	1.760434759	sp,n
element	Mn	moles	1.902143E-02	sp,n
DISSOLUTION LAW	3			
rate constant rk1	8.706300e-012	csigma1		
TEMPERATURE (C)	25.0			234
PRECIPITATION LAW	0			

REACTANT	GPC_304L	status	0	
moles remaining	5.4943	destroyed	0.00000	
reactant type	special	sk	141.4645	
surface type	0	fk	1.00000	
end-member		moles		ss,n
volume	12.5945			sp
element	C	moles	2.497710E-03	sp,n
element	N	moles	7.139420E-03	sp,n
element	Si	moles	2.670417E-02	sp,n
element	P	moles	1.452843E-03	sp,n
element	S	moles	9.355704E-04	sp,n
element	Fe	moles	1.218418E+00	sp,n
element	Cr	moles	3.654120E-01	sp,n
element	Mn	moles	3.640464E-02	sp,n
element	Ni	moles	1.703868E-01	sp,n
DISSOLUTION LAW	3			
rate constant rk1	2.516000e-014	csigma1		
TEMPERATURE (C)	25.0			
PRECIPITATION LAW	0			

REACTANT	DOE_SNF_CAN_316L	status	0	
moles remaining	0.8592	destroyed	0.00000	
reactant type	special	sk	22.6701	
surface type	0	fk	1.00000	
end-member		moles		ss,n
volume	12.5313			sp
element	C	moles	2.497710E-03	sp,n
element	N	moles	7.139420E-03	sp,n
element	Si	moles	3.560556E-02	sp,n
element	P	moles	1.452843E-03	sp,n
element	S	moles	9.355704E-04	sp,n
element	Fe	moles	1.169177E+00	sp,n
element	Cr	moles	3.269476E-01	sp,n
element	Mn	moles	3.640464E-02	sp,n
element	Mo	moles	2.605795E-02	sp,n
element	Ni	moles	2.044641E-01	sp,n
DISSOLUTION LAW	3			
rate constant rk1	2.528700e-014	csigma1		
TEMPERATURE (C)	25.0			234

PRECIPITATION LAW	0				
REACTANT	J-13_water		status	0	
moles remaining	1.00000E+06		destroyed	0.0000	
reactant type	DISPLACER		sk	1.0000	
surface type	0		fk	1.0000	
end-member			moles		ss,n
volume	0.00000				sp
element	O	moles	5.551831245952758E+01		sp,n
element	Al	moles	2.552925442142962E-08		sp,n
element	B	moles	1.238820352587119E-05		sp,n
element	Ba	moles	9.999999999562674E-17		sp,n
element	Ca	moles	3.243674988170862E-04		sp,n
element	Cl	moles	2.013951078234399E-04		sp,n
element	Cr	moles	1.000000000032547E-16		sp,n
element	Cu	moles	1.000000000144320E-16		sp,n
element	F	moles	1.147465104190493E-04		sp,n
element	Fe	moles	3.599898362633903E-12		sp,n
element	Gd	moles	1.000000000319854E-16		sp,n
element	H	moles	1.110189627726903E+02		sp,n
element	C	moles	2.094090326853263E-03		sp,n
element	P	moles	1.260688562573650E-06		sp,n
element	K	moles	1.289058664798220E-04		sp,n
element	Li	moles	6.915430381772644E-06		sp,n
element	Mg	moles	8.269903704973302E-05		sp,n
element	Mn	moles	3.053653213911434E-16		sp,n
element	Mo	moles	9.999999999999966E-17		sp,n
element	N	moles	1.416016274998283E-04		sp,n
element	Na	moles	1.992190534111455E-03		sp,n
element	Ni	moles	1.000000000004491E-16		sp,n
element	Np	moles	1.000000000454101E-16		sp,n
element	Pb	moles	1.000000000000987E-16		sp,n
element	Pu	moles	1.000000000407232E-16		sp,n
element	S	moles	1.915397806679813E-04		sp,n
element	Si	moles	1.014741003820566E-03		sp,n
element	Tc	moles	1.000000000000003E-16		sp,n
element	Ti	moles	1.000000000000003E-16		sp,n
element	U	moles	9.999999997784918E-17		sp,n
element	Zr	moles	1.000000000089727E-16		sp,n
DISSOLUTION LAW	3				
rate constant rk1	1.158800e-011		csigma1		
TEMPERATURE (C)	25.0				234
PRECIPITATION LAW	0				

options

- SOLID SOLUTIONS -
  ignore solid solutions
  * process solid solutions
- LOADING OF SPECIES INTO MEMORY -
  * don't print
  lists species loaded into memory
- LIST DERIVATIVES OF BASIS ELEMENTS AT EACH PRINT POINT -
  * don't print
  print
- LIST ALL SPECIES LOADED INTO MEMORY AND THEIR LOG K VALUES -
  * don't print

```
    print
- LIST DISTRIBUTION OF AQUEOUS SPECIES AT EACH PRINT POINT -
  * only species > 10**-12 molal
    all species
    don't print
- LIST CATION/H+ ACTIVITY RATIOS AT EACH PRINT POINT -
  * don't print
    print
- LIST BULK ELEMENT AND OXIDE COMPOSITION AT EACH PRINT POINT -
  * don't print
    print
- MINERAL SATURATION STATES -
  * print if affinity > -10 kcals
    print all
    don't print
- LIST GAS SPECIES SUMMARY AT EACH PRINT POINT -
    don't print
  * print
- PRINT AQUEOUS MASS AND CONCENTRATION TOTALS -
  * don't print
    print
- TAB FILES -
  * write
    append to previous tabx file
    don't write
- WRITE PICKUP FILE -
  * write pickup file at end of run
    don't write pickup file
    write pickup file for each print point
- PHYSICALLY REMOVED SUBSYSTEM -
  * does nothing
    transfer minerals but leave trivial mass in the system
    transfer minerals
- CLEAR INITIAL PHYSICALLY REMOVED SUBSYSTEM -
  * does nothing
    clear p.r.s. before first reaction progress advance
- PHASE BOUNDARY SEARCH -
  * step size constrained by predicted phase boundaries
    phase boundaries estimated from Taylor's series and printed
    locations of phase boundaries ignored
- AUTO BASIS SWITCHING -
  * off
    on
- SUPPRESS REDOX REACTIONS -
  * does nothing
    suppress all redox reactions
- LINEAR OR LOGARITHMIC TAYLOR'S SERIES -
  * linear for kcol = 1,kdim, logarithmic for kcol = 1,kbt
    logarithmic for kcol = 1,kbt
    linear for kcol = 1,kdim
- AZERO AND HYDRATION NUMBERS -
  * no change
    read in new azero and hydration numbers
- PRINT MEAN MOLAL ACTIVITY COEFFICIENTS FOR DISSOLVED SPECIES -
  * does nothing
    print
- PITZER DATABASE INFORMATION -
```

```
|   * print only warnings                                                    |
|     print species in model and number of Pitzer coefficients               |
|     print species in model and names of Pitzer coefficients                |
| - PRINT DIAGNOSTIC MESSAGES -                                              |
|   * don't print                                                            |
|     print level 1 messages                                                 |
|     print level 2 messages                                                 |
| - PRINT PRE-NEWTON-RAPHSON OPTIMIZATION -                                  |
|   * don't print                                                            |
|     print summary information                                              |
|     print detailed information                                             |
| - PRINT STEP SIZE AND ORDER -                                              |
|   * don't print                                                            |
|     print scale factor                                                     |
|     print orders and step size scaling factors                             |
| - CONTROL STEP SIZE AND ORDER PRINT -                                      |
|   * does nothing                                                           |
|     print step size and order when delzi .le. dlzmx1                       |
| - NEWTON ITERATIONS -                                                      |
|   * don't print                                                            |
|     print summary of newton iterations                                     |
|     print summary, residual functions and correction terms                 |
|     print summary, residual functions, correction terms and matrix         |
| - PRINT SEARCH ITERATIONS -                                                |
|   * don't print                                                            |
|     print                                                                  |
| - PRINT HPSAT ITERATIONS -                                                 |
|   * don't print                                                            |
|     print                                                                  |
| - PRINT FINITE DIFFERENCE AND DERIVATIVE DATA -                            |
|   * don't print                                                            |
|     print computations from RDERIV, and RTAYLR                             |
|     print computations from RDERIV, RTAYLR, DERIV and TAYLOR               |
| - PRINT KINETICS DIAGNOSTIC MESSAGES -                                     |
|   * don't print                                                            |
|     print level 1 diagnostics                                              |
|     print level 1 and level 2 diagnostics                                  |
| - PRINT AKMATR -                                                           |
|   * don't print                                                            |
|     print level 1 diagnostics                                              |
| - KILL ITERATION VARIABLES -                                               |
|   * does nothing                                                           |
|     allow selection of variables to remove                                 |
|----------------------------------------------------------------------------|
| development options  (used for code development)                           |
|----------------------------------------------------------------------------|
|    0 check finite difference and Taylor series expression                  |
|    0 check reaction rate finite difference and Taylor series               |
|----------------------------------------------------------------------------|
| tolerances                        desired values - defaults info-only      |
|----------------------------------------------------------------------------|
| number of N-R iterations          |                  |  40      itermx   |
| p.r.s. transfer interval          |                  |  varies  dlzidp   |
| residual magnitude                |                  |  1.0e-06 tolbt    |
| correction magnitude              |                  |  1.0e-06 toldl    |
| search/find tolerance             |                  |  varies  tolx     |
| supersaturation                   |                  |  varies  tolsat   |
```

```
| supersaturation set size                |                | varies  tolsst |
| max. size Taylor's series term          |                | 1.0e-04 screw1 |
| max. initial value betamx               |                | n/a     screw2 |
| max. Taylor's series term (kin.)        |                | 1.0e-04 screw3 |
| corrector iteration                     |                | 1.0e-04 screw4 |
| max. size of N-R correction term        |                | 4.0     screw5 |
| step size (economy mode)                |                | 4.0     screw6 |
| log mass of phases                      |                | varies  zklogu |
| decrement mass (p.r.s.)                 |                | 2.0     zklogl |
| min. left after p.r.s.                  |                | .98     zkfac  |
| initial step size                       |                | varies  dlzmx1 |
| upper limit step size                   | 0.200000       | varies  dlzmx2 |
| maximum order                           |                | 6       nordlm |
| num. attempted assemblages              |                | 25      ntrymx |
| slide -> over phase bound.              |                | 8       npslmx |
| slide -> over redox insta.              |                | 3       nsslmx |
| fo2 scan control                        |                | none    ioscan |
|-----------------------------------------------------------------------------|
c pickup file written by EQ3NR.7.2bR139
c supported by eqlib.7.2bR168
|EQ3NR input file name= j13noc30.3i
| Ca++ not fixed by CALcite, Log10fCO2 fixed -3.0 (hence the "30").
|==== j13[cal,noc][25,30,35].3i General Series Notes: ================|
|2-10-99 HWStockman xcif3 Wolery's J13wsf.3i to Davelar format, then
|  determine sensitivity to CO2, O2 constraints as cross-check on the
|  variants used by PLCloke. HPO4-- corrected for H; 120 PO4--- from
|  Harrar et al. mul by 95.979/94.971 MolWts from EQ6 DB.
|==== j13hws??.3i specific comments for versions ======================|
| 2-10-99 j13hws03: Like 02, but set log fCO2 = -3.5, pH init=8.5, and
|  balance on H+.
| 2-10-99 j13hws02: Like 01, but raise init pH from 7.5 to 7.6.
| 2-10-99 j13hws01: Like 00, but raise pH slightly.
|==== TJWolery original comments on J13wsf.3i below ==================|
|Description= "J-13 well water, with traces of spent fuel components"
|Version level= 7.2
|Revised 08/08/95    Revisor= T. J. Wolery
|This is part of the EQ3NR Test Case Library (EQ3/6-V7-EQ3NR-TST-R04)
|
|  Water from well J-13 at the Nevada Test Site, spiked with
|trace amounts of spent nuclear fuel components. The composition
|is otherwise identical to that in the EQ3NR test case input file
|J13W.3I, which is based on data reported by Harrar et al. (1990).
|Water from this well is commonly used to represent the groundwater
|at the proposed high-level nuclear waste repository at Yucca
|Mountain, Nevada.
|
|  Purpose: to initialize the EQ6 test case input file J13WSF.6I,
|which simulates the interaction of J-13 well water with spent
|nuclear fuel. This test case also tests the ability of EQ3NR to
|handle a system containing many components.
|
|
|                              References
|
|Harrar, J. E., Carley, J. F., Isherwood, W. F., and Raber, E., 1990,
|  Report of the Committee to Review the Use of J-13 Well Water in
|  Nevada Nuclear Waste Storage Investigations: UCID-21867, Lawrence
```

Livermore National Laboratory, Livermore, California. TIC# 209096. (HWStockman adds TIC # 2-10-99 above)			
temperature (C)	25.000		
electrical imbalance	6.198072111975040E-15		
number of aqueous master species	32		
position of last pure mineral	32		
position of last solid solution	32		
suppressed species	(suppress,replace,augmentk,augmentg)		value
Quartz	mineral	suppress	.00000E+00
Tridymite	mineral	suppress	.00000E+00
CaZrO3	mineral	suppress	.00000E+00
BaZrO3	mineral	suppress	.00000E+00
SrZrO3	mineral	suppress	.00000E+00
Muscovite	mineral	suppress	.00000E+00
Celadonite	mineral	suppress	.00000E+00
Zircon	mineral	suppress	.00000E+00
Dolomite	mineral	suppress	.00000E+00
Dolomite-dis	mineral	suppress	.00000E+00
Dolomite-ord	mineral	suppress	.00000E+00
Annite	mineral	suppress	.00000E+00
Phlogopite	mineral	suppress	.00000E+00

iopg options

- pH SCALE CONVENTION -
  * modified NBS
    internal
    rational
- ACTIVITY COEFFICIENT OPTIONS -
  * use B-dot equation
    Davies' equation
    Pitzer's equations

elements, moles and moles aqueous		
O	5.551831245952758E+01	0.000000000000000E+00
Al	2.552925442142962E-08	0.000000000000000E+00
B	1.238820352587119E-05	0.000000000000000E+00
Ba	9.999999999562674E-17	0.000000000000000E+00
Ca	3.243674988170862E-04	0.000000000000000E+00
Cl	2.013951078234399E-04	0.000000000000000E+00
Cr	1.000000000032547E-16	0.000000000000000E+00
Cu	1.000000000144320E-16	0.000000000000000E+00

F	1.147465104190493E-04	0.000000000000000E+00
Fe	3.599898362633903E-12	0.000000000000000E+00
Gd	1.000000000319854E-16	0.000000000000000E+00
H	1.110189627726903E+02	0.000000000000000E+00
C	2.094090326853263E-03	0.000000000000000E+00
P	1.260688562573650E-06	0.000000000000000E+00
K	1.289058664798220E-04	0.000000000000000E+00
Li	6.915430381772644E-06	0.000000000000000E+00
Mg	8.269903704973302E-05	0.000000000000000E+00
Mn	3.053653213911434E-16	0.000000000000000E+00
Mo	9.999999999999966E-17	0.000000000000000E+00
N	1.416016274998283E-04	0.000000000000000E+00
Na	1.992190534111455E-03	0.000000000000000E+00
Ni	1.000000000004491E-16	0.000000000000000E+00
Np	1.000000000454101E-16	0.000000000000000E+00
Pb	1.000000000000987E-16	0.000000000000000E+00
Pu	1.000000000407232E-16	0.000000000000000E+00
S	1.915397806679813E-04	0.000000000000000E+00
Si	1.014741003820566E-03	0.000000000000000E+00
Tc	1.000000000000003E-16	0.000000000000000E+00
Ti	1.000000000000003E-16	0.000000000000000E+00
U	9.999999997784918E-17	0.000000000000000E+00
Zr	1.000000000089727E-16	0.000000000000000E+00

master species and logarithmic basis variables		
H2O	H2O	1.744358983526984E+00
Al+++	Al+++	- 1.688678142712154E+01
B(OH)3(aq)	B(OH)3(aq)	- 4.939182887195578E+00
Ba++	Ba++	-

1.600206749676945E+01		
Ca++	Ca++	-
3.510825142307810E+00		
Cl-	Cl-	-
3.696119793904588E+00		
CrO4--	CrO4--	-
1.600893068061055E+01		
Cu++	Cu++	-
1.793528542476122E+01		
F-	F-	-
3.941442675845588E+00		
Fe++	Fe++	-
2.313336636121568E+01		
Gd+++	Gd+++	-
1.913958509063167E+01		
H+	H+	-
8.067223257067396E+00		
HCO3-	HCO3-	-
2.692996014218606E+00		
HPO4--	HPO4--	-
6.015465230149174E+00		
K+	K+	-
3.890196358153585E+00		
Li+	Li+	-
5.160546465137654E+00		
Mg++	Mg++	-
4.106607560999163E+00		
Mn++	Mn++	-
1.571499105086488E+01		
MoO4--	MoO4--	-
1.600000000000000E+01		
NO3-	NH3(aq)	-
3.849454346786642E+00		
Na+	Na+	-
2.702461892988562E+00		
Ni++	Ni++	-
1.600652502212401E+01		
Np++++	Np++++	-
4.996264105337004E+01		
Pb++	Pb++	-
1.600242157584094E+01		
Pu++++	Pu++++	-
4.300735480158046E+01		
SO4--	SO4--	-
3.737766888575554E+00		
SiO2(aq)	SiO2(aq)	-
3.000483264317265E+00		
TcO4-	TcO4-	-
1.600000000000000E+01		
Ti(OH)4(aq)	Ti(OH)4(aq)	-
1.600000000000000E+01		
UO2++	UO2++	-
2.332660231214583E+01		
Zr(OH)2++	Zr(OH)2++	-
3.084644536722611E+01		
O2(g)	O2(g)	-7.000000000000000E-01

physically removed subsystem (solid solution, mineral, moles)		
none		

File: ratefacs.in

```
glassratefac= .5 1 2 3
steelratefac= .1 1 2 3
fuelratefac=.1 1 10 100
dripratefac=.1 1 2 10
```

Attachment III. Listing of Files on Electronic Media.

This attachment contains the MS-DOS directory for files placed on the electronic media (Ref. 12). The files are of 8 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 t???????.6i;
3) EQ6 output files (text, extension = 6o);
4) Tab-delimited text files (extension = txt), with names t???????.elem????.txt. as discussed in Section 5.3.2; these contain total aqueous moles (*.elem_aqu.txt), total moles in minerals and aqueous phase (*.elem_m_a.txt), total moles in minerals, aqueous phase, and remain 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;
5) FORTRAN source files (extension = for) for the version of EQ6 used in the calculations; and
6) 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;
7) EQ6 data files used for the calculations, with the text file data0.nuc.R8a, and the binary version data1.nuc; and
8) Eqsetup files (name=*.in, *junk.txt, test.txt, triga.txt)

```
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.

BINARY~1        <DIR>          10-06-99  5:04p binary for pp plots
EQ6_6O~1        <DIR>          10-07-99  3:14p EQ6_6o_6i_txt
eqsetup         <DIR>          10-06-99  4:32p eqsetup
EXCELF~1        <DIR>          10-06-99  4:32p excel files
PROGRA~1        <DIR>          10-06-99  5:02p program files

Directory of binary for pp plots:
t!1a1111 bin    22,197,552  05-24-99  7:12p t!1a1111.bin

Directory of EQ6_6o_6i_txt:

t!1a1111 6i         47,557  05-24-99  7:15p t!1a1111.6i
t!1a1111 6o      3,977,782  05-24-99  7:12p t!1a1111.6o
T!1A11~1 TXT        39,311  05-24-99  7:12p t!1a1111.elem_aqu.txt
T!1A11~2 TXT        37,206  05-24-99  7:12p t!1a1111.elem_min.txt
T!1A11~3 TXT        37,219  05-24-99  7:12p t!1a1111.elem_tot.txt
t!1a1113 6i         47,557  05-24-99  7:15p t!1a1113.6i
t!1a1113 6o      8,002,008  05-24-99  8:06p t!1a1113.6o
T!1A11~4 TXT        71,351  05-24-99  8:06p t!1a1113.elem_aqu.txt
T!DC15~1 TXT        67,518  05-24-99  8:06p t!1a1113.elem_min.txt
```

```
T!E249~1 TXT        67,531  05-24-99  8:06p t!1a1113.elem_tot.txt
t!1a1122 6i         47,557  05-24-99  7:17p t!1a1122.6i
t!1a1122 6o      8,409,068  05-24-99 10:50p t!1a1122.6o
T!0145~1 TXT        72,241  05-24-99 10:50p t!1a1122.elem_aqu.txt
T!FC35~1 TXT        68,360  05-24-99 10:50p t!1a1122.elem_min.txt
T!0369~1 TXT        68,373  05-24-99 10:50p t!1a1122.elem_tot.txt
t!1a1133 6i         47,557  05-24-99  7:15p t!1a1133.6i
t!1a1133 6o      8,000,014  05-24-99  9:56p t!1a1133.6o
T!2125~1 TXT        71,351  05-24-99  9:56p t!1a1133.elem_aqu.txt
T!1D15~1 TXT        67,518  05-24-99  9:56p t!1a1133.elem_min.txt
T!2349~1 TXT        67,531  05-24-99  9:56p t!1a1133.elem_tot.txt
t!1a1211 6i         47,557  05-24-99  7:15p t!1a1211.6i
t!1a1211 6o      4,189,991  05-24-99 11:21p t!1a1211.6o
T!1A12~2 TXT        40,201  05-24-99 11:20p t!1a1211.elem_aqu.txt
T!1A12~3 TXT        38,048  05-24-99 11:20p t!1a1211.elem_min.txt
T!1A12~4 TXT        38,061  05-24-99 11:20p t!1a1211.elem_tot.txt
t!1a1213 6i         47,557  05-24-99  7:15p t!1a1213.6i
t!1a1213 6o      8,352,049  05-25-99 12:20a t!1a1213.6o
T!E0F4~1 TXT        70,461  05-25-99 12:20a t!1a1213.elem_aqu.txt
T!DCE4~1 TXT        66,676  05-25-99 12:20a t!1a1213.elem_min.txt
T!E219~1 TXT        66,689  05-25-99 12:20a t!1a1213.elem_tot.txt
t!1a1222 6i         47,557  05-24-99  7:15p t!1a1222.6i
t!1a1222 6o      8,012,739  05-25-99  2:48a t!1a1222.6o
T!0155~1 TXT        71,796  05-25-99  2:48a t!1a1222.elem_aqu.txt
T!1A12~1 TXT        67,939  05-25-99  2:48a t!1a1222.elem_min.txt
T!0379~1 TXT        67,952  05-25-99  2:48a t!1a1222.elem_tot.txt
t!1a1231 6i         47,557  05-24-99  7:15p t!1a1231.6i
t!1a1231 6o      4,166,632  05-25-99 12:55a t!1a1231.6o
T!2135~1 TXT        39,756  05-25-99 12:55a t!1a1231.elem_aqu.txt
T!1D25~1 TXT        37,627  05-25-99 12:55a t!1a1231.elem_min.txt
T!2359~1 TXT        37,640  05-25-99 12:55a t!1a1231.elem_tot.txt
t!1a1233 6i         47,557  05-24-99  7:15p t!1a1233.6i
t!1a1233 6o      8,064,654  05-25-99  1:53a t!1a1233.6o
T!21F4~1 TXT        69,571  05-25-99  1:53a t!1a1233.elem_aqu.txt
T!1DE4~1 TXT        65,834  05-25-99  1:53a t!1a1233.elem_min.txt
T!2319~1 TXT        65,847  05-25-99  1:53a t!1a1233.elem_tot.txt
t!1a2022 6i         43,852  05-24-99  8:57p t!1a2022.6i
t!1a2022 6o      5,609,398  06-02-99  9:25p t!1a2022.6o
T!1A20~1 TXT        49,546  06-02-99  9:25p t!1a2022.Elem_aqu.txt
T!1A20~2 TXT        46,889  06-02-99  9:25p t!1a2022.Elem_min.txt
T!1A20~3 TXT        46,902  06-02-99  9:25p t!1a2022.Elem_tot.txt
t!1a2111 6i         47,557  05-24-99  7:15p t!1a2111.6i
t!1a2111 6o      4,123,300  05-25-99  3:09a t!1a2111.6o
T!1A21~1 TXT        41,536  05-25-99  3:09a t!1a2111.elem_aqu.txt
T!1A21~2 TXT        39,311  05-25-99  3:09a t!1a2111.elem_min.txt
T!1A21~3 TXT        39,324  05-25-99  3:09a t!1a2111.elem_tot.txt
t!1a2113 6i         47,557  05-24-99  7:15p t!1a2113.6i
t!1a2113 6o      8,138,423  05-25-99  4:07a t!1a2113.6o
T!1A21~4 TXT        71,796  05-25-99  4:07a t!1a2113.elem_aqu.txt
T!EC15~1 TXT        67,939  05-25-99  4:07a t!1a2113.elem_min.txt
T!F249~1 TXT        67,952  05-25-99  4:07a t!1a2113.elem_tot.txt
t!1a2122 6i         47,557  05-24-99  7:15p t!1a2122.6i
t!1a2122 6o      8,775,281  05-25-99  6:24a t!1a2122.6o
T!1145~1 TXT        76,246  05-25-99  6:24a t!1a2122.elem_aqu.txt
T!0D35~1 TXT        72,149  05-25-99  6:24a t!1a2122.elem_min.txt
T!1369~1 TXT        72,162  05-25-99  6:24a t!1a2122.elem_tot.txt
t!1a2131 6i         47,557  05-24-99  7:15p t!1a2131.6i
```

```
t!1a2131 6o      4,173,190  05-25-99  4:28a t!1a2131.6o
T!31E5~1 TXT        41,981  05-25-99  4:28a t!1a2131.elem_aqu.txt
T!2DD5~1 TXT        39,732  05-25-99  4:28a t!1a2131.elem_min.txt
T!330A~1 TXT        39,745  05-25-99  4:28a t!1a2131.elem_tot.txt
t!1a2133 6i         47,557  05-24-99  7:15p t!1a2133.6i
t!1a2133 6o      8,213,493  05-25-99  5:26a t!1a2133.6o
T!3125~1 TXT        72,686  05-25-99  5:26a t!1a2133.elem_aqu.txt
T!2D15~1 TXT        68,781  05-25-99  5:26a t!1a2133.elem_min.txt
T!3349~1 TXT        68,794  05-25-99  5:26a t!1a2133.elem_tot.txt
t!1a2211 6i         47,557  05-24-99  7:16p t!1a2211.6i
t!1a2211 6o      4,041,012  05-25-99  7:02a t!1a2211.6o
T!1A22~2 TXT        38,866  05-25-99  7:02a t!1a2211.elem_aqu.txt
T!1A22~3 TXT        36,785  05-25-99  7:02a t!1a2211.elem_min.txt
T!1A22~4 TXT        36,798  05-25-99  7:02a t!1a2211.elem_tot.txt
t!1a2213 6i         47,557  05-24-99  7:16p t!1a2213.6i
t!1a2213 6o      8,870,960  05-25-99  8:02a t!1a2213.6o
T!F0F4~1 TXT        76,691  05-25-99  8:01a t!1a2213.elem_aqu.txt
T!ECE4~1 TXT        72,570  05-25-99  8:01a t!1a2213.elem_min.txt
T!1A22~1 TXT        72,583  05-25-99  8:01a t!1a2213.elem_tot.txt
t!1a2222 6i         47,557  05-24-99  7:16p t!1a2222.6i
t!1a2222 6o      8,240,986  05-25-99 10:31a t!1a2222.6o
T!1155~1 TXT        69,571  05-25-99 10:31a t!1a2222.elem_aqu.txt
T!0D45~1 TXT        65,834  05-25-99 10:31a t!1a2222.elem_min.txt
T!1379~1 TXT        65,847  05-25-99 10:31a t!1a2222.elem_tot.txt
t!1a2231 6i         47,557  05-24-99  7:16p t!1a2231.6i
t!1a2231 6o      3,978,038  05-25-99  8:34a t!1a2231.6o
T!3135~1 TXT        38,421  05-25-99  8:34a t!1a2231.elem_aqu.txt
T!2D25~1 TXT        36,364  05-25-99  8:34a t!1a2231.elem_min.txt
T!3359~1 TXT        36,377  05-25-99  8:34a t!1a2231.elem_tot.txt
t!1a2233 6i         47,557  05-24-99  7:16p t!1a2233.6i
t!1a2233 6o      8,576,921  05-25-99  9:33a t!1a2233.6o
T!31F4~1 TXT        75,801  05-25-99  9:32a t!1a2233.elem_aqu.txt
T!2DE4~1 TXT        71,728  05-25-99  9:32a t!1a2233.elem_min.txt
T!3319~1 TXT        71,741  05-25-99  9:32a t!1a2233.elem_tot.txt
t!1b1131 6i         46,197  06-29-99  1:31p t!1b1131.6i
t!1b1131 6o      1,393,680  06-29-99  1:39p t!1b1131.6o
T!1B11~1 TXT        13,946  06-29-99  1:39p t!1b1131.elem_aqu.txt
T!1B11~2 TXT        13,209  06-29-99  1:39p t!1b1131.elem_min.txt
T!1B11~3 TXT        13,222  06-29-99  1:39p t!1b1131.elem_tot.txt
t!1c1131 6i         38,965  06-29-99  1:31p t!1c1131.6i
t!1c1131 6o      1,375,671  06-29-99  1:50p t!1c1131.6o
T!1C11~1 TXT        12,611  06-29-99  1:50p t!1c1131.elem_aqu.txt
T!1C11~2 TXT        11,946  06-29-99  1:50p t!1c1131.elem_min.txt
T!1C11~3 TXT        11,959  06-29-99  1:50p t!1c1131.elem_tot.txt
t!1g1021 6i         44,254  05-24-99  7:57p t!1g1021.6i
t!1g1021 6o      2,266,361  05-25-99 11:32a t!1g1021.6o
T!1G10~1 TXT        22,401  05-25-99 11:32a t!1g1021.elem_aqu.txt
T!1G10~2 TXT        21,208  05-25-99 11:32a t!1g1021.elem_min.txt
T!1G10~3 TXT        21,221  05-25-99 11:32a t!1g1021.elem_tot.txt
t!1g2021 6i         44,006  05-24-99  7:57p t!1g2021.6i
t!1g2021 6o      2,179,492  05-25-99 11:20a t!1g2021.6o
T!1G20~2 TXT        21,066  05-25-99 11:20a t!1g2021.elem_aqu.txt
T!1G20~3 TXT        19,945  05-25-99 11:20a t!1g2021.elem_min.txt
T!1G20~4 TXT        19,958  05-25-99 11:20a t!1g2021.elem_tot.txt
t!1g2022 6i         43,924  05-24-99  7:57p t!1g2022.6i
t!1g2022 6o      5,752,846  05-25-99 11:10a t!1g2022.6o
T!1125~1 TXT        51,326  05-25-99 11:10a t!1g2022.elem_aqu.txt
```

```
T!1G20~1 TXT        48,573  05-25-99 11:10a t!1g2022.elem_min.txt
T!1349~1 TXT        48,586  05-25-99 11:10a t!1g2022.elem_tot.txt
t02a2204 6i         39,584  05-23-99 12:03p t02a2204.6i
T02A22~1 TXT        35,751  05-23-99 12:37p t02a2204.elem_aqu.txt
T02A22~2 TXT        33,838  05-23-99 12:37p t02a2204.elem_min.txt
T02A22~3 TXT        33,851  05-23-99 12:37p t02a2204.elem_tot.txt
t02g1203 6i         39,660  05-23-99 12:02p t02g1203.6i
T02G12~1 TXT        20,621  05-23-99  1:33p t02g1203.elem_aqu.txt
T02G12~2 TXT        19,524  05-23-99  1:33p t02g1203.elem_min.txt
T02G12~3 TXT        19,537  05-23-99  1:33p t02g1203.elem_tot.txt
t02g2203 6i         39,658  05-23-99 12:03p t02g2203.6i
T02G22~2 TXT        23,291  05-23-99  1:19p t02g2203.elem_aqu.txt
T02G22~3 TXT        22,050  05-23-99  1:19p t02g2203.elem_min.txt
T02G22~4 TXT        22,063  05-23-99  1:19p t02g2203.elem_tot.txt
t02g2204 6i         39,658  05-23-99 12:03p t02g2204.6i
T04DAE~1 TXT        34,861  05-23-99  1:06p t02g2204.elem_aqu.txt
T02G22~1 TXT        32,996  05-23-99  1:06p t02g2204.elem_min.txt
T03FC0~1 TXT        33,009  05-23-99  1:06p t02g2204.elem_tot.txt
t@1a1111 6i         47,635  06-03-99 11:55a t@1a1111.6i
T@1A11~2 TXT        39,756  06-09-99  5:28p t@1a1111.elem_aqu.txt
T@1A11~3 TXT        37,627  06-09-99  5:28p t@1a1111.elem_min.txt
T@1A11~1 TXT        37,640  06-09-99  5:28p t@1a1111.elem_tot.txt
t@1a1222 6i         47,633  06-03-99 10:47a t@1a1222.6i
T@1A12~1 TXT        70,906  06-09-99  6:33p t@1a1222.elem_aqu.txt
T@1A12~2 TXT        67,097  06-09-99  6:33p t@1a1222.elem_min.txt
T@1A12~3 TXT        67,110  06-09-99  6:33p t@1a1222.elem_tot.txt
t@1a2113 6i         47,633  06-09-99  3:42p t@1a2113.6i
T@1A21~1 TXT        70,461  06-09-99  5:04p t@1a2113.elem_aqu.txt
T@1A21~2 TXT        66,676  06-09-99  5:04p t@1a2113.elem_min.txt
T@1A21~3 TXT        66,689  06-09-99  5:04p t@1a2113.elem_tot.txt

Directory of eqsetup:
atwts    in          1,020  07-06-99  3:13p atwts.in
eqsetup  c          42,392  07-07-99 11:27a eqsetup.c
ratefacs in            100  05-26-99  9:57p ratefacs.in
template in         39,196  05-29-99  6:37p template.in
test     txt         1,657  07-07-99  2:54p test.txt
testjunk txt         1,064  07-07-99  2:55p testjunk.txt
Triga    txt         4,116  09-08-99  3:19p Triga.txt
TRIGAJ~1 TXT         3,662  07-07-99  2:36p trigajunk.txt

Directory of excel files:
CHANGE~1 XLS       164,864  08-18-99  3:54p changes_to_fftf.xls
DENSIT~1 XLS       237,056  07-14-99  3:24p density_triga.xls
EQSETU~1 XLS        30,208  09-28-99  3:13p eqsetup qualify.xls
FFTF_S~1 XLS     3,695,616  07-28-99  1:39p fftf_short.xls
TRIGA_~1 XLS       425,472  10-05-99  4:59p TRIGA_common_items.xls

Directory of program files:
AUTOEXEC BAT           624  09-12-99  1:20p AUTOEXEC.BAT
CONFIG   SYS           463  06-17-98  2:04p CONFIG.SYS
DATA0N~1 R8A     2,299,784  11-25-98  4:15p data0.nuc.R8a
data1    nuc       791,620  04-22-99  4:22p data1.nuc
data1    R8a       791,200  08-18-99  8:20a data1.R8a
data1    weg       792,936  01-19-99 11:34a data1.weg
Eq3nr    exe     2,169,333  08-18-95  5:47p Eq3nr.exe
eq6      exe     1,056,485  12-11-98  1:27p eq6.exe
```

```
eq6new    for     1,322,545  12-11-98 10:50a eq6new.for
eqlibnew  for       492,613  07-01-98  6:34p eqlibnew.for
EQPT      EXE     2,337,701  08-18-95  5:47p EQPT.EXE
EXTERNAL  FNT         9,900  06-29-95  8:27p EXTERNAL.FNT
HELP_PP              50,724  03-31-98  6:04p HELP_PP
PP        EXE       308,609  10-10-98  4:15p PP.EXE
PREFER    PP             62  01-20-99 10:25a PREFER.PP
program   txt             0  10-07-99  3:27p program.txt
Readme    txt           505  09-12-99  1:51p Readme.txt
Runeq3    exe       388,005  08-18-95  5:46p Runeq3.exe
RUNEQ6    EXE       392,181  08-18-95  5:46p RUNEQ6.EXE
RUNEQPT   EXE       334,517  08-18-95  5:46p RUNEQPT.EXE
```