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Title: Hanford Cs-Sr Repository Disposal Performance Analysis Using the TSPA-FEIS Model

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5. Purpose:

Efforts to accelerate cleanup at the Hanford Site include feasibility evaluations of disposing existing cesium chloride and strontium fluoride-filled containers (referred to as capsules) to the proposed repository at Yucca Mountain, Nevada. These materials were produced from Hanford high-level waste. The capsules are in a different disposal form than what is being considered for the present repository license application.

This report details a feasibility study conducted to determine the transport of materials through the repository if the capsules were to be direct disposed in the repository without further treatment. This study consists of a specific disposal scenario, since a design for disposal of the capsules does not exist, and definition of specific analysis cases. This study analyzes the effect of disposition of these materials on the waste package chemistry and the transport of these materials through the repository to the accessible environment.

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SUMMARY

Efforts to accelerate cleanup at the Hanford Site include evaluating repository direct disposal (i.e., disposal without further treatment) of existing containers (referred to as capsules) of cesium chloride and strontium fluoride previously produced from Hanford high-level waste. To support the disposal evaluation, a study of the behavior of these materials in the proposed repository was conducted to determine the chemical changes to the repository waste packages containing the capsule materials and the transport of these materials through the repository. The capsules are known to contain contaminant metals that may be of regulatory concern at disposal, and one of the key questions for disposal of the capsules is how these contaminants transport through the repository system. This report details the results of a feasibility study that analyzes the transport of these materials through the proposed repository if they were to be direct disposed.

This study is not a final determination of acceptability of the capsule materials in the repository, but is a feasibility study indicating how the materials would transport through the repository after breach of the waste package containing the materials after assumed placement in the repository. This study does not address other significant issues related to the direct disposal of the capsules to the repository, but rather only analyzes the chemical and transport effects of the capsule material. Issues that need to be addressed for a full evaluation of the direct disposal of the capsules include transportation studies, studies of container handling at the repository, packaging studies, and others.

No designs for repository direct disposal of the capsules exist. To conduct this feasibility study, a scenario for packaging the capsules was defined using existing spent nuclear fuel standardized canister and repository waste package designs. This allowed scenario specific definition of per package contents and the number of waste packages. Also, the U.S. Department of Energy, Richland Operations Office, the study requestor, provided concentration limits for the five metal contaminants (barium, cadmium, chromium, lead, and silver). The basis of these limits come from EPA National Primary Drinking Water Regulation, and National Secondary Drinking Water Regulation. The concentration for these five metals were calculated at the site boundary similar to the radionuclide dose calculations. The calculated concentrations were then compared to the EPA's 40 CFR 141 National Primary Drinking Water Regulation, 141.62 Maximum Contaminant levels for inorganic contaminants (Barium, Cadmium and Chromium), Subpart I Control of Lead and Copper, 141.80, (c),(1) (lead) and 40 CFR 143, National Secondary Drinking Water Regulation, 143.3 (silver). Only one packaging scenario, which does not reflect pending changes to waste package design by Yucca Mountain, was analyzed in this study. If a decision is made to proceed with direct disposal, the studies in this report will need to be repeated after disposal designs and updated analysis software are available.

This feasibility study is composed of two complementary evaluations. First, a predictive geochemistry analysis evaluates changes in the repository waste package chemistry due to interactions of the materials in the waste package and infiltrating groundwater from the repository. Second, a Total System Performance Assessment, which is a complex predictive analysis of radionuclide and material transport through the repository, analyzes the disposal packages containing commercial and United States Department of Energy spent nuclear fuel, the cesium and strontium capsules in this study, and high-level waste glass material.

Geochemical analyses were performed for waste package materials and contents interacting with infiltrating ground water. The focus of the geochemical analysis is the interaction of cesium chloride and strontium fluoride capsule constituents within the breached repository waste packages, which may cause

changes in the waste package chemistry and potentially alter the solution pH ranges and maximum constituent solubilities that help to define solubility limits in the Total System Performance Assessment. For the geochemical calculation, a previous analysis of high-level waste glass and spent nuclear fuel disposal was used as a baseline analysis. The baseline was then modified to replace Department of Energy spent nuclear fuel with the cesium chloride or strontium fluoride capsules while leaving all other package constituents unchanged. Similar to the baseline analysis, these simulations consider one ground water inflow rate into and out of the waste package with mean waste package material degradation rates, which are material dependent. Two separate waste package configurations were evaluated, one for the cesium chloride capsules and vitrified high-level waste glass and one for the strontium fluoride capsules and vitrified high-level waste glass. Each waste package configuration is evaluated for a worst-case scenario (no decay of short-lived radioisotopes prior to a waste package breach) and a most-likely scenario (short-lived radionuclides decayed prior to a package breach).

A pronounced drop in solution pH is observed during the first few years of the waste package simulations in this study. This pH response is affected by acid producing reactions involving metals (e.g., chromium, iron, boron, phosphorous) rapidly dissolved into package solution from the highly soluble capsules. The low initial pH conditions may be minimized by surface complexation effects involving iron corrosion products (e.g., hydrous ferric oxides) and hydrogen ions are expected to buffer pH during the first few hundred years of waste package failure. The pH buffering is expected to be sustained by a relatively high iron corrosion rate during early time. Bulk solution chemistry (i.e., pH, ionic strength, and redox potential) predicted for all waste package simulations is within the evaluated range of the model and the results from this modeling compare well to the baseline indicating no major changes in expected chemical state of the disposed waste package.

With the exception of strontium, rapid capsule degradation results in maximum constituent concentrations occurring within the first few years in all waste package simulations. The exception for maximum strontium concentration timing results from the precipitation of solid phase strontium fluoride that is predicted during strontium fluoride capsule degradation. Due to the solubility of precipitated strontium fluoride, maximum strontium concentrations occur on the order of thousands of years later than for other capsule constituents.

The Total System Performance Assessment is a complex computer model of material release and transport in the repository. The release and transport of identified contaminant metals was simulated using a surrogate specie in the computer model. Specific inventories and properties for each metal contaminant were used as input to the computer model. Solubility values for the materials were set based on information from the geochemical analysis. No other simulation settings were changed for this study.

For the analysis of radionuclide transport, the Total System Performance Assessment model was run for both nominal and igneous event (i.e., a volcanic eruption in the repository) scenarios. Model input settings were modified to simulate the amount of additional radionuclides placed into the waste package from the Hanford capsules. In some cases, the capsule inventory was added to the existing waste package inventory to provide a conservative dose at the accessible environment. As has been previously done by repository personnel, a conservative case eliminating the engineered barrier system (i.e., the waste package shell and repository drip shield) was run to determine the effectiveness of the natural repository system. The analysis results indicate no increase in repository dose by the addition of the materials in the cesium/strontium capsules to the existing repository inventory. This is because the relative dose contributions from the radionuclides in the capsules are very minor compared to the existing dose from commercial and United States Department of Energy spent nuclear fuel, and high-level waste material.

For the analysis of contaminant metal transport and release, the Total System Performance Assessment model was run for each individual metal and each capsule type using both nominal and igneous event scenarios. One contaminant metal in the capsules, barium, is generated by decay of cesium isotopes. The Total System Performance Assessment model does not track generation of decay products that are non-radioactive. To perform the evaluation of the barium release and transport, decay of cesium isotopes was externally calculated and the resulting barium amount entered into the input data at the start of the simulation, thus defining a maximum barium amount in the capsules. As was done with the radionuclide transport analysis, a conservative case eliminating the waste package and drip shield was run to determine the effectiveness of the natural repository system at retaining these materials. The analyses results indicate that, in all cases, the concentration of contaminant metals in water at the repository boundary remain below EPA's National Primary Drinking Water Regulation, and National Secondary Drinking Water Regulation limits, specified for this study by the U.S. Department of Energy, Richland Operations Office.

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ACRONYMS

ASM	American Society of Metals
ASTM	American Society for Testing Materials
atm	atmosphere
CRWMS	Civilian Radioactive Waste Management System
DHLW	DOE high-level waste
DOE	U.S. Department of Energy
FEIS	Final Environmental Impact Statement
HLW	high-level waste
M&O	Maintenance and Operating
NG	Nuclear Grade
NSNFP	National Spent Nuclear Fuel Program
SCFT	solid-centered flow-through
SNF	spent nuclear fuel
SR	site recommendation
SRL	Savannah River Laboratory
TSPA	Total System Performance Assessment
WP	waste package
WESF	Waste Encapsulation and Storage Facility

NOMENCLATURE

Term	Description
Base Case	Simulation used to define release and dose for the basic planned repository layout. The Base Case examines radionuclide dose from all waste packages which contain either commercial SNF waste packages or codisposal waste packages with DOE SNF and DOE HLW glass as discussed below. The Base Case is used as a basis for comparison of other model runs.
Codisposal	Codisposal is a concept of placing DOE SNF and DOE HLW glass in the same waste package for disposal. In this analysis, all DOE materials are placed in a waste package in a codisposal configuration using five HLW glass canisters surrounding one DOE standardized canister containing DOE SNF.
Dose	Regulations controlling the repository specify limits on dose as 15 millirem per year for 10,000 years. The basis for demonstrating compliance with the dose limit assumes that a certain size person drinks a specific amount of water from a hypothetical well located at the site boundary, which is 18 kilometers from the physical repository. In addition, a certain rate of consumption of food materials that are grown in that region using that well water is assumed. The biosphere dose conversion factors were developed by repository personnel using the environmental and agricultural parameters characteristic of the Amargosa Valley Region and the dietary lifestyle characteristics of the receptor consistent with those specified in controlling regulations. For this analysis, this basis is not changed.
Early Failure of a Waste Package	Those waste packages that fail early due to manufacturing or material defects or to pre-emplacement operations, including improper heat treatment.
Engineered Barrier System	The principal features of the engineered barrier system are a drip shield and a waste package. The engineered barrier system also includes ground support, a corrosion resistant waste emplacement that supports a pallet, and an invert at the base of the drift, which will have a steel infrastructure and will be filled with crushed welded tuff.

Term	Description
Full Range Inventory	Material inventory using the full range of known values. The specific value for a specific realization within a simulation is selected using the triangular distribution.
Igneous Scenario	This scenario describes igneous activity that could affect repository performance. It includes igneous intrusion that addresses the possibility that magma, in the form of a dike, could intrude into the repository and disrupt the expected repository performance. Also, it includes volcanic eruption that describes a volcanic conduit (or conduits) that invades the repository, destroys waste packages, and erupts at the land surface. The dose for this scenario is weighted by the probability of an actual event occurring.
Nominal Scenario	This scenario describes the expected natural conditions prevailing at the Yucca Mountain site. The nominal scenario is used for the majority of the simulations because it is the expected set of conditions.
Specie	A chemical constituent that is of interest for the analysis. In GoldSim, the species element defines all of the contaminant species being simulated (and their properties).
Triangular Distribution	The Triangular Distribution is used as a subjective description of a population for which there is limited sample data. It is based on knowledge of the minimum and maximum values of the population, and uses an estimate for the modal value. Despite being a simplistic description of a population, it is a very useful distribution for modeling processes where the relationship between variables is known, but data are scarce. Generally in this study, the distribution is defined by the range of analyzed data for a specific variable, such as a chemical concentration.

1. QUALITY ASSURANCE

1.1 Quality Program Applicability

This document was developed and is controlled in accordance with National Spent Nuclear Fuel Program (NSNFP) procedures. Unless otherwise noted, information must be evaluated for adequacy relative to its specific use if relied on to support design or decisions important to safety or waste isolation. Current procedures at the time of work were used. All the information in this report was derived from available references.

The NSNFP procedures applied to this activity implement DOE/RW-0333P, "Quality Assurance Requirements and Description" and are part of the NSNFP Quality Assurance Program. The NSNFP Quality Assurance Program has been assessed and accepted by representatives of the Office of Quality Assurance within the Office of Civilian Radioactive Waste Management for the work scope of the NSNFP. The NSNFP work scope extends to the work presented in this report.

The current principal NSNFP procedures applied to this activity include the following:

- NSNFP Procedure 6.01, "Review and Approval of NSNFP Internal Documents"
- NSNFP Procedure 6.03, "Managing Document Control and Distribution"
- NSNFP Procedure 3.04, "Engineering Documentation"
- NSNFP Procedure 19.01, "Software Control."

1.2 Software Use and Control

Modeling software used to generate data for this study and controls on that software are described in Section 3.1 for the Geochemical Analysis software and in Section 4.1 for the Total System Performance Assessment software. For preparation of this report, only commercial software (Microsoft Office 2003 and SigmaPlot 8), which is exempt from the software controls outlined in NSNFP procedures, was used to reduce specific existing data, model output data, and to prepare this report.

2. INTRODUCTION AND BACKGROUND INFORMATION

2.1 Introduction

Efforts to accelerate cleanup at the Hanford Site include evaluating direct disposal (i.e., disposal without further treatment) of existing containers (referred to as capsules) of cesium chloride and strontium fluoride, produced from Hanford high-level waste (HLW), in the proposed repository at Yucca Mountain, Nevada. The capsules are a different disposal form than is considered in the present repository license application (LA) evaluations. This report presents the results of a feasibility study to evaluate the material release from capsule direct disposal in the repository. Regulatory requirements specify that the analysis of material placement in the repository be performance-based. The term "performance-based" means evaluating various parameters, such as radionuclide release, through analysis of the as-packaged material response to the repository environment.

The analyses discussed in this report are performed using methods like those used at the repository for similar analysis work. The supporting information for the analyses is discussed in different sections of this report. The relation between the supporting information in Section 2 and the analyses in Sections 3 and 4 is depicted in Figure 1, which also shows the information flows between the various analyses. A predictive geochemical analysis evaluates changes in the waste package chemistry due to interactions of the materials in the waste package with infiltrating repository groundwater. The geochemical analysis defines any changes to chemical parameters for the Total System Performance Assessment, which is a complex predictive analysis of radionuclide and material transport through the repository, modeling the disposal package (containing commercial/Department of Energy (DOE) spent nuclear fuel (SNF), and HLW) material degradation and transport in the repository. Different TSPA analyses are performed to evaluate the effect of transport of radionuclides and specific contaminant metals in the capsules.

2.2 Capsule History

Chemical reclamation of materials from DOE SNF, known as reprocessing, generated liquid by-product streams containing radionuclides and other materials requiring disposal. At the Hanford Site, spent fuel from production reactors was reprocessed using the PUREX process. Cesium-137, strontium-90, and other fission products from the spent fuel exited the PUREX process in the high-level acid waste stream, which was neutralized and stored in tanks. The Waste Encapsulation and Storage Facility (WESF) produced capsules that were filled with materials extracted from these by-product streams. The cesium and strontium recovery and purification took place in B-plant, while the material conversion, encapsulation, and storage took place at WESF.

A brief description of the cesium chloride process[1] indicates that after recovery of the cesium from the PUREX waste, the cesium was reacted to a carbonate in solution. The cesium carbonate solution was reacted with hydrochloric acid to produce a cesium chloride solution. The solution was evaporated to solid cesium chloride, which was heated to produce a molten material. The molten cesium chloride salt was placed in an inner capsule (see Section 2.3 for a capsule description). The capsule lid was put in place and welded. Each capsule was then leak checked and placed inside an outer capsule, which then had a cap welded to it. After leak testing, the completed capsule was weighed, the contents were evaluated by calorimetry, and the capsule was placed in storage.

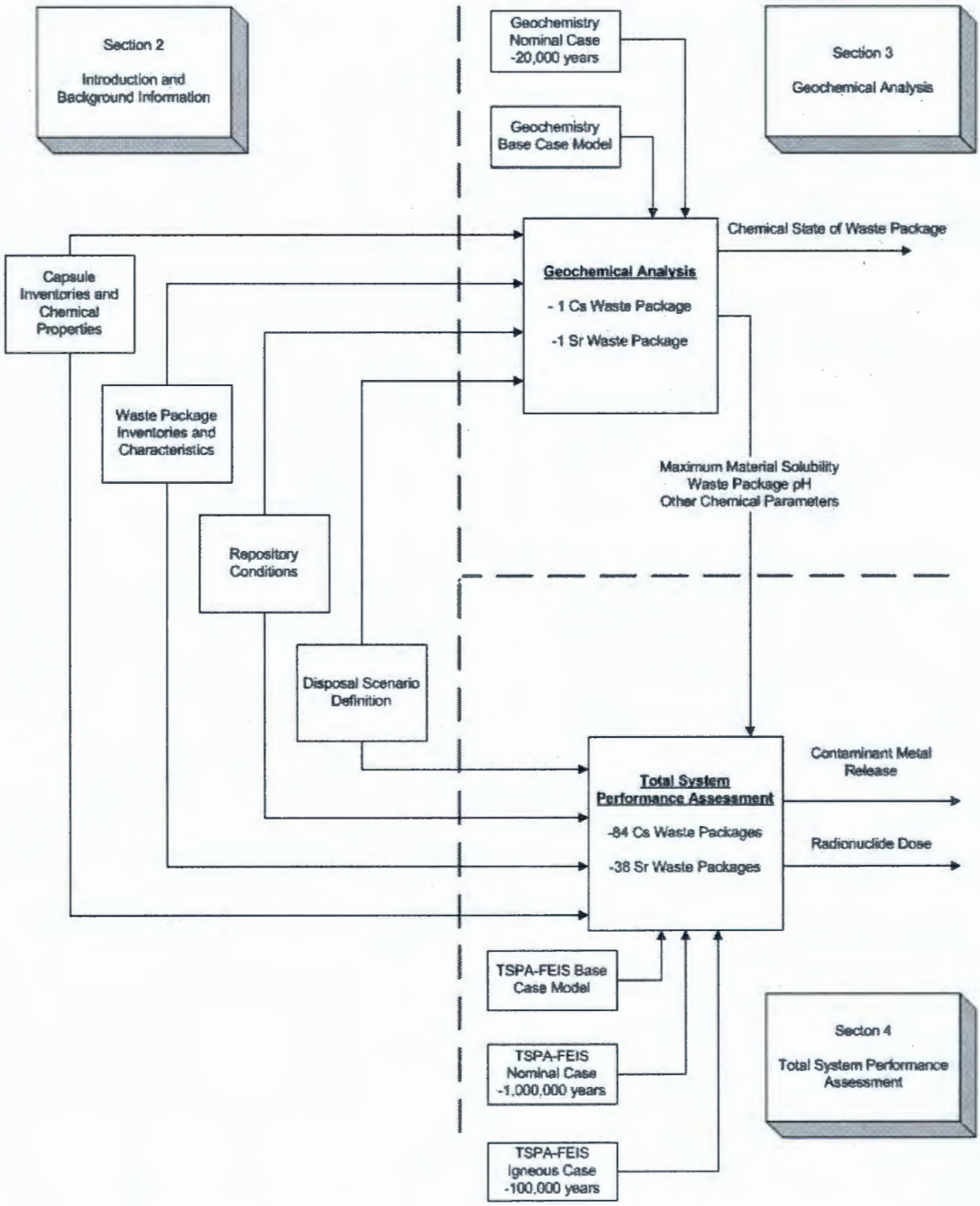

Figure 1. Relation between the supporting information and analyses for the evaluation of cesium-strontium capsule repository direct disposal.

A brief description of the strontium fluoride capsule process (See Reference 1) indicates the strontium was recovered from the PUREX acid waste solution. A volume of the waste solution containing 3 to 5 kg

of strontium was neutralized to a pH of 8 to 9 with a sodium hydroxide solution. Solid sodium fluoride was added to the solution to precipitate strontium fluoride. The resulting slurry was heated with mixing for 1 hour and was then filtered. The filter cake was washed with water and fired at a high temperature in argon for several hours. After cooling, the strontium fluoride was pulverized to minus 1/2-in. granules and loaded into an inner capsule by impact consolidation, which was essentially a cold-step-pressing operation. The capsule was closed by welding a lid in place. The capsule was leak checked and decontaminated. The cleaned capsule was sealed in an outer capsule. After the weld checking, weighing, and calorimetry to determine the heat output, the capsule was stored in a water-filled basin.

2.3 Capsule Descriptions

The cesium chloride and strontium fluoride capsules, illustrated in Figure 2, are similar. Dimensions (which changed three times during production) and schematics for the cesium chloride capsules are shown in Figure 3 and Table 1; a similar drawing for the strontium fluoride capsules is shown in Figure 4. The capsule materials are 316L stainless steel except for the strontium inner capsules, which are made from Hastelloy C-276. There are indications that some of the strontium fluoride outer capsules were inadvertently made from Hastelloy (see Reference 1). Hastelloy reacts more slowly than 316L stainless, so these studies assume a uniform outer capsule material of 316L stainless steel.

Twenty-three of the cesium-containing capsules failed for various reasons over the years. These capsules were placed inside an overpack, known as a type W overpack, to provide a new containment boundary. The overpack is constructed of 316L stainless steel and contains approximately 50% of the steel mass of any one overpacked capsule, but only contributes approximately 1.5% of the total steel mass for the inventory of all cesium capsules. The dimensions of the type W overpack are shown in Figure 3.

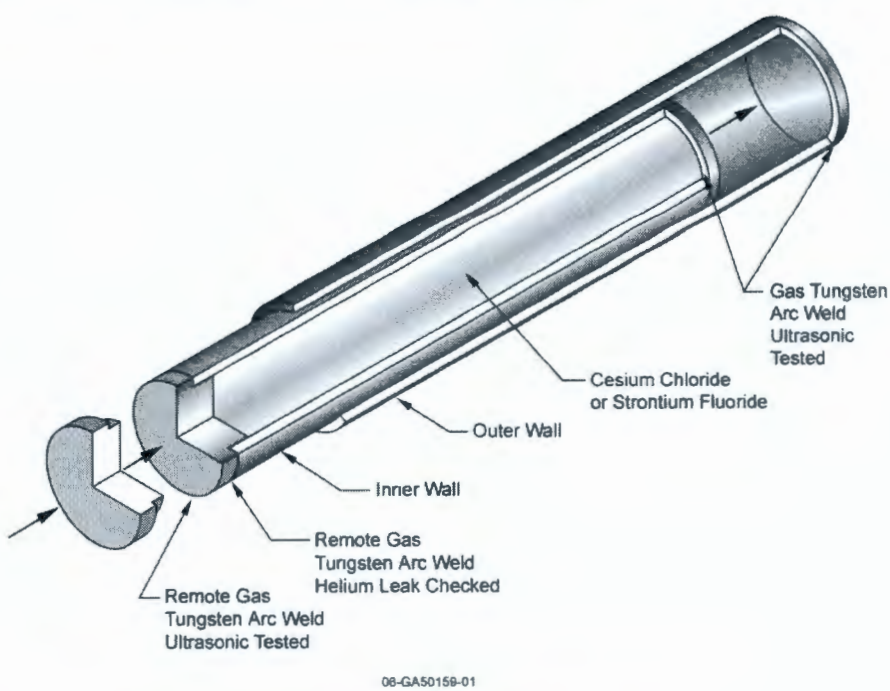

Figure 2. A schematic of the cesium chloride/strontium fluoride capsules.

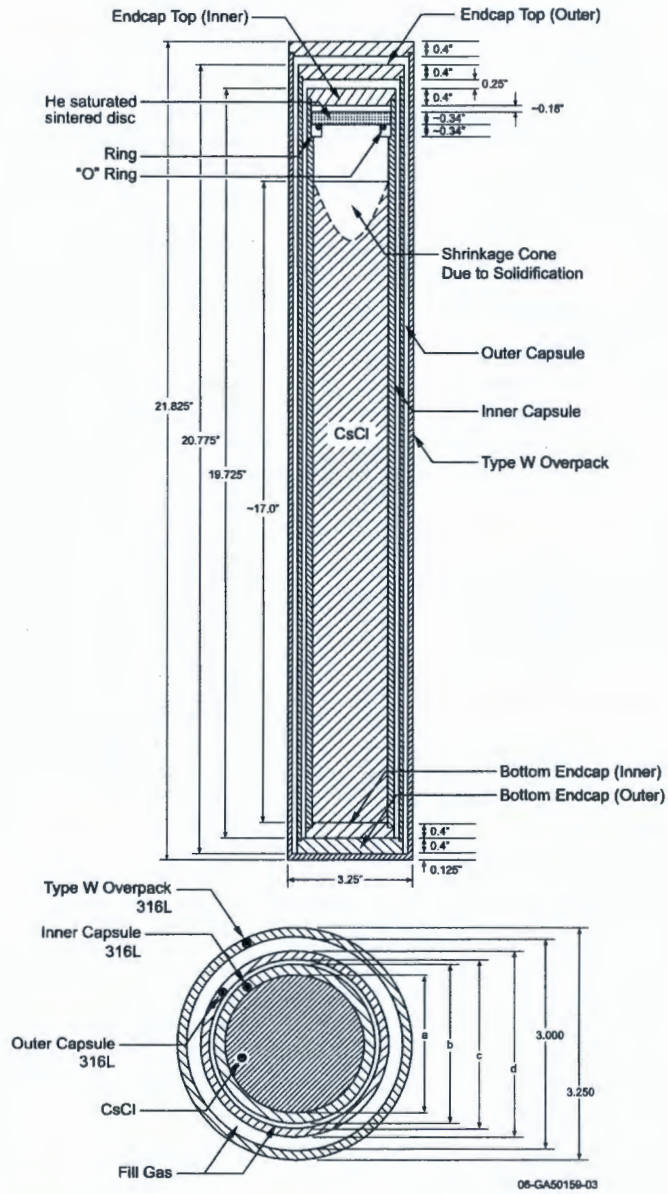

Figure 3. A schematic of the cesium chloride capsules.

Table 1. Diameters of the cesium chloride capsules.

Capsule Type	Inner Capsule Inner Diameter (a) (see Figure 3)	Inner Capsule Outer Diameter (b) (see Figure 3)	Outer Capsule Inner Diameter (c) (see Figure 3)	Outer Capsule Outer Diameter (d) (see Figure 3)
1	2.060 in.	2.250 in.	2.407 in.	2.625 in.
2	2.044 in.	2.250 in.	2.407 in.	2.645 in.
3	1.983 in.	2.255 in.	2.385 in.	2.657 in.

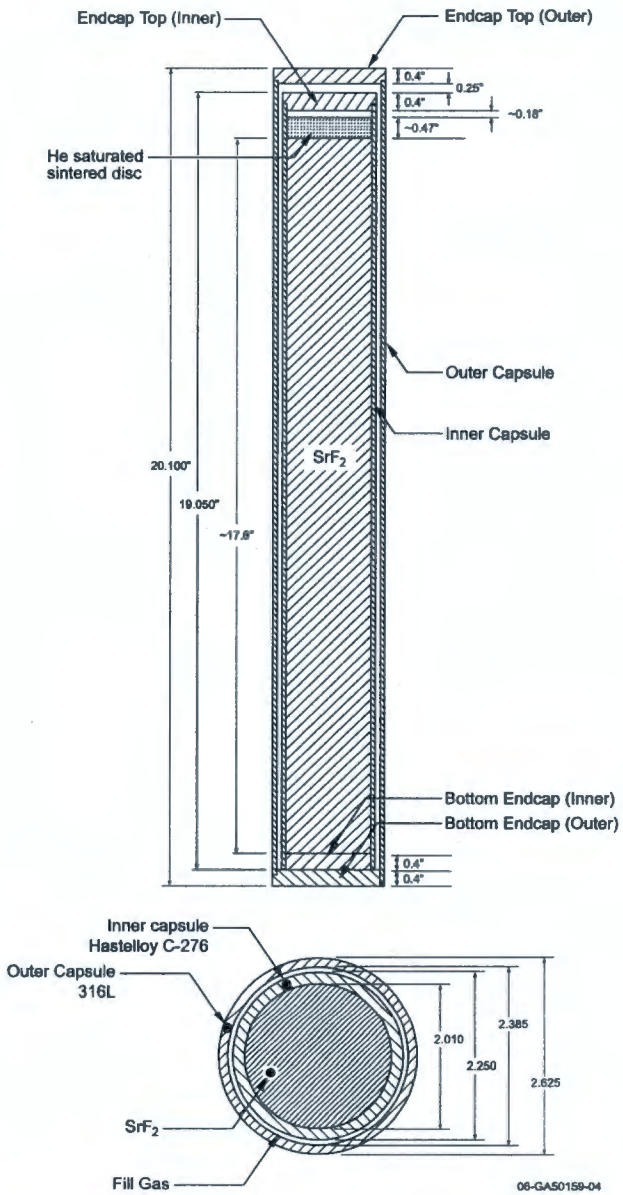

Figure 4. A schematic of the strontium fluoride capsules.

2.4 Analysis Scenario and Assumptions

A capsule disposal design has not been developed. For this analysis, a disposal scenario was developed to define required parameters for the analysis. This scenario is a best estimate of repository disposal packaging, but it is not a formal design. This section discusses the scenario-specific data and assumptions that are common to both the geochemical and TSPA analyses. Data and assumptions that are specific to only one of the analyses are detailed in that specific section of the report.

2.4.1 Repository Disposal Packaging

There are 1,335 cesium chloride capsules and 601 strontium fluoride capsules to be disposed (see Reference 1). For this conceptual scenario, a design is used that places the capsules in a basket inside a 316L stainless steel container, which is placed inside of a DOE standardized canister. The standardized canister is then placed inside a repository waste package.

2.4.1.1 Capsule Disposal Basket and Container

A basket conceptual design, illustrated in Figure 5, was provided by Hanford.[a] This design places up to eight capsules in each basket and two baskets within a shell inside of a DOE standardized canister (see Section 2.4.1.2) for 16 available capsule positions per standardized canister.

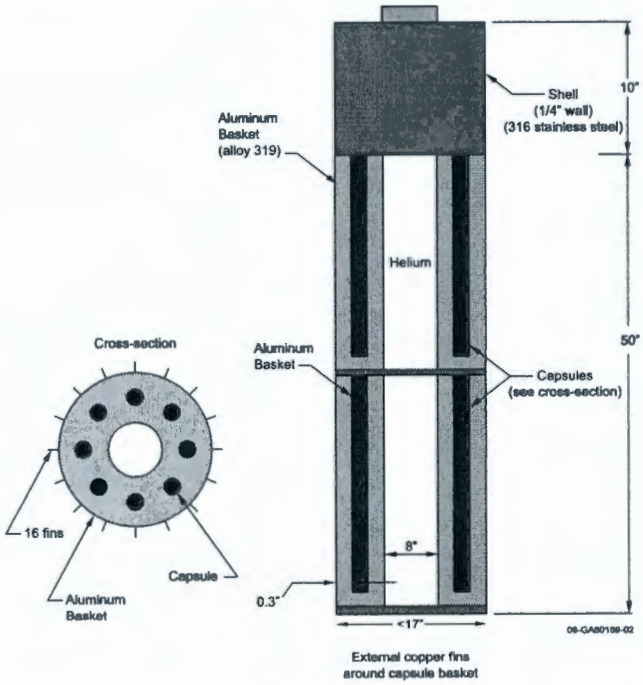

Figure 5. Conceptual basket assembly for placing cesium and strontium capsules in a storage container.

The basket assembly is made from aluminum alloy 319 and has a 316L stainless steel shell. The stacked rack assembly has a 25.4-cm (10-in.) plug. The basket has a void in the center filled with helium, and the void is 20.3 cm (8 in.) in diameter with a volume of 20,490 cm^3 (1,250 $in.^3$) in each basket. The volume occupied by eight capsules placed in a basket is 14,260 cm^3 (870.2 $in.^3$). This is based on the smaller strontium fluoride capsule (leaving a conservatively high-metal volume in the basket). Subtracting this volume from the basket volume results in a basket metal volume of 55,520 cm^3 (3,388 $in.^3$). Aluminum 319 has a density of 2.768 g/cm^3, which results in a per basket aluminum mass of 153.7 kg (338.8 lb).[2]

a. Roger McCormack, personal communication, January 2006.

The basket shell will hold two stacked baskets with a plug in the end of the basket. The basket shell is made from 316L stainless steel. It is anticipated that copper fins will be placed on the outside of the shell for heat dissipation. Those fins are not expected to be a significant mass. Therefore, the mass of the copper from the fins is neglected in this study. The wall thickness of the shell is 0.318 cm (0.125 in.) with a volume of 7,446 cm^3 (454.4 $in.^3$). Using a density of 8 g/cm^3, the mass of the shell is 348.4 kg (768.2 lb). The plug that sits on top of the baskets in the shell is also made of 316L stainless steel. The plug volume is 36,110 cm^3 (2,204 $in.^3$). The steel mass in the plug is 288.9 kg (636.9 lb).

2.4.1.2 DOE Standardized Canister

Previous studies of DOE SNF repository disposal have resulted in the design of a DOE standardized canister, illustrated in Figure 6. The standardized canister has an approximate diameter of 45.7 cm (18 in.) in both 300-cm (118.1-in.) and 457-cm (179.9-in.) lengths, referred to as the 10-ft canister and the 15-ft canister, respectively. The DOE 10-ft standardized canister is used in this study to contain the capsule racks and baskets. The capsule disposal baskets in the outer shell container, discussed above, will fit in the canister and fill the 10-ft canister to approximately half of its overall length.

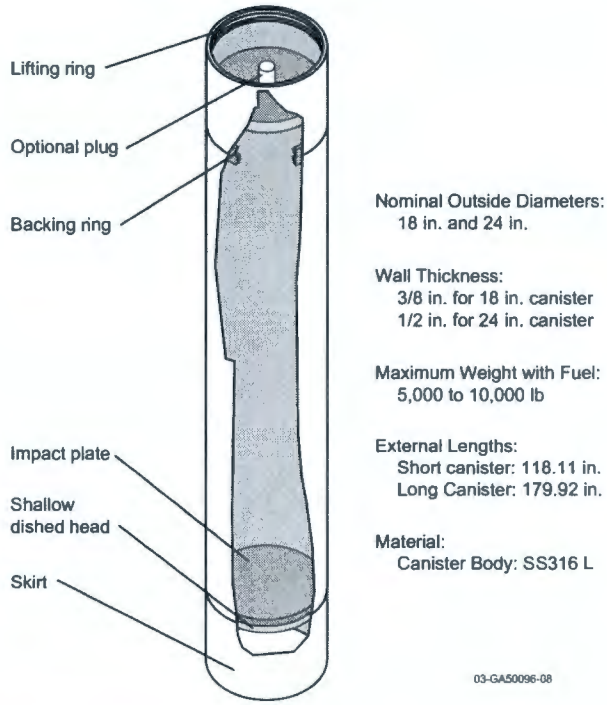

Figure 6. The DOE standardized canister.

A spacer is used inside the standardized canister to hold the shell and fill the standardized canister. A simple conceptual design for the spacer, consisting of a hollow right cylinder with a wall thickness of 0.635 cm (0.25 in.) and a 1-in.-thick lid on each end, is shown in Figure 7. The spacer has a void volume

of 216,000 cm^3 (13,200 $in.^3$). The metal volume of the spacer, which is made from 316L stainless steel, is 19,940 cm^3 (1,217 $in.^3$) with an approximate metal mass of 159.5 kg (351.7 lb).

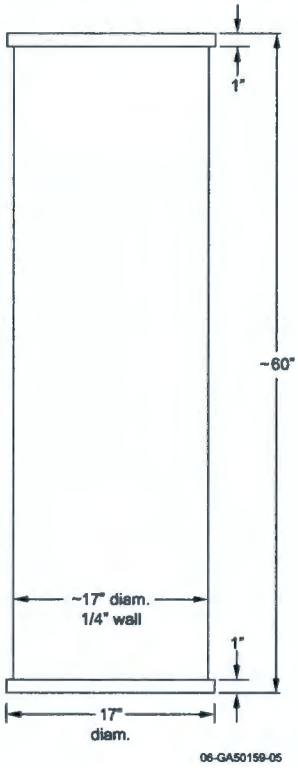

Figure 7. Spacer assembly for placing the capsules in the DOE standardized canister.

2.4.1.3 Waste Package Configurations

Although there have been changes made to the repository design over the past several years, the current design is based on fundamentally different waste package designs, specific to the materials to be placed in them. There are two basic waste package designs to handle the various DOE SNF and HLW canisters in the repository.[3] Because the two designs will accommodate both DOE SNF and HLW, these waste package configurations are sometimes referred to as the "DOE waste package" or "DOE codisposal waste package." In addition to these, there is one designed specifically to accommodate the Hanford Multi-Canister Overpack, which make three waste package designs for DOE SNF.

The codisposal design allows the placement of five 61-cm (24-in.)-diameter DHLW canisters surrounding one 45.7-cm (18-in.)-diameter DOE SNF canister in the center. This design has an approximate internal length of 3.04 m (10 ft) or 4.6 m (15 ft) to accommodate the 10 or 15-ft-long DOE SNF and HLW canisters. This configuration has been called the 5-DHLW/DOE SNF short or long-waste package, respectively. Figure 8 shows a cross section of the 5-DHLW/DOE SNF waste package design.[4]

The scenario for packaging the capsules in this study is the codisposal concept in a 5-DHLW/DOE SNF short-waste package. The canister containing the capsules would replace the SNF canister in the center of

the package. It is assumed that the properties of the HLW glass in the waste packages, previously derived for similar calculations at the repository, are constant and that no changes will be made to those properties for this study.

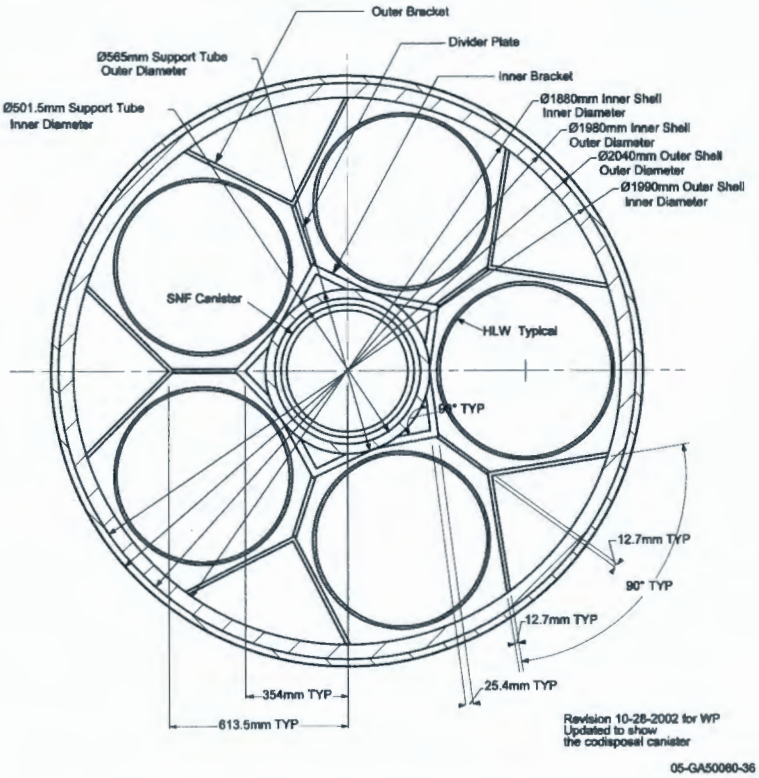

Figure 8. Cross section of the 5-DHLW/DOE SNF codisposal waste package.

Four primary components make up the DOE codisposal waste package: (1) the internal basket assemblies that facilitate loading of the DOE SNF and HLW to ensure proper geometry, (2) an inner stainless steel vessel, (3) an outer corrosion-resistant vessel, and (4) the trunnion collar used for lifting and handling of the waste package. Figure 9 shows these four waste package components.[5]

The internal basket assemblies will be fabricated of A-516 carbon steel grade 70. The inner vessel will be made of 50-mm-thick Type 316 NG stainless steel with additional restrictions on the amount of carbon and nitrogen. The inner vessel will be designed and fabricated in accordance with the American Society of Mechanical Engineers Code, Section III, Division 1, Subsection NC. The outer vessel will be made of 25-mm-thick Alloy 22. The outer vessel fabrication and examination will be in accordance with the American Society of Mechanical Engineers Code, Section III, Division 1, Subsection NC. In addition, the outer vessel will have two, not one, Alloy 22 closure lids to provide additional margin against early waste package failure. The trunnion collar is removable and will be fabricated of 17-4 PH stainless steel.

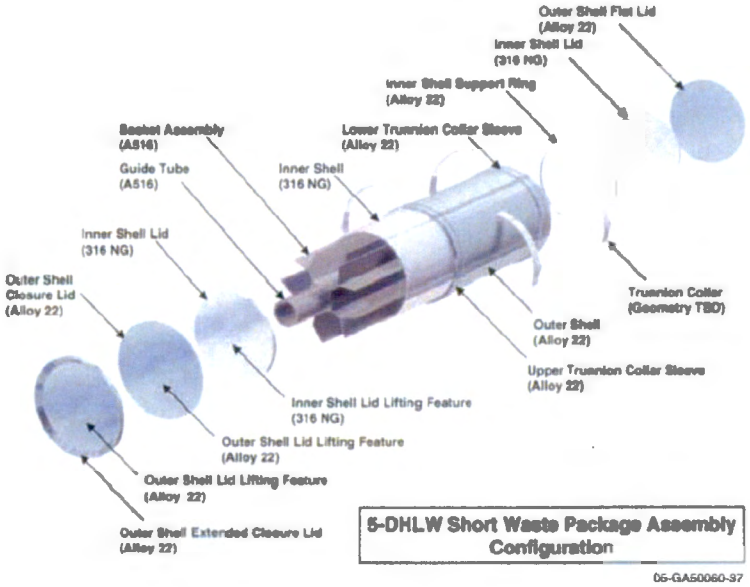

Figure 9. Components of the 5-DHLW/DOE SNF codisposal waste package.

2.4.1.4 Number of Capsules in the Waste Package

The number of capsules per waste package is controlled by either the maximum available openings in the capsule basket or the thermal loading of the package. Because the radionuclides, and thus the heat load, from the capsules will decay rapidly, the assumption was made that the capsules will be packaged for disposal sometime after 2018, discounting the heat loading in the near term. This allows 16 capsules of either type to be placed in the standardized canister, resulting in 84 standardized canisters to contain the cesium chloride capsules and 38 standardized canisters to contain the strontium fluoride capsules. Because the waste package will be loaded with one standardized canister containing the capsules, this will result in the same number of waste packages as standardized canisters.

2.4.2 Capsule Contents Composition

The composition of the materials in the capsule defines the chemistry of the system, and hence, the form of the materials as they are released from the waste package. Material composition also defines the material physical transport parameters. The versions of the geochemical and TSPA models used in this study do not track the generation of radionuclide decay daughter products of interest to this study. Since some of those daughter products are of interest to the results of this study, amounts for those were calculated and included in the capsule compositions, to assure that the chemical effects and transport of these daughters was included in the studies. The daughters were added on top of the existing inventories, which resulted in somewhat different material compositions than shown in Reference 1.

2.4.2.1 *Cesium Chloride and Strontium Fluoride Composition*

The capsule chemical compositions are taken from Reference 1. As discussed in Reference 1, material amounts in the capsule were calculated by computing a weight percentage of each compound based on the amounts of metals reported by previous work. The presence of silver is inferred from PUREX process knowledge, prior to the separation of the capsule materials from the PUREX HLW. For this study, the amount of silver was defined as the lower analytical detection limit when the material was analyzed.[b] The metal weight percentages were converted to compound weight percentages, corrected to include the amount of silver specified. The calculations assume that the species in the capsules are in their thermodynamically favored state (e.g., barium produced from cesium decay would be in the form $BaCl_2$) and that no ions exist in the capsule (i.e., there is chloride and fluoride available to bond with the materials generated). These assumptions, which are in line with those made for the analysis of capsule corrosion, induce small differences in the calculated values of non-radionuclide capsule contents. This difference can be seen by comparing values in Tables 2 and 3 and Tables 4 and 5. For the non-radioactive elements that do not bond with the radioactive elements, the maximum calculated difference ranges from 0 grams (for silver) to ~2.9 grams (for sodium) in a cesium chloride capsule package and from 0 grams (for silver) to ~3.9 grams (for sodium) in a strontium fluoride capsule. For the materials that interact with the radionuclides as they decay, the changes are higher. The total amount of materials in the capsule is unchanged. The weight percent calculations only change the distribution of material within the defined total weight of the capsules.

Because of the above assumptions and calculations, for purposes of this study, the higher value set for any given specie was used as the values for the specie in the TSPA (in all cases except barium, this is the Year 2006 value. Because the TSPA does not track barium generation from decay, the Year 2275 values for barium were used in the TSPA.) Separate geochemistry runs were made for each data set for each year, and the most conservative solubilities from the analysis of the capsule types were used in the TSPA. The results of the TSPA discussed later in this report therefore represent conservative evaluations in response to base data anomalies.

Analysis of the radionuclide quantities in the capsules are as of the Year 1975 (see Reference 1). Using this base, the amounts of the chemicals and isotopes in the capsules at Year 2006 and at Year 2275 (after 10 cesium-137 half-lives) were calculated. Ten half-lives were selected to allow for essentially the total decay of cesium-137 (half-life = 30.07 years)[6], strontium-90 (half-life = 28.78 years) and resulting daughter products to their decay products.

The results of these calculations are shown in Tables 2 and 3 for the cesium chloride capsules, and Tables 4 and 5 for the strontium fluoride capsules. The quantities are presented as grams per capsule and grams per standardized canister packed with the number of capsules discussed in Section 2.4.1.4. The weights reported for each element are the minimum, average, and maximum values of the weight ranges of all of the cesium chloride or strontium fluoride capsules. The shorter-lived radioisotopes of cesium and strontium are shown separately from the stable or very long-lived isotopes to facilitate analysis of the specific isotopes behavior.

b. S. Moy, personal communication, March 2006.

2.4.2.2 *Contaminant Metals*

A concern with capsule disposal is the presence of contaminant metals that are controlled under various hazardous material disposal regulations. The contaminant metals detected in the capsules are barium, cadmium, chromium, lead, and silver. (See Reference 1). The contaminants, shown with asterisks in Tables 2, 3, 4, and 5, are present in low amounts, but have potential to migrate through the repository.

Table 2. Estimated nominal element mass in the cesium chloride capsules at Year 2006.

Element	Weight in Capsule (g)				Weight in Standardized Canister (16 capsules) (g)		
	Minimum	Average	Maximum		Minimum	Average	Maximum
Aluminum	9.4E-01	7.9E+00	1.0E+01		1.5E+01	1.3E+02	1.6E+02
Barium*	3.6E+01	3.1E+02	3.9E+02		5.8E+02	4.9E+03	6.3E+03
Boron	2.5E+00	2.1E+01	2.7E+01		4.0E+01	3.3E+02	4.3E+02
Cadmium*	5.7E-02	4.8E-01	6.2E-01		9.2E-01	7.7E+00	9.9E+00
Calcium	3.1E+00	2.6E+01	3.4E+01		5.0E+01	4.2E+02	5.4E+02
Cerium	1.8E-02	1.5E-01	1.9E-01		2.8E-01	2.4E+00	3.1E+00
Cesium -135	1.9E+01	1.6E+02	2.1E+02		3.1E+02	2.6E+03	3.4E+03
Cesium-137	3.5E+01	2.9E+02	3.8E+02		5.6E+02	4.7E+03	6.0E+03
Cesium, Other	8.5E+01	7.1E+02	9.1E+02		1.4E+03	1.1E+04	1.5E+04
Chromium*	4.4E+00	3.7E+01	4.7E+01		7.0E+01	5.8E+02	7.5E+02
Cobalt	3.1E-01	2.6E+00	3.4E+00		5.0E+00	4.2E+01	5.4E+01
Copper	6.2E-01	5.2E+00	6.7E+00		9.9E+00	8.3E+01	1.1E+02
Iron	1.6E+00	1.3E+01	1.7E+01		2.5E+01	2.1E+02	2.7E+02

Element	Weight in Capsule (g)				Weight in Standardized Canister (16 capsules) (g)		
	Minimum	Average	Maximum		Minimum	Average	Maximum
Lanthanum	1.8E-02	1.5E-01	1.9E-01		2.8E-01	2.4E+00	3.0E+00
Lead*	4.4E+00	3.6E+01	4.7E+01		7.0E+01	5.8E+02	7.5E+02
Magnesium	7.8E-01	6.5E+00	8.4E+00		1.2E+01	1.0E+02	1.3E+02
Manganese	1.5E-01	1.3E+00	1.6E+00		2.4E+00	2.0E+01	2.6E+01
Molybdenum	6.6E-02	5.5E-01	7.1E-01		1.0E+00	8.8E+00	1.1E+01
Nickel	1.0E+00	8.6E+00	1.1E+01		1.6E+01	1.4E+02	1.8E+02
Palladium	5.6E-02	4.7E-01	6.0E-01		9.0E-01	7.5E+00	9.7E+00
Phosphorus	3.1E-01	2.6E+00	3.4E+00		5.0E+00	4.2E+01	5.4E+01
Potassium	2.5E+00	2.1E+01	2.7E+01		3.9E+01	3.3E+02	4.3E+02
Rubidium	1.5E+00	1.3E+01	1.7E+01		2.5E+01	2.1E+02	2.7E+02
Silicon	1.3E+00	1.1E+01	1.4E+01		2.1E+01	1.8E+02	2.3E+02
Silver*	3.2E-02	2.7E-01	3.4E-01		5.1E-01	4.3E+00	5.5E+00
Sodium	9.7E+00	8.1E+01	1.0E+02		1.5E+02	1.3E+03	1.7E+03
Strontium	5.7E-01	4.8E+00	6.1E+00		9.1E+00	7.6E+01	9.8E+01
Sulfur	0.0E+00	0.0E+00	0.0E+00		0.0E+00	0.0E+00	0.0E+00
Titanium	2.1E-01	1.8E+00	2.3E+00		3.4E+00	2.9E+01	3.7E+01
Zirconium	2.4E-01	2.0E+00	2.6E+00		3.9E+00	3.3E+01	4.2E+01

Element	Weight in Capsule (g)				Weight in Standardized Canister (16 capsules) (g)		
	Minimum	Average	Maximum		Minimum	Average	Maximum
Chlorine	1.0E+02	8.3E+02	1.1E+03		1.6E+03	1.3E+04	1.7E+04
Oxygen	7.7E+00	6.4E+01	8.3E+01		1.2E+02	1.0E+03	1.3E+03
Total Weight	3.2E+02	2.7E+03	3.4E+03		5.1E+03	4.3E+04	5.5E+04

Table 3. Estimated nominal element mass in the cesium chloride capsules at Year 2275.

Element	Weight in Capsules (g)				Weight in Standardized Canister (16 capsules) (g)		
	Minimum	Average	Maximum		Minimum	Average	Maximum
Aluminum	9.19E-01	7.69E+00	9.91E+00		1.5E+01	1.2E+02	1.6E+02
Barium*	6.94E+01	5.81E+02	7.48E+02		1.1E+03	9.3E+03	1.2E+04
Boron	2.43E+00	2.03E+01	2.62E+01		3.9E+01	3.2E+02	4.2E+02
Cadmium*	5.57E-02	4.66E-01	6.00E-01		8.9E-01	7.5E+00	9.6E+00
Calcium	3.03E+00	2.53E+01	3.27E+01		4.8E+01	4.1E+02	5.2E+02
Cerium	1.72E-02	1.44E-01	1.86E-01		2.8E-01	2.3E+00	3.0E+00
Cesium-135	1.89E+01	1.58E+02	2.04E+02		3.0E+02	2.5E+03	3.3E+03
Cesium-137	6.96E-02	5.83E-01	7.51E-01		1.1E+00	9.3E+00	1.2E+01
Chromium*	4.24E+00	3.55E+01	4.58E+01		6.8E+01	5.7E+02	7.3E+02
Cesium, Other	8.23E+01	6.89E+02	8.87E+02		1.3E+03	1.1E+04	1.4E+04
Cobalt	3.02E-01	2.53E+00	3.26E+00		4.8E+00	4.0E+01	5.2E+01
Copper	6.02E-01	5.04E+00	6.50E+00		9.6E+00	8.1E+01	1.0E+02
Iron	1.52E+00	1.27E+01	1.64E+01		2.4E+01	2.0E+02	2.6E+02
Lanthanum	1.71E-02	1.43E-01	1.85E-01		2.7E-01	2.3E+00	3.0E+00
Lead*	4.24E+00	3.55E+01	4.57E+01		6.8E+01	5.7E+02	7.3E+02
Magnesium	7.57E-01	6.34E+00	8.17E+00		1.2E+01	1.0E+02	1.3E+02

Element	Weight in Capsules (g)				Weight in Standardized Canister (16 capsules) (g)		
	Minimum	Average	Maximum		Minimum	Average	Maximum
Manganese	1.45E-01	1.22E+00	1.57E+00		2.3E+00	1.9E+01	2.5E+01
Molybdenum	6.38E-02	5.34E-01	6.88E-01		1.0E+00	8.5E+00	1.1E+01
Nickel	1.00E+00	8.38E+00	1.08E+01		1.6E+01	1.3E+02	1.7E+02
Palladium	5.45E-02	4.56E-01	5.88E-01		8.7E-01	7.3E+00	9.4E+00
Phosphorus	3.03E-01	2.54E+00	3.27E+00		4.8E+00	4.1E+01	5.2E+01
Potassium	2.40E+00	2.01E+01	2.58E+01		3.8E+01	3.2E+02	4.1E+02
Rubidium	1.50E+00	1.25E+01	1.61E+01		2.4E+01	2.0E+02	2.6E+02
Silicon	1.27E+00	1.07E+01	1.37E+01		2.0E+01	1.7E+02	2.2E+02
Silver*	3.19E-02	2.67E-01	3.44E-01		5.1E-01	4.3E+00	5.5E+00
Sodium	9.39E+00	7.86E+01	1.01E+02		1.5E+02	1.3E+03	1.6E+03
Strontium	5.52E-01	4.62E+00	5.95E+00		8.8E+00	7.4E+01	9.5E+01
Sulfur	0.00E+00	0.00E+00	0.00E+00		0.0E+00	0.0E+00	0.0E+00
Titanium	2.07E-01	1.74E+00	2.24E+00		3.3E+00	2.8E+01	3.6E+01
Zirconium	2.37E-01	1.98E+00	2.56E+00		3.8E+00	3.2E+01	4.1E+01
Chlorine	1.06E+02	8.84E+02	1.14E+03		1.7E+03	1.4E+04	1.8E+04
Oxygen	7.46E+00	6.24E+01	8.05E+01		1.2E+02	1.0E+03	1.3E+03
Total Weight	3.19E+02	2.67E+03	3.44E+03		5.1E+03	4.3E+04	5.5E+04

Table 4. Estimated nominal element mass in the strontium fluoride capsules at Year 2006.

Element	Weight in Capsule (g)				Weight in Standardized Canister (16 Capsules) (g)		
	Minimum	Average	Maximum		Minimum	Average	Maximum
Aluminum	5.4E-01	3.7E+00	5.0E+00		8.7E+00	6.0E+01	8.0E+01
Barium*	5.3E+00	3.6E+01	4.9E+01		8.4E+01	5.8E+02	7.8E+02
Cadmium*	2.5E-01	1.7E+00	2.3E+00		4.0E+00	2.8E+01	3.7E+01
Calcium	3.5E+00	2.4E+01	3.23E+01		5.5E+01	3.8E+02	5.1E+02
Chromium*	8.0E-01	5.5E+00	7.4E+00		1.3E+01	8.9E+01	1.2E+02
Copper	2.6E-02	1.8E-01	2.4E-01		4.1E-01	2.9E+00	3.8E+00
Fluorine	1.3E+02	9.0E+02	1.2E+03		2.1E+03	1.4E+04	1.9E+04
Iron	1.0E+00	6.9E+00	9.3E+00		1.6E+01	1.1E+02	1.5E+02
Lanthanum	4.8E-01	3.3E+00	4.4E+00		7.6E+00	5.3E+01	7.1E+01
Lead*	5.7E-01	3.9E+00	5.3E+00		9.1E+00	6.3E+01	8.4E+01
Magnesium	6.6E-01	4.5E+00	6.1E+00		1.1E+01	7.2E+01	9.7E+01
Manganese	2.0E-01	1.4E+00	1.8E+00		3.2E+00	2.2E+01	2.9E+01
Nickel	1.0E+00	7.0E+00	9.5E+00		1.6E+01	1.1E+02	1.5E+02
Potassium	2.3E-02	1.6E-01	2.1E-01		3.6E-01	2.5E+00	3.4E+00
Silicon	1.8E-01	1.3E+00	1.7E+00		2.9E+00	2.0E+01	2.7E+01
Silver*	3.6E-02	2.5E-01	3.3E-01		5.8E-01	4.0E+00	5.3E+00

Element	Weight in Capsule (g)				Weight in Standardized Canister (16 Capsules) (g)		
	Minimum	Average	Maximum		Minimum	Average	Maximum
Sodium	7.4E+00	5.1E+01	6.8E+01		1.2E+02	8.1E+02	1.1E+03
Strontium-90	5.4E+01	3.7E+02	5.0E+02		8.6E+02	5.9E+03	7.9E+03
Strontium,Other	9.2E+01	6.4E+02	8.5E+02		9.2E+01	6.4E+02	8.5E+02
Zirconium	6.2E+01	4.3E+02	5.7E+02		9.9E+02	6.8E+03	9.1E+03
Total Weight	3.6E+02	2.5E+03	3.3E+03		5.8E+03	4.0E+04	5.3E+04

Table 5. Estimated nominal element mass in the strontium fluoride capsules at Year 2275.

Element	Weight in Capsule (g)				Weight in Standardized Canister (16 Capsules) (g)		
	Minimum	Average	Maximum		Minimum	Average	Maximum
Aluminum	5.1E-01	3.5E+00	4.7E+00		8.2E+00	5.6E+01	7.5E+01
Barium*	5.0E+00	3.4E+01	4.6E+01		8.0E+01	5.5E+02	7.4E+02
Cadmium*	2.4E-01	1.6E+00	2.2E+00		3.8E+00	2.6E+01	3.5E+01
Calcium	3.3E+00	2.2E+01	3.0E+01		5.2E+01	3.6E+02	4.8E+02
Chromium*	7.6E-01	5.2E+00	7.0E+00		1.2E+01	8.3E+01	1.1E+02
Copper	2.4E-02	1.7E-01	2.3E-01		3.9E-01	2.7E+00	3.6E+00
Fluorine	1.4E+02	9.9E+02	1.3E+03		2.3E+03	1.6E+04	2.1E+04
Iron	9.4E-01	6.5E+00	8.7E+00		1.5E+01	1.0E+02	1.4E+02

Element	Weight in Capsule (g)				Weight in Standardized Canister (16 Capsules) (g)		
	Minimum	Average	Maximum		Minimum	Average	Maximum
Lanthanum	4.5E-01	3.1E+00	4.2E+00		7.2E+00	5.0E+01	6.7E+01
Lead*	5.4E-01	3.7E+00	5.0E+00		8.6E+00	5.9E+01	7.9E+01
Magnesium	6.2E-01	4.3E+00	5.7E+00		9.9E+00	6.8E+01	9.2E+01
Manganese	1.9E-01	1.3E+00	1.7E+00		3.0E+00	2.1E+01	2.8E+01
Nickel	9.6E-01	6.6E+00	8.9E+00		1.5E+01	1.1E+02	1.4E+02
Potassium	2.1E-02	1.5E-01	2.0E-01		3.4E-01	2.4E+00	3.2E+00
Silicon	1.7E-01	1.2E+00	1.6E+00		2.7E+00	1.9E+01	2.5E+01
Silver*	3.6E-02	2.5E-01	3.3E-01		5.8E-01	4.0E+00	5.3E+00
Sodium	6.9E+00	4.8E+01	6.4E+01		1.1E+02	7.7E+02	1.0E+03
Strontium-90	7.6E-02	5.2E-01	7.0E-01		1.2E+00	8.4E+00	1.1E+01
Strontium,Other	8.7E+01	6.0E+02	8.0E+02		1.4E+03	9.6E+03	1.3E+04
Zirconium	1.1E+02	7.5E+02	1.0E+03		1.7E+03	1.2E+04	1.6E+04
Total Weight	3.6E+02	2.5E+03	3.3E+03		5.8E+03	4.0E+04	5.3E+04

3. GEOCHEMICAL ANALYSIS

The geochemical analysis in this study calculates in-package[c] solution concentrations for contaminant metals (silver, barium, cadmium, chromium, and lead), cesium isotopes (cesium-133, cesium-135, cesium-137), and strontium (strontium-87 and strontium-90) in two separate breached codisposal waste packages interacting with infiltrating ground water. As previous analyses have assumed, both waste packages contain Savannah River Laboratory (SRL) HLW glass. This is because of the conservative chemical properties of SRL HLW glass, compared to other DOE HLW glass. Additionally, the geochemical analysis supports the evaluation of the chemistry inside the capsule containing waste and allows comparison to previous calculations of waste package chemistry. Since no significant changes to the waste package chemistry were encountered, the applicability of the TSPA-FEIS model to this study is confirmed.

3.1 Geochemical Analysis Software and Model

The computer software used in this study is EQ3/6 (EQ3/6, V. 7.2b) and Version 7.2bLV of EQ6. This software was obtained from Yucca Mountain for use in other work and is suitable for use in this study. Software validation was performed at Yucca Mountain. Installation and maintenance of the software was performed under quality controls outlined in the Yucca Mountain installation instructions accompanying the software. Software validated under the quality program at Yucca Mountain is referred to as "qualified."

EQ6 version 7.2bLV does not contain a solid-centered flow-through mode (SCFT). However, the functionality of a SCFT mode is provided, as in previous analyses at the repository, by including waste package materials as "special reactants" in EQ6 input files. In this SCFT mode, an increment of aqueous displacer solution is added continuously to the waste package system and a like volume of the existing solution is removed simulating a well-mixed batch reactor.

Table 6 describes the computer software used to carry out the calculations discussed in this report. The software was only used within the qualified data range and without modification of the source code, subroutines, and/or executables. The EQ3/6 calculations were executed on two different computers:

- EQ3/6 calculations were performed using a Windows 95 operating system on a Dell OptiPlex GX1P computer.
- EQ6 calculations were performed using a Windows NT Version 4.0 operating system on a Dell OptiPlex GX1P computer.

[c] The term "in-package" defines that the geochemical studies discussed in this report evaluate chemistry changes only for materials inside the waste package. This evaluation does not explicitly look at the chemistry of the repository. The purpose of this evaluation is to assure that changes to previous waste package chemistry analyses, which the overall repository chemistry is based upon, are small enough to expect no impact to the repository chemistry from the changes caused by inclusion of the cesium and strontium capsules.

Table 6. Computer software used in the geochemical calculations.

Software	Version	Status of Software	Description and Components Used
EQ3/6	7.2b	Qualified on Windows 95	EQ3NR is a speciation-solubility code used to determine the starting fluid composition for EQ6 reaction-path calculations
			EQPT is a database file preprocessor
			EQPP is an output file data extraction program
EQ6	7.2bLV	Qualified on Windows NT 4.0	EQ6 is a reaction path code which models water/rock interaction or fluid mixing in either a pure reaction progress mode or a time mode providing estimation of concentrations remaining in an aqueous solution

3.2 Geochemical Analysis File Nomenclature

The cesium chloride and strontium fluoride waste package cases evaluated in this study are summarized in Table 7. In this table, the capsule type, capsule mass loading, and amount of isotope decay (i.e., Year 2006 versus Year 2275) for each case are used for the case the name. The case name has the form [capsule type][mass loading][isotope decay year] where:

capsule type = Corresponds to either cesium chloride or strontium fluoride

mass loading = Corresponds to the total mass of 16 capsules in a waste package

isotope decay year = Corresponds to current year/no decay (Year 2006) or 10 half-life decay of short-lived isotopes (Year 2275)

For example, the cesium chloride capsule waste package simulation, considering a maximum capsule mass loading with no isotopic decay (i.e., Year 2006), has the name CsClMax2006. A simulation of the cesium chloride capsule waste package with minimum capsule mass loading and complete isotopic decay (i.e., Year 2275) has the name CsClMin2275.

Table 7. Case names for cesium chloride and strontium fluoride waste package cases.

Waste Package[a]	16 Capsule Mass Loading (g)[b]	Isotope Decay Year	Case Name
Cesium Chloride-HLW Glass	55,040 g	2006	CsClMax2006
	55,040 g	2275	CsClMax2275
	5,104 g	2006	CsClMin2006
	5,104 g	2275	CsClMin2275
Strontium Fluoride-HLW Glass	53,281 g	2006	SrF2Max2006
	53,281 g	2275	SrF2Max2275
	5,760 g	2006	SrF2Min2006
	5,760 g	2275	SrF2Min2275

a. The EQ6 file used as the source of suppressed species for this calculation was originated by E. Thomas, in 2004, for *In-Package Chemistry Abstraction* (see Reference 7).

b. Mass of cesium and strontium isotopes and progeny given in Tables 9 through 12.

3.3 Geochemical Analysis Approach

This study uses the geochemical modeling program EQ3/6 (described in Section 3.1) to calculate in-package solution chemistry as waste package materials and contents interacting with infiltrating ground water over a 20,000-year period. This period is consistent with the previous baseline analysis. All cases evaluated include five HLW glass-filled canisters co-disposed with either 16 cesium chloride or 16 strontium fluoride capsules. Calculations include the HLW glass to provide a similar waste package configuration to the baseline. Since the focus of this study is an estimation of aqueous concentrations of cesium chloride and strontium fluoride capsule constituents dissolved into package solution, only cursory consideration is given to HLW glass constituents. Cases are evaluated for maximum and minimum cesium chloride and strontium fluoride capsule mass loading as well as changes in capsule composition resulting from complete decay of short-lived cesium and strontium isotopes to barium and zirconium. Isotopic decay is assumed to occur prior to waste package failure (see Section 3.5.11). Only sensitivity to capsule mass loading and compositions are examined in this study. Sensitivity to HLW glass composition, water composition, water infiltration rate, and material degradation rates are not within the scope of this study. However, sensitivity studies have been performed in the past for the DOE-SNF/HLW waste package, those studies should also be applicable to this study.

EQ3/6 simulations in this study modify previous DOE-SNF and HLW glass codisposal evaluations[7]. These simulations were modified for the replacement of DOE-SNF with cesium chloride or strontium fluoride capsules. Details of input file modification are given in Section 3.4. Calculations for this study involve the following steps:

- Determine the initial cesium chloride and strontium fluoride waste package solution compositions

- Calculate initial amount (moles), average composition (moles constituent/gram material), and surface area of cesium chloride and strontium fluoride capsule material (i.e., reactant) placed in waste packages
- Calculate initial amount (moles) and surface area of waste package steels, alloys, and HLW glass (i.e., reactants)
- Calculate the in-package water mass and normalize each reactant's amount and surface area to that mass
- Calculate the waste package aqueous "displacer" rates using a water infiltration rate of 0.001 m^3/year (1.0 L/year)
- Perform calculations using the solid-centered flow-through mode (discussed in Section 3.1) to continuously add an increment of the displacer solution (J-13 well water[d]) to the waste package system and remove a like volume of existing solution, which simulates a well-mixed batch reactor
- Repeat calculations for all HLW glass-cesium chloride and HLW glass-strontium fluoride waste package cases
- Calculate the in-package solution concentration of capsule constituents during 20,000-year simulations.

3.4 Calculation Approach

This simulation used conceptual and computational methods from previous geochemical waste package analyses (see Reference 7). The previous approach considers a scenario where the waste package's inner and outer shells have been breached and the drip shield has been damaged such that seepage flow is directed into the waste package through openings near the upper surface. The shells remain intact allowing ground water to enter and exit the waste package via these openings. Given this conceptual model, the waste package is treated as a well-mixed batch reactor where all waste package materials and contents (reactants) simultaneously interact with the in-package solution. This approach simulates a titration in which reactants are added to the system according to their kinetic degradation rate and exposed surface area.

Previous analyses calculated the bulk in-package chemistry resulting from degradation of HLW glass and DOE-SNF interacting with infiltrating ground water in approximately 5-m (15-ft)-long waste packages. Included in those analyses is a base case, which considers the mean or most likely parametric values of chemical and physical parameters. That base case is the geochemical baseline to compare results for this study.

d. J-13 well water is the standard water used in these types of calculations and in supporting laboratory experimentation for water/material interaction analysis at the repository. It is named after a specific sampling well on the repository site (J-13) and has a specified composition that is discussed Section 3.6.3.1.

The current waste package calculations estimate bulk in-package solution chemistry and the aqueous concentration of capsule constituents on an appropriate time scale relative to the regulatory period. This solution chemistry is compared to the baseline analysis. The mass of cesium and strontium in the waste package will decrease over time due to radioactive decay. The study approach includes estimation of cesium and strontium isotope concentrations for maximum and minimum capsule mass loading of two capsule composition cases: early waste package failure occurring before significant isotopic decay occurs, and late waste package failure occurring after relatively short-lived isotopes have completely decayed. Normalized capsule compositions are given for all cases in Tables 9 through 12. In all, eight cases are evaluated (cases are defined in Table 7). There are two cases for each of the two waste package types (i.e., cesium chloride and strontium fluoride). Each of these cases is evaluated at Year 2006 and Year 2275, as discussed in Section 2.4.2.

This approach is taken because EQ6 lacks the capability to differentiate or track decay for multiple isotopes of an individual element. The four current time cases include simulations considering both the maximum and minimum capsule mass loading and the capsule compositions for Year 2006. These cases represent the highest potential isotope concentrations in solution. In order to maximize concentrations conservatively, radioactive decay is neglected. The four most likely cases (Year 2275) are simulated by modifying the maximum and minimum mass-loading cases to account for radionuclide decay changing the amount of cesium-137, strontium-90, barium, and zirconium following a complete decay of the short-lived isotopes in the capsules. The decay of relatively long-lived cesium-135 (a half-life 2.3 million years) and the initial cesium-133/total cesium mass ratio is used with simulation results to calculate the maximum in-package concentrations of those cesium isotopes (see Section 3.5.5). The only strontium isotope in the most likely cases is strontium-87, which is radioactively stable.

To ensure meaningful comparisons to the baseline, current calculations use data for material and HLW glass compositions, degradation rates, and mineral suppression (see Sections 3.5.3 and 3.5.6) taken from the baseline analysis. Because the current calculations consider an approximately 3-m (10-ft)-long codisposal waste package, values of waste package material and HLW glass mass, volumes, and surface areas are taken from a second previous geochemical analyses that involved a short-waste package.[8] Data for cesium chloride and strontium fluoride capsule and associated capsule packaging material (e.g., capsule baskets) degradation rates are provided in Reference 1.

The waste package loading configuration for this calculation includes the placement of five 0.61-m (24-in.)-diameter by approximately 3-m-long HLW canisters constructed of 304L stainless steel and filled with HLW glass around one 0.46-m (18-in.)-diameter DOE standardized canister constructed of 316L stainless steel containing either 16 cesium chloride or 16 strontium fluoride capsules within the short codisposal waste package.

The molar quantities and surface areas of waste package materials, other than those related to the capsule package, used in these calculations were originally normalized to the void volume of a waste package containing SNF and HLW glass. Due to an increased in-package void volume, resulting from replacement of SNF with the capsules, data normalized to that previous void volume must be re-normalized to the "new" waste package void volume (the new normalization factor) prior to running simulations. The new normalization factor is calculated as one-half (see Section 3.5.8) of the total waste package void volume. Previous waste package molar quantities and surface areas are renormalized to the current water mass as

follows:

$$normalized_value = \frac{(previous_normalized_value) * (previous_normalization_factor)}{new_normalization_factor}$$

Normalized molar quantities and surface areas for cesium chloride and strontium fluoride waste package simulations are given in Table 8. Relative to this, high normalized strontium fluoride capsule surface areas result from the use of laboratory estimates of effective surface areas (400 cm^2/g) that are based on observed strontium fluoride dissolution rates (see Reference 1, Section 5.3.3). In all tables in this section, the number of digits reported does not necessarily reflect the accuracy or precision of the calculation. In most tables, three to four digits after the decimal place have been retained to prevent round-off errors in subsequent calculations. Other than the capsule composition, cesium chloride and strontium fluoride waste package calculations are identical with respect to moles and surface areas of waste package materials. Therefore, values for waste package material moles and surface areas in Table 8 are applicable to all waste package calculations. The molar quantities and surface areas of 316L stainless steel capsule package components are combined to simplify input to EQ6. A summary of the compositions, densities, and degradation rates of steels and alloys used in the simulations is provided in Section 3.6.3. Simulation inputs for cesium chloride capsule composition, density, and degradation rates are given in Table 9. Those inputs for the strontium fluoride capsule are given in Table 10.

To simplify input into EQ3/6, the molecular weight of all waste package materials and components is normalized to 100 grams/mole. This is done because compositions are given in weight percentages, and doing so eliminates the need to calculate a molecular weight for each material. The molecular weights are set to 100 grams/mole using the fractional weight distribution of elements in each material. This is done by normalizing elemental weight fractions to a total of 1 and then multiplying those normalized values by the element's molecular weight of 100 grams.

Table 8. Normalized geochemical simulation waste package mole and surface area values.

Waste Package	Reactant	Previous Normalized Moles[a,b] (moles/kg water)	Previous Normalized Surface Area[a,b] (cm^2/kg water)	Re-Normalized Moles[b] (moles/kg water)	Re-Normalized Surface Area[b] (cm^2/kg water)
All	Inner Vessel[a] (316NG SS)	27.51	57.31	49.089	102.26
	Capsule Canister[a] (Std. DOE, 316L SS)	0.8592	22.67	1.5332	40.45
	Basket Assembly and Canister Impact Plates[a] (A516 Carbon Steel)	9.48	121.615	16.92	217.01
	HLW Canister[a] (304L SS)	5.494	141.5	9.80	252.49
	HLW Glass[a,c]	21.82	1228.5	38.94	417.55
	Capsule Canister Components (316L SS)			2.6374	81.83

Waste Package	Reactant	Previous Normalized Moles[a,b] (moles/kg water)	Previous Normalized Surface Area[a,b] (cm^2/kg water)	Re-Normalized Moles[b] (moles/kg water)	Re-Normalized Surface Area[b] (cm^2/kg water)
	Capsule Baskets[b] (Al-319)			1.3370	20.586
Cesium Chloride[b]	Cesium chloride Min Mass Loading (16 Capsules)[c]			2.2203E-02	4.8588E-01
	Cesium chloride Max Mass Loading (16 Capsules)[c]			2.3943E-01	5.2396E+00
Strontium Fluoride[b]	Strontium fluoride Min Mass Loading (16 Capsules)[c]			2.5057E-02	1.0023E+03
	Strontium fluoride Max Mass Loading (16 Capsules)[c]			2.3178E-01	9.2711E+03

[a] Previous and new in-package water volumes (normalization factors) = 4102 liters and 2298.8 liters, respectively. Previous water volume and normalized moles and surface areas originate from Reference 8.
[b] To determine the total capsule mass (g), multiply the normalized moles by 100g/mole and the normalization factor of 2298.8 liters. To determine the true capsule surface area (cm^2), multiply the normalized surface area by the normalization factor of 2298.8 liters.
c. Normalized mole and surface area values for HLW glass are from Reference 8, Table 3. The surface area includes the most likely exposure factor (i.e., 4), which accounts for an increase in surface area due to fractures in the glass.

3.5 Geochemical Analysis Assumptions

Because these simulations are based on previous waste analyses, assumptions relevant to the previous and current analyses are listed and include assumptions specific to the replacement of SNF with cesium chloride or strontium fluoride capsules in the waste package analyses. Appendix A contains this list of assumptions amplified with the rationale behind each assumption.

3.5.1 Water Flux and Circulation

The waste package configuration is discussed in Section 2.4.1. Based on this configuration, the geochemical calculations assume: (1) the corrosion-resistant shell remains intact except for openings near the upper surface that allow dripping ground water to enter and exit the waste package via these openings; (2) the rate of water ingress and egress (i.e., flux) are consistent and equivalent to the rate at which infiltrating ground water drips onto the waste package; and (3) the water circulates freely enough within the partially filled waste package that all the waste package components and degradation products may react with each other through the aqueous solution.

3.5.2 Insoluble Metals

The waste package drip shield (Titanium Grade 7) and the outer corrosion-resistant shell (Alloy 22) will have a negligible effect on the in-package chemistry. Thus, these materials are neglected in geochemical calculations.

3.5.3 Waste Package Component Properties

The component properties (i.e., composition, mass, surface area, volume, and degradation rates) of the waste package used in these calculations are represented to a degree that closely approximates their true properties.

3.5.4 Capsule Properties

Based on the capsule descriptions in Section 2, the geochemical calculations assume: (1) The chemical and physical properties (e.g., composition, mass, surface area, and volume) of capsules used in these calculations are represented to a degree that closely approximates their true properties, (2) the cesium chloride capsules degrade and dissolve into waste package solution very quickly, within the first few days of EQ6 simulations, (3) impurities in the cesium chloride capsules (e.g., $PbCl_2$) and strontium fluoride capsules (e.g., PbF_2) will dissolve at rates consistent with those prescribed for the bulk capsules, and (4) the inner strontium fluoride canister material, Hastelloy C-276, will have a negligible effect on the in-package chemistry and may be substituted with 316L stainless steel in these calculations.

3.5.5 Cesium and Strontium Isotopes

The initial cesium and strontium isotopic mass ratios may be used for post EQ6 determination of individual isotope in-package solution concentrations.

3.5.6 Mineral Phase Suppression

This study assumes goethite may be suppressed in favor of hematite formation.

3.5.7 Capsule and HLW Glass Exposure

The cesium chloride capsule, strontium fluoride capsule, and HLW glass canisters are initially completely breached (allowing 100% of the surface areas to be exposed to degradation) to allow for damage that may occur due to future events and processes.

3.5.8 In-Package Water Content and Composition

Based on the overall system configuration and the baseline analysis comparison, the geochemical calculations assume: (1) The volume of an aqueous solution in the waste package is maintained at one-half of the total in-package void volume. (2) The solid volume initially occupied by the 16 capsules can be added to the total initial waste package void volume (i.e., mass of water). (3) The solutions that drip into the waste packages will have the major ion composition of J-13 well water as given in DTN: MO0006J13WTRCM.000 for at least 20,000 years. (4) And the addition of small amounts (1.0E-16 molal) of trace elements present in the waste package to the EQ3NR input file used to calculate initial in-

package solution composition will not affect the nature or extent of subsequent EQ6 geochemical calculations.

3.5.9 Thermodynamic Equilibrium

All reactions between the in-package solution and precipitating solids are in equilibrium. In addition, all gas-solution reactions are reversible and are at equilibrium with the ambient atmosphere outside the waste package, and the latter will be characterized by specific partial pressures (fugacities) of carbon dioxide and oxygen, respectively, of $10^{-3.0}$ and $10^{-0.7}$ atm.[9]

3.5.10 Thermodynamic Database

The thermodynamic database, data0.ymp.R4, used for the previous base case analysis (see Reference 7), is sufficiently accurate for these geochemical calculations. The additions and changes made to the database for previous base case analyses will not compromise the results of the geochemical calculations.

3.5.11 Changes to the Capsule Composition

Highly reactive chemical species of barium and zirconium produced by radioactive decay will react with capsule impurities, forming metals of those materials and stable species of those decay products prior to waste package failure. Using chloride or fluoride to balance the electrochemical charge of the capsule's molar composition will have a negligible effect on in-package chemistry.

3.6 Geochemical Analysis Input Data

3.6.1 Cesium Chloride Capsule Composition and Degradation Rate

A high cesium chloride capsule degradation rate was conservatively selected to affect rapid dissolution into the in-package solution (see Section 3.5.4). Year 2006 data (Section 3.5.5) for the normalized molar composition and characteristics used in simulation calculations are summarized in Table 9. Table 10 summarizes the normalized molar composition and characteristics used for Year 2275 calculations. Mass and composition data given in Tables 9 and 10 are based on inventory average values shown in Section 2.4. The number of capsules placed in each waste package is discussed in Section 2.4. However, uncertainty of the cesium chloride mass within individual capsules facilitates an evaluation of minimum and maximum cesium chloride mass-loading scenarios. The minimum and maximum normalized cesium chloride molar mass and surface area for 16 cesium chloride capsules are given in Table 8.

Table 9. Year 2006 cesium chloride capsule composition and degradation rate.

Element	Normalized Constituent Moles per 100 grams of Capsule (EQ6 Reactant Inputs)[a]
Aluminum	1.1007E-02
Boron	7.2521E-02
Barium	8.3443E-02
Calcium	2.4421E-02
Cadmium	1.6013E-04
Cerium	3.9699E-05
Cesium-137	Intentionally Blank
Cesium-135	
Other Cesium	
Cesium (Total)	3.2562E-01
Chromium	2.6384E-02
Cobalt	1.6579E-03
Copper	3.0640E-03
Iron	8.8003E-03
Lanthanum	3.9895E-05
Lead	6.6145E-03
Magnesium	1.0071E-02
Manganese	8.5529E-04
Molybdenum	2.1489E-04
Nickel	5.5117E-03
Palladium	1.6554E-04
Phosphorus	3.1633E-03
Potassium	1.9819E-02
Rubidium	5.6643E-03
Silicon	1.4657E-02
Silver	9.2983E-05
Sodium	1.3205E-01
Strontium	2.0369E-03
Sulfur	0.0000E+00
Titanium	1.4003E-03
Zirconium	8.3977E-04

Element	Normalized Constituent Moles per 100 grams of Capsule (EQ6 Reactant Inputs)[a]
Chlorine[b]	8.8701E-01
Oxygen	1.5075E-01
Totals[c]	1.7981E+00

Molecular Weight[d]	100.00 g/mole
Density	3.99 g/cm^3
Cesium Chloride Capsule Degradation Rate Constant[e], at 25°C	1.0E-07 mole/cm^2 s

a. Component weights used to calculate this column originate from Table 2, Column "Average Weight in Standardized Canister for 16 capsules."

b. Charge was balanced using chloride. As a result, the Cl mass (g) used is 47.67g greater than that given in Table 2 (i.e., 13,346.3g).

c. Totals represent the average constituent mass used to calculate average capsule composition. The total mass (g) includes "total cesium" (i.e., cesium-137 + cesium-135 + "other" cesium). ("other" cesium is assumed to be cesium-133.)

d. The molecular weight of all waste package components is normalized to 100 g/mole to simplify inputs to EQ6.

e. Arbitrarily selected to affect rapid dissolution into the in-package solutions.

Table 10. Year 2275 cesium chloride capsule composition and degradation rate.

Element	Normalized Moles of Constituent per 100 grams of Capsule (EQ6 Reactant Inputs)[a]
Aluminum	1.0675E-02
Barium	1.5833E-01
Boron	7.0331E-02
Cadmium	1.5529E-04
Calcium	2.3684E-02
Cerium	3.8500E-05
Cesium-137	Intentionally Blank
Cesium-135	
Other Cesium	
Cesium - Total	2.3798E-01
Chromium	2.5588E-02
Cobalt	1.6079E-03

Element	Normalized Moles of Constituent per 100 grams of Capsule (EQ6 Reactant Inputs) [a]
Copper	2.9714E-03
Iron	8.5345E-03
Lanthanum	3.8690E-05
Lead	6.4147E-03
Magnesium	9.7673E-03
Manganese	8.2946E-04
Molybdenum	2.0840E-04
Nickel	5.3452E-03
Palladium	1.6054E-04
Phosphorus	3.0678E-03
Potassium	1.9220E-02
Rubidium	5.4932E-03
Silicon	1.4214E-02
Silver	9.2711E-05
Sodium	1.2806E-01
Strontium	1.9754E-03
Sulfur	0.0000E+00
Titanium	1.3581E-03
Zirconium	8.1440E-04
Chlorine[b]	9.3724E-01
Oxygen	1.4619E-01
Totals [c]	1.8204E+00

Molecular Weight[e]	100.00 g/mole
Density	3.99 g/cm^3
Cesium Chloride Capsule Degradation Rate Constant[e], at 25°C	1.0E-07 mole/cm^2 s

a. Component weights used to calculate this column originate from Table 3, Column "Average Weight in Standardized Canister for 16 capsules."

b. Charge was balanced using chloride. As a result, the Chlorine mass (g) used is 43.99 g greater than that given Table 3 (14,149.9 g).

c. Totals represent the average constituent mass used to calculate average capsule composition. The total mass (g) includes total cesium (i.e., cesium-135 + other cesium). (Other cesium is assumed to be cesium-133).

d. The molecular weight of all waste package components is normalized to 100 g/mole to simplify inputs to EQ6.

e. Conservatively selected to affect rapid dissolution into the in-package solution.

3.6.2 Strontium Fluoride Capsule Composition and Degradation Rate

The strontium fluoride capsule containment is conservatively assumed to be breached (waste package failure) at the start of geochemical simulations. Year 2006 data (Section 3.5.5) for the normalized molar composition and characteristics used in simulation calculations are summarized in Table 11. Table 12 summarizes the normalized molar composition and characteristics used for Year 2275 calculations. Mass and composition data given in Tables 11 and 12 are based on the inventory average values shown in Section 2.4. The number of capsules placed in each waste package is discussed in Section 2.4. However, uncertainty of the strontium fluoride mass within the individual capsules facilitates an evaluation of minimum and maximum strontium fluoride mass loading scenarios. The minimum and maximum normalized strontium fluoride molar mass and surface areas for 16 strontium fluoride capsules are given in Table 8.

Table 11. Year 2006 strontium fluoride capsule composition and degradation rate.

Element	Normalized Moles of Constituent per 100 grams of Capsule (EQ6 Reactant Inputs) [a]
Aluminum	4.7730E-03
Barium	9.1449E-03
Cadmium	5.3296E-04
Calcium	2.0536E-02
Chromium	3.6775E-03
Copper	9.7114E-05
Fluorine[b]	2.1963E+00
Iron	4.2711E-03
Lanthanum	8.1842E-04
Lead	6.5387E-04
Magnesium	6.4347E-03
Manganese	8.6258E-04
Nickel	4.1461E-03
Potassium	1.3798E-04
Silicon	1.4211E-01
Silver	9.3019E-05
Sodium	7.6368E-02
Strontium-90	Intentionally Blank
Strontium - Other	
Strontium - Total[c]	3.9267E-01
Zirconium	1.6120E-01
Totals [c]	3.0249E+00

Molecular Weight[d]	100.00 g/mole
Density	4.24 g/cm^3
Strontium Fluoride Capsule Degradation Rate Constant[e], at 25°C	1.1E-12 mole/cm^2 s

a. Component weights used to calculate this column originate from Table 4, Column "Average Weight in Standardized Canister for 16 Capsules."

b. Charge was balanced using fluoride. As a result, the fluorine mass (g) used is 0.82 g less than that given in Table 4 (i.e., 16,502.3 g).

c. Totals represent the average constituent mass used to calculate average capsule composition. The total mass (g) includes total strontium (i.e., Strontium-90 + strontium - Other [assumed to be Strontium-87]).

d. The molecular weight of all waste package components was normalized to 100 g/mole to simplify inputs to EQ6.

e. Calculated based on laboratory estimation of strontium fluoride effective surface area (400 cm^2/g) and dissolution rate (1.4x10^{-4} μg/cm^2 s) given in Reference 1.

Table 12. Year 2275 strontium fluoride capsule composition and degradation rate.

Element	Normalized Moles of Constituent per 100 grams of Capsule (EQ6 Reactant Inputs)[a]
Aluminum	5.2496E-03
Barium	1.0058E-02
Cadmium	5.8619E-04
Calcium	2.2586E-02
Chromium	4.0448E-03
Copper	1.0681E-04
Fluorine[b]	2.1002E+00
Iron	4.6977E-03
Lanthanum	9.0015E-04
Lead	7.1917E-04
Magnesium	7.0772E-03
Manganese	9.4872E-04
Nickel	4.5601E-03
Potassium	1.5176E-04
Silicon	1.6943E-03
Silver	9.2730E-05
Sodium	8.3995E-02
Strontium-90	Intentionally Blank
Strontium - Other	

Strontium - Total	2.7575E-01
Zirconium	3.3111E-01
Totals [c]	2.8545E+00

Molecular Weight[d]	100.00 g/mole
Density	4.24 g/cm^3
Strontium Fluoride Capsule Degradation Rate Constant[e], at 25°C	1.1E-12 mole/cm^2 s

a. Component weights used to calculate this column originate from Table 5, Column "Average Weight in Standardized Canister for 16 Capsules."

b. Charge was balanced using fluoride. As a result, the fluorine mass (g) used is 2.40g less than that given in Table 5 (i.e., 15,830.8g).

c. Totals represent the average constituent mass used to calculate average capsule composition. The total mass (g) includes total strontium (i.e., strontium-90 + strontium - other [assumed to be strontium-87]).

d. The molecular weight of all waste package components was normalized to 100 g/mole to simplify inputs to EQ6.

e. Calculated based on laboratory estimation of strontium fluoride effective surface area (400 cm^2 /g) and dissolution rate (1.4x10^{-4} μg/cm^2 s) given in Reference 1.

3.6.3 Steel, Alloy, and HLW Glass Compositions and Degradation Rates

Tables 13 and 14 provide summaries of the compositions, densities, and degradation rates of the steels and alloys used in calculations. Degradation rates in Table 14 represent recently published values (see Reference 7). The steel and alloy degradation rates are assumed to be unaffected by a one-half void volume water content (Section 3.5.8). Table 15 provides a summary of the normalized HLW glass composition, density, and degradation rate input as the complex mineral "GlassSRL" in the database associated with these calculations. The composition and degradation rates discussed represent recently published values (see Reference 7). The initial normalized moles and surface areas of waste package materials and contents (e.g., steel, alloys, HLW glass) are given in Table 8.

Table 13. Steel and alloy compositions used for geochemical simulations.

Element	A516 Carbon Steel[a]		304L Stainless Steel[a]		316L Stainless Steel[a]		316NG Stainless Steel[b,c]		Aluminum-319 Alloy[d]	
	Wt%	Moles per 100 g of Reactant	Wt%	Moles per 100 g of Reactant	Wt%	Moles per 100 g of Reactant	Wt%	Moles per 100 g of Reactant	Wt%	Moles per 100 g of Reactant
Aluminum	NA	NA	NA	NA	NA	NA	NA	NA	87.30	3.236
Carbon	0.28	0.023	0.03	0.002	0.08	0.007	0.02	0.002	NA	NA
Chromium	NA	NA	19.00	0.365	17.00	0.327	17.00	0.327	NA	NA
Copper	NA	NA	NA	NA	NA	NA	NA	NA	3.50	0.055
Iron	98.3	1.760	68.05	1.218	65.50	1.173	65.58	1.174	1.00	0.018
Magnesium	NA	NA	NA	NA	NA	NA	NA	NA	0.10	0.004
Manganese	1.03	0.019	2.00	0.036	2.00	0.036	2.00	0.036	0.50	0.009
Molybdenum	NA	NA	NA	NA	2.50	0.026	2.50	0.026	NA	NA
Nickel	NA	NA	10.00	0.170	12.00	0.204	12.00	0.204	0.35	0.006
Nitrogen	NA	NA	0.10	0.007	0.10	0.007	0.08	0.006	NA	NA
Phosphorus	0.04	0.001	0.05	0.001	0.05	0.001	0.05	0.001	NA	NA
Silicon	0.29	0.010	0.75	0.027	0.75	0.027	0.75	0.027	6.00	0.214
Sulfur	0.04	0.001	0.03	0.001	0.03	0.001	0.03	0.001	NA	NA
Titanium	NA	NA	NA	NA	NA	NA	NA	NA	0.25	0.005
Zinc	NA	NA	NA	NA	NA	NA	NA	NA	1.00	0.015
Total	100.00	—	100.00	—	100.00	—	100.00	—	100.00	—
Density (g/cm^3)	7.85		7.94		7.98		7.98		2.77	

a. Pasupathi, V. 1999. Waste Package Materials Properties. BBA000000-01717-0210-00017 REV 00. Las Vegas: M&O. MOL.19990407.0172.

b. ASTM A 276-91a, 1991, *Standard Specification for Stainless and Heat-Resisting Steel Bars a nd Shapes*, Philadelphia, Pennsylvania: American Society for Testing and Materials, p. 2, Table 1, TIC: 240022

c. ASM International, 1987, *Corrosion*. Volume 13 of *Metals Handbook*, 9th Edition, Metals Park, Ohio: ASM International, TIC: 209807.

d. Type 319 Aluminum ASTM B108-03a, Table 1 for 319.0.

Table 14. Steel and alloy degradation rates used for geochemical simulations.

	A516 Carbon Steel[a]	304L Stainless Steel[a]	316L Stainless Steel[a]	Aluminum319 Alloy[a,b]	316NG Stainless Steel[c]
Mean rate (μm/year)	102.7	11.44	1.94	12.95	1.94
Mean rate constant (mole/cm^2 s)[c]	3.00E-11	3.00E-12	5.00E-13	1.00E-12	5.00E-13

a. Pasupathi, V. 1999. Waste Package Materials Properties. BBA000000-01717-0210-00017 REV 00. Las Vegas:M&O. MOL.19990407.0172.

b. The mean 319 aluminum degradation rate is uncertain for the conditions simulated. However, the compositions of 319 and 1100 aluminum are similar. For the purpose of this calculation the degradation rate of 1100 aluminum (see Reference 7. Section 6.3.1.3.2. Table 6-5, p. 6-14) is assumed for 319 aluminum in EQ6 calculations).

c. CRWMS M&O, 1997, *Criticality Evaluation of Degraded Internal Configurations for the PWR AUCF waste package Design,* BBA000000-01717-0200-00056, Rev. 00, Las Vegas, Nevada: CRWMS M&O, ACC: MOL.19971231.025

Table 15. High level waste glass composition and degradation rate.

Element	Moles per 100g of HLW Glass[a] (Database Mineral: GlassSRL)
Aluminum	8.6300E-02
Barium	1.0800E-03
Boron	2.9100E-01
Calcium	1.6200E-02
Fluorine	1.6600E-03
Iron	1.7200E-01
Magnesium	3.3300E-02
Oxygen	2.7000E+00
Phosphorus	4.8900E-04
Potassium	7.5100E-02
Silicon	7.7600E-01
Sodium	5.7700E-01
Sulfur	4.0100E-03
Uranium	7.8200E-03
Density (g/cm^3)	2.85
Total degradation rate[b] = $k_1[H^+]^{-0.4} + k_2[H^+]^{0.6}$ (moles/cm^2 s)	
Rate constant k_1	2.7E-22 moles/cm^2 s
Rate constant k_2	3.6E-13 moles/cm^2 s

a. Values from Reference 7, Table 4-5.
b. Rate values from Reference 7 Table 6-8 for 25 degrees.

3.6.3.1 *Water Composition and Flux Rate*

It is assumed (see Section 3.5.8) that the water entering the waste package has the composition of J-13 well water summarized in Table 16. The rate at which this water enters a waste package is believed to be the same as the rate of water dripping onto the waste package (Section 3.5.1). Geochemical calculations are performed for all waste package simulations using one constant inflow water rate. The rate used (1 L/yr or 0.001 m^3/yr) is consistent with the baseline analysis (see Reference 7, Section 6.5.1.2, p. 6-42). This rate represents the midpoint of the range evaluated in the previous waste package analyses (see Reference 7, Section 6.3.1.3.1, p. 6-11). Consistency of in-package solution retention time is maintained between this and the baseline analysis by normalization of the water flow rate to the in-package solution content. The flow rate used in these waste package simulations is normalized to one-half (i.e., 2298.8 liters) of the current waste package's total void volume (Section 3.5.8). The water flow rate and initial in-package solution's pH are given in Table 16.

Table 16. Major elements of J-13 well water and water flux used for EQ3/6 input.

Parameter	J-13 Well Water (mg/L)	Initial In-Package Solution Parameter[a]
Temperature	25°C	25°C
Ca^{2+}	13.0	
Cl^-	7.14	
F^-	2.18	
HCO_3^-	Used for charge balance of initial in-package solution[b]	
K^+	5.04	
Mg^{2+}	2.01	
Na^+	45.8	
NO_3^-	8.78	
SiO_2	61.0	
SO_4^{2-}	18.4	
pH	7.41	8.09[c]
Inflow Water Flux (L/yr)		1.0
Inflow Water Flux (moles/s)[d]		1.38E-11

a. Molal concentrations of initial in-package aqueous species equilibrated using EQ3NR

b. The initial in-package solution is electrically balanced on $HCO3^-$ by EQ3NR (see Reference 7, Section 6.3.1.3.1 for logic).

c. The initial in-package solution pH represents the pH value after the solution is equilibrated to $\log fCO_2$ = -3.0atm and fO_2 = -0.7atm by EQ3NR.

d. The rate is normalized to one-half the total waste package void volume.

3.7 Geochemistry Simulation Results and Analysis

Results of the geochemical simulation are presented for maximum and minimum in-package solution concentrations of cesium, strontium, and the contaminant metal materials in the waste packages during 20,000-year simulations. Results of bulk in-package solution chemistry are presented for comparison to the baseline. Maximum in-package aqueous concentrations of capsule constituents are presented for use as input to the TSPA. The mass of constituents retained in-package by mineral phase precipitation and/or released from the packages by in-package solution discharge are not used in the TSPA and are not presented. Constituent concentrations and bulk chemistry are presented in response to changes of initial capsule mass loading and isotopic compositions while the amount of water, waste package materials, and HLW glass are consistent for all cases simulated. The range of maximum and minimum values for ionic strength, pH, and redox potential, represented as Eh, are presented as an indication of bulk in-package solution chemistry during the 20,000-year simulations.

In all cases, there is corrosion of waste package materials and content to produce mineral assemblages comprised primarily of metal oxides and clay minerals. Surface complexation/adsorption effects involving iron corrosion products (e.g., hydrous ferric oxides) and hydrogen ions are expected to buffer pH during the first few hundred years of waste package failure. The pH buffering is expected to be sustained by a relatively high iron corrosion rate during early time. Corrosion products and mineral phases of capsule constituents predicted to form are defined for cesium chloride and strontium fluoride cases in Section 3.7.1 and 3.7.2, respectively.

Both the cesium chloride and strontium fluoride waste package simulations consider mean values of steel/alloy degradation rates, a pH-dependent HLW glass degradation rate, and a 1.0 liter per year water flux (Tables 14, 15, and 16) consistent with the baseline analysis for comparison with current results. HLW glass, included in the waste package as previously discussed, is retained in these calculations to provide an appropriate representation of how the capsules may be disposed. However, these calculations focus on estimating the aqueous concentrations of constituents dissolved from cesium chloride and strontium fluoride capsules into a package solution. Therefore, only cursory consideration is given to the HLW glass constituents (i.e., uranium) in this calculation.

3.7.1 Cesium Chloride Capsule Waste Packages

Cesium chloride waste package calculations are performed for four cases. Two maximum and two minimum capsule mass loading cases are simulated for an estimation of solution concentrations of cesium-133, cesium-135, cesium-137 and impurities that would result from a waste package failure happening before isotopic decay occurs. These two analyses are referred to as maximum and minimum current year (e.g., Year 2006), mass loading cases. These Year 2006 failure cases are highly unlikely under the conditions simulated and are intended merely to bracket the highest possible in-package solution concentrations of cesium isotopes. For this reason, the time series data of these simulations are not presented, but the results are summarized in Table 17. Individual cesium isotope solubility is calculated by multiplying the initial isotope weight fraction by the maximum total cesium solubility predicted for maximum and minimum mass loading cases in Table 17 and Table 18.

Table 17. Year 2006 cesium chloride waste package results summary for maximum and minimum in-package constituent concentrations and bulk chemistry.

Cesium Chloride WP at Year 2006	Max Mass Loading	Min Mass Loading
Initial Solution Eh =	7.40E-01	7.40E-01
Max Eh =	1.07E+00	1.01E+00
Max Ionic Strength =	6.40E-01	5.25E-01
Max/initial pH =	8.09	8.09
Min. pH =	2.49	3.54
Element	(mg/L)	(mg/L)
Barium	2.7165E+03	2.2762E+02
Cadmium	4.3093E+00	3.9961E-01
Cesium-133	6.3060E+03	5.8477E+02
Cesium-135	1.4498E+03	1.3444E+02
Cesium-137	2.6046E+03	2.4153E+02
Cesium-Total	1.0360E+04	9.6073E+02
Chlorine	7.5351E+03	7.0484E+02
Chromium	3.1717E+02	8.2528E-02
Lead	1.7044E+02	8.1169E+00
Silver	1.0236E+00	1.1696E-01
Strontium	4.2726E+01	3.9621E+00
Uranium	9.9056E-01	1.2644E-01

Degradation of waste package materials and contents from waste package failure is shown in Figure 10 for the CsClMax2275 and CsClMin2275 cases. Figure 10 represents all cesium chloride waste package cases because, with the exception of differing initial capsule mass loading, the degradation history of waste package components is identical for all cesium chloride package simulations. Waste package material degradation is in good agreement with that of the baseline analysis (see Reference 7, Figure 6-12, p. 6-43), with the exception of additional components (e.g., capsule packaging materials) and differences of initial material moles resulting from the use of the short waste package.

The most pronounced system response is that of solution pH. The evolution of pH is complex and initially controlled by capsule degradation and subsequent oxidation and mineral precipitation reactions. A comparison of CsClMin2275 and CsClMax2275 pH histories shows a significant difference in pH response resulting from differences of initial capsule mass and subsequent precipitation reactions. The oxidation of metals, rapidly dissolved into a package solution from the highly soluble cesium chloride capsules (Section 3.5.2), drives down the pH through acid-producing reactions and results in a sudden increase of protons that overwhelms the system's buffering capacity during approximately the first 5 days of the simulations. Dissolution of chromium and iron with subsequent eskolaite (Cr_2O_3) and hematite (Fe_2O_3) formation are the primary acid-producing precipitation reactions affecting low pH during the

initial simulation. (Six moles of protons are created for each mole of either eskolaite or hematite formed). However, the formation of boric and phosphoric acids by the respective oxidation of boron and phosphorous released from the capsules also contribute to low pH conditions. Respective minimum pH values of approximately 3.6 and approximately 2.5 for CsClMin2275 and CsClMax2275 cases correspond with capsule exhaustion at approximately 5 days (1.45×10^{-2} years in Figure 10). After the capsules are exhausted, the pH remains low until proton consuming reactions and displacement processes allow the pH to increase sharply. Those reactions and processes include the dissolution of soluble precipitated phases, the displacement of boric acid, and the addition of alkalinity by HLW glass degradation and water flux. The sharp rise in pH is followed by a gradual decline affected by the relatively slow corrosion of carbon and stainless steel waste-package materials, after which the pH remains at about 5.5. The pH step observed at approximately 2 years in the CsClMax2275 case is due partially to a change of calculation step size determined automatically within EQ6 by reaction progress and primarily to decreased eskolaite and hematite precipitation, presented in Figures 11 and 12. The decrease of eskolaite and hematite precipitation is not readily apparent as concentration time series data are plotted in log scale.

Lower pH values are predicted in the first few years of the CsClMin2275 and CsClMax2275 simulations with minima of approximately 3.6 and 2.5 pH, respectively (Figure 10). The extreme values of these relatively brief pH minima may be increased (i.e., the pH value increased) by corrosion product surface complexing effects which are expected to buffer pH in the first few hundred years of waste package material corrosion. The buffering of pH by surface complexation effects is not included in this model, but is suggested in previous waste package analyses (see Reference 7, Section 6.8.4). After the first few years, the current predicted pH response is in good agreement with the range of pH predicted for the baseline analysis (see Reference 7, Section 6.6.1, Figure 6-27). Over all, the current bulk solution chemistry is in good agreement with the baseline (see Reference 7, Section 6.5). Summary data for range of pH, Eh, and ionic strength are given as representative of bulk solution chemistry with maximum impurity concentrations and cesium isotope concentrations for Year 2006 and Year 2275 cases in Tables 17 and 18. Ionic strength and Eh time series data are presented with pH histories for CsClMin2275 and CsClMax2275 cases in Figures 13 and 14.

The ionic strength maxima are observed to correspond with exhaustion of the stainless steel (316L) capsule canister and capsule packaging components at ~2,000 years in Figure 13.

Oxidation-reduction (redox) reactions are the primary processes by which waste package materials and components corrode and the in-package solution is altered. The solution Eh (volts), a measure of redox potential, is uniform (0.74 volts) for air-saturated water entering the failed waste package (Assumption 3.4.9). Therefore, in-package changes of Eh can be attributed to reactions affecting the assemblage of corrosion products. The results show how the Eh varies between approximately 0.7 to 1.0 volts; these are oxidizing conditions as the presence of metal oxide phases also indicates (Figure 12). Consistent with the base line, the Eh changes only in response to pH changes (Figure 14) indicating uniformly oxidizing conditions even during the period of rapid capsule degradation.

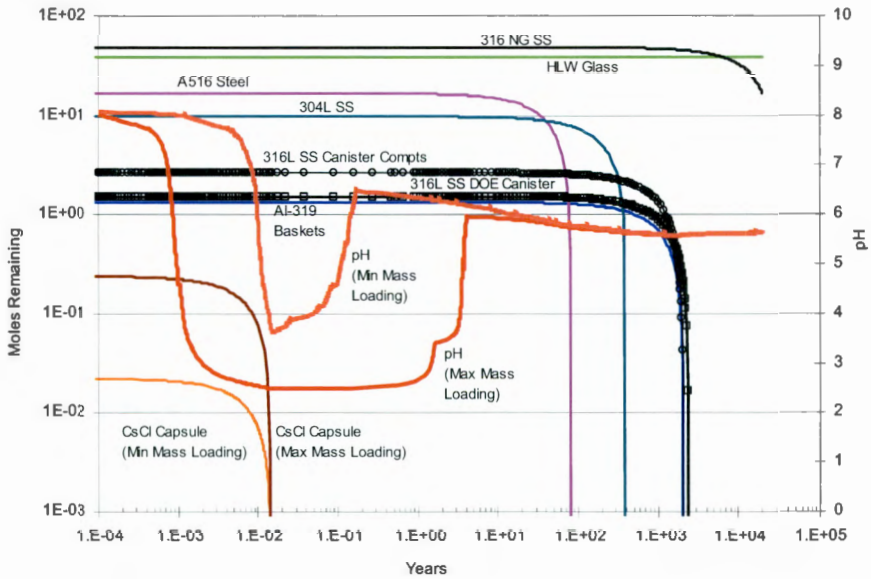

Figure 10. Degradation of cesium chloride waste package for Year 2275 maximum and minimum cesium chloride mass loading case.

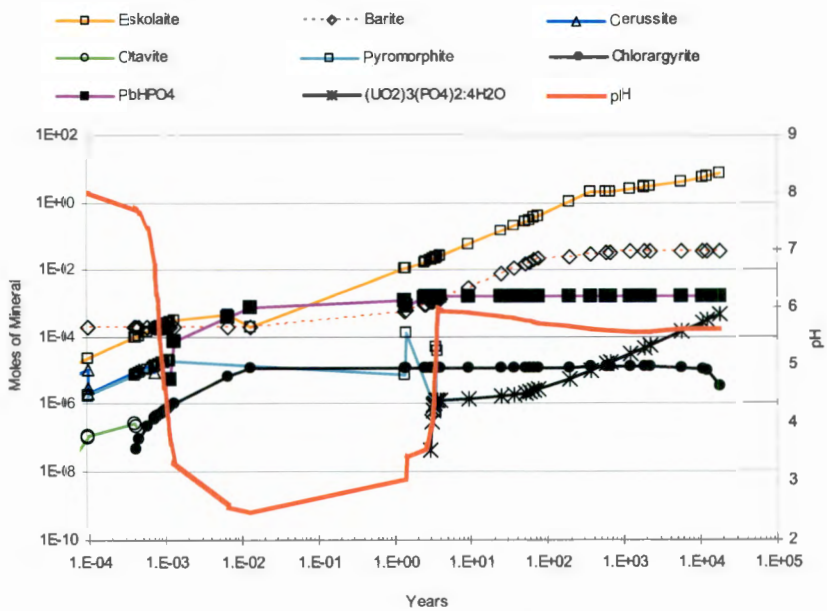

Figure 11. Mineralized capsule constituents for Year 2275 maximum loading cesium chloride waste package case.

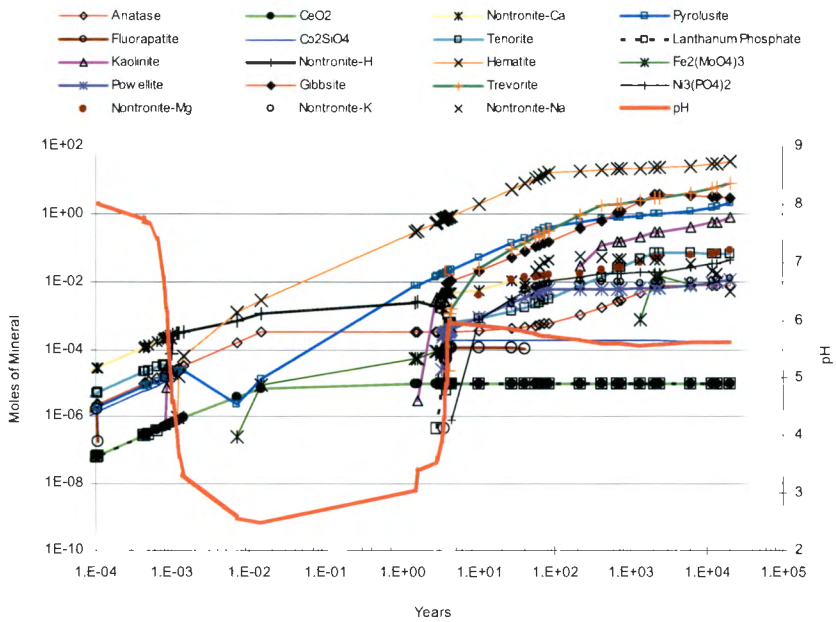

Figure 12. Major minerals forming in Year 2275 maximum loading cesium chloride case, excluding capsule constituents.

Table 18. Year 2275 cesium chloride waste package results summary.

Cesium chloride WP at Year 2275	Maximum Mass Loading	Minimum Mass Loading
Initial Solution Eh =	7.40E-01	7.40E-01
Max Eh =	1.07E+00	1.00E+00
Max Ionic Strength =	6.32E-01	5.20E-01
Max/Initial pH =	8.09	8.09
Min. pH =	2.50	3.63
Element	(mg/L)	(mg/L)
Barium	5.1785E+03	4.5591E+02
Cadmium	4.1790E+00	3.8753E-01
Ceium-137	0.0000E+00	0.0000E+00
Cesium Total	7.5719E+03	7.0215E+02
Cesium-135	1.4152E+03	1.3123E+02
Cesium-135	6.1567E+03	5.7092E+02
Chlorine	7.9613E+03	7.4433E+02
Chromium	3.0602E+02	5.0527E-02
Lead	1.6527E+02	6.1860E+00
Silver	1.1047E+00	1.2136E-01
Strontium	4.1436E+01	3.8425E+00
Uranium	9.3943E-01	1.2522E-01

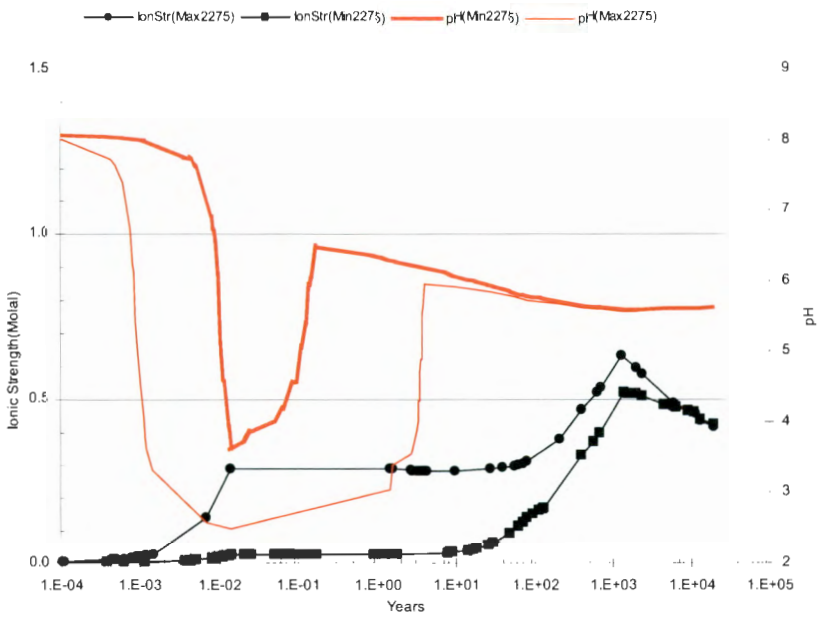

Figure 13. Comparison of pH and ionic strength for the cesium chloride Year 2275 cases.

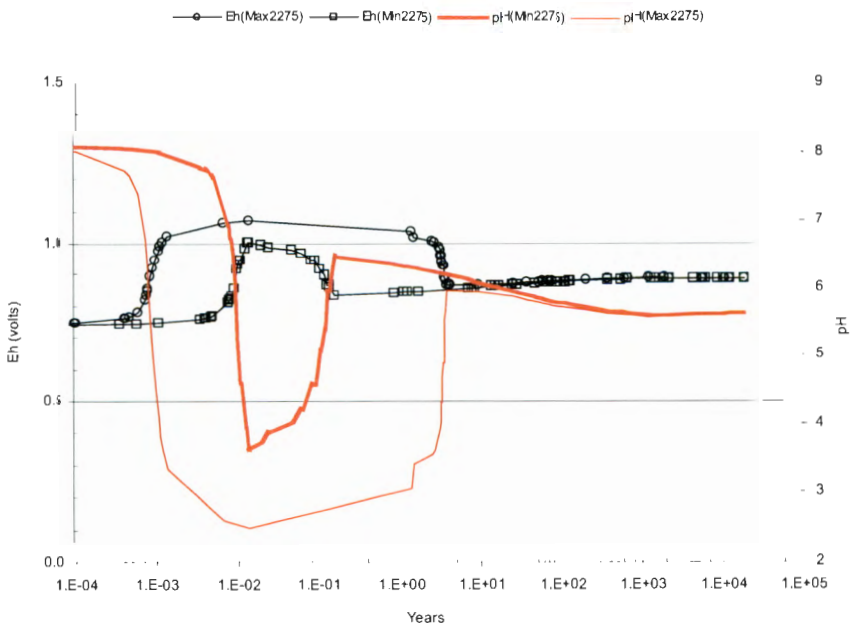

Figure 14. Comparison of pH and Eh for the cesium chloride Year 2275 cases.

The Year 2275 simulations are intended to provide most likely maximum and minimum solution concentrations of capsule constituents as inputs to the TSPA. For this purpose, knowledge of the timing of maximum constituent concentrations is not essential. These concentration histories are presented to provide insight into the controls of constituent concentrations. Figures 15 and 17 show the predicted solution concentrations of the contaminant metals, cesium, and pH histories from waste package failure for CsClMin2275 and CsClMax2275 cases, respectively. The timing of maximum solution concentrations, given in Tables 17 and 18, is dependent on either the capsule degradation rate (Section 3.4.4) or the solubility of mineral phases predicted to form with an individual capsule constituent. Constituents predicted to precipitate as solid mineral phases are shown with pH histories for CsClMax2275 and CsClMin2275 cases in Figures 11 and 16. With the exception of cesium, mineral phases are predicted to form for all capsule constituents during at least some portion of the simulation period. Those minerals include chlorargyrite (AgCl), barite ($BaSO_4$), eskolatite (Cr_2O_3), cerussite ($PbCO_3$), pyromorphite ($Pb_5(PO_4)_3Cl$), lead phosphate ($PbHPO_4$), and otavite ($CdCO_3$). Maximum solution concentrations are observed to occur within the first $1x10^{-2}$ years of both Year 2275 cases (Figures 15 and 16). This timing corresponds with capsule exhaustion (Figure 10) suggesting maximum solution concentrations are controlled by the capsule's physical properties with little influence imposed by water flux. No mineral phase is predicted to form for highly water-soluble cesium. Therefore, the timing and maximum solution concentrations of cesium are determined solely by the capsule degradation rate and the amount of cesium initially added to the simulations. With exception of cesium, following capsule exhaustion, constituent solution concentrations are controlled at least to some degree by mineral solubility. This solubility control is most evident in the chromium and lead-time series data after 1 year (Figures 15 and 17).

Major mineral assemblages, excluding capsule constituents, predicted to form in CsClMax2275 and CsClMin2275 cases are shown in Figures 12 and 18. Other than differences in the timing of formation and the formation of antlerite ($Cu_3(SO_4)(OH)_4$), absent in the CsClMax2275 case, mineral assemblages are consistent for both CsClMin2275 and CsClMax2275 cases. This result indicates that the difference and duration of pH minimums predicted during the first few years of capsule degradation will not influence the later time mineral assemblage. Further, with the exception of mineral phases forming as a direct result of capsule degradation (e.g., anatase and CeO_2), there is good agreement between the current mineral assemblage and that of the baseline analysis (see Reference 7, Section 6.5.1.2, Figure 6-13). This agreement implies that replacement of SNF with cesium chloride capsules in the waste packages will have a minimal impact on the assemblage of minerals and corrosion products forming by waste package material corrosion.

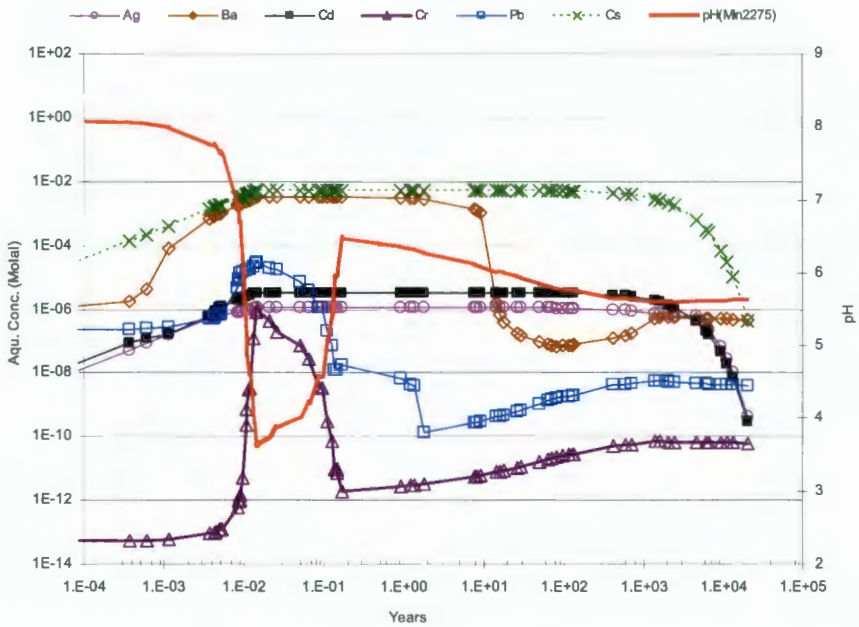

Figure 15. Year 2275 waste package concentrations of capsule constituents for the minimum cesium chloride mass loading case.

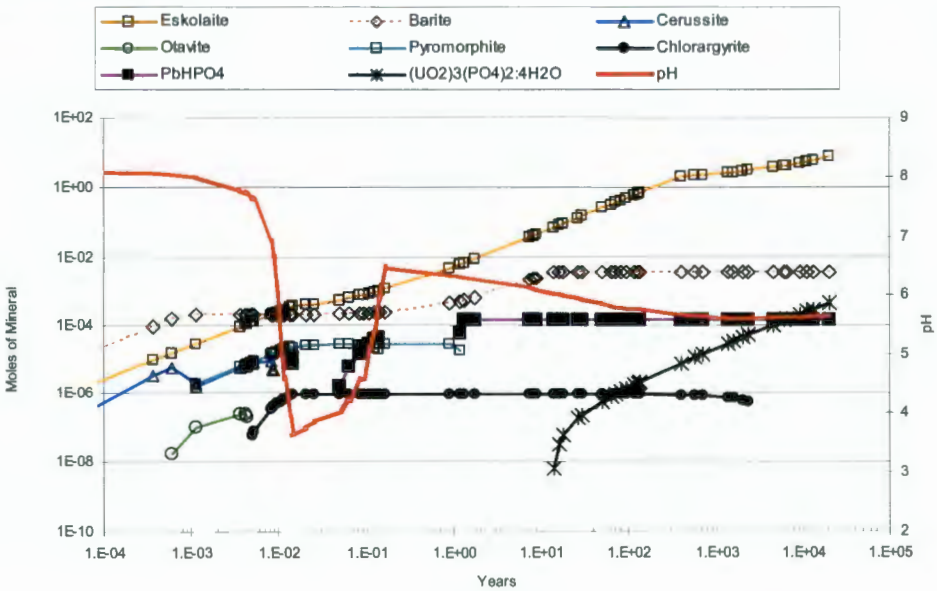

Figure 16. Mineralized capsule constituents for the Year 2275 minimum mass loading cesium chloride case.

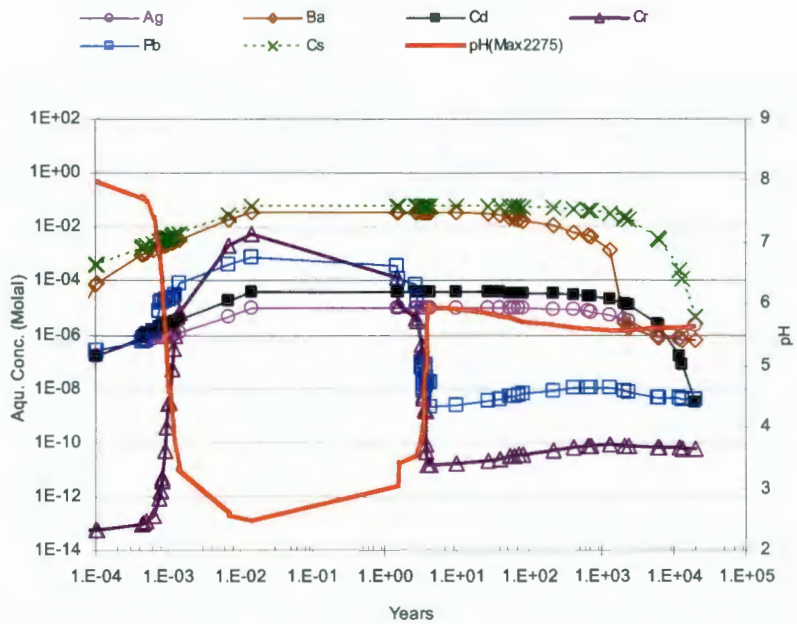

Figure 17. Year 2275 waste package concentrations of capsule constituents for the maximum cesium chloride mass loading case.

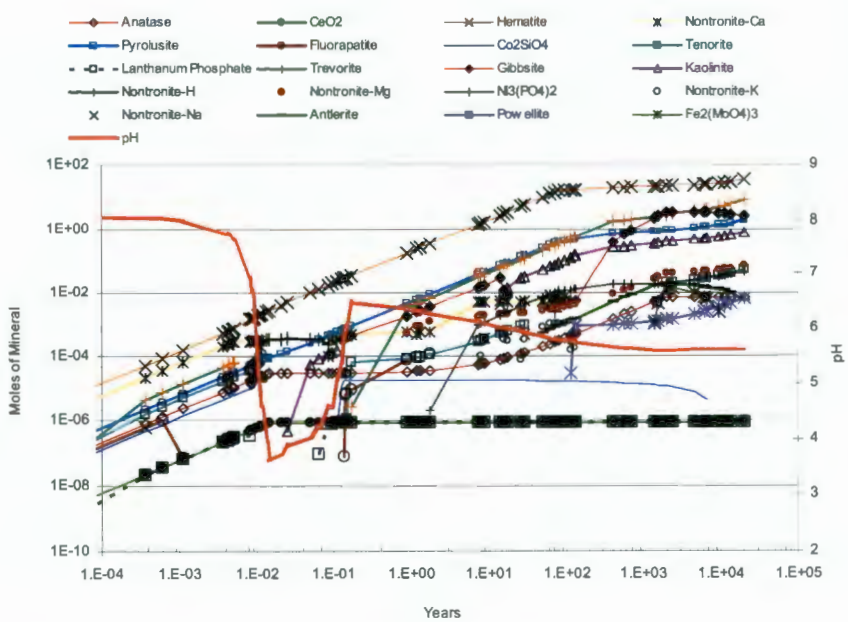

Figure 18. Major minerals forming in the Year 2275 minimum mass loading cesium chloride case, excluding capsule constituents.

3.7.2 Strontium Fluoride Capsule Waste Packages

Similar to cesium chloride waste package simulations, strontium fluoride waste package simulations are performed for four cases. Two maximum and two minimum strontium fluoride capsule mass loading cases are simulated for the estimation of the in-package solution concentration of strontium isotopes (i.e., strontium-87 and strontium-90) and the contaminant metals that would result from waste package failure happening before strontium-90 decay occurs. These Year 2006 failure cases are highly unlikely under the conditions simulated and are intended merely to bracket the highest possible in-package solution concentrations of strontium isotopes. For this reason, time series data of these simulations are not presented, but results are summarized in tabular form for the maximum and minimum solution concentrations of capsule constituents and bulk solution chemistry in Table 19. Maximum Strontium-90 isotope solubility is calculated by multiplying the initial isotope weight fraction by the maximum total strontium solubility predicted for maximum and minimum mass loading cases in Table 19. Strontium-90 has been decayed to its progeny for Year 2275 evaluations (Assumption 3.4.5).

Table 19. Year 2006 strontium fluoride waste package results summary for in-package constituent concentrations and bulk chemistry.

Strontium Fluoride WP at Year 2006	Maximum Mass Loading	Minimum Mass Loading
Initial Solution Eh =	7.40E-01	7.40E-01
Max Eh =	9.51E-01	9.34E-01
Max Ionic Strength =	5.47E-01	5.35E-01
Max/initial pH =	8.09	8.09
Min. pH =	4.52	4.81
Element	(mg/L)	(mg/L)
Barium	2.89980E+02	3.89913E-01
Cadmium	1.62647E+01	1.76126E+00
Chromium	1.66668E-04	4.17560E-05
Fluorine	4.31169E+03	1.02677E+03
Lead	1.47386E-01	6.18658E-02
Silver	2.80115E-01	2.28540E-01
Strontium Total	1.15001E+03	7.21963E+02
Strontium-87	7.27113E+02	4.56472E+02
Strontium-90	4.22900E+02	2.65491E+02
U-Total	2.12886E+00	8.79517E-01
Zirconium	3.39698E+03	4.32238E+02

These geochemical simulations consider the strontium fluoride capsule degradation rates and compositions given in Tables 11 and 12. A 1.0 liter per year water flux, mean values of steel/alloy degradation rates and pH-dependent HLW glass degradation rate (Tables 13, 14, 15, and 16) consistent with the baseline analysis are used for comparison with current results. Two additional maximum and minimum mass loading cases are simulated to estimate constituent concentrations resulting from waste package failure occurring after the relatively short-lived strontium-90 isotope has completely decayed to zirconium. These two analyses, referred to as Year 2275 minimum (hereafter, SrF2Min2275) and maximum (hereafter, SrF2Max2275) mass loading cases, represent a more likely in-package chemistry scenario. Capsule compositions input to these calculations are consistent with those of the Year 2006 mass loading cases, with the exception of changes in composition resulting from decay of strontium-90 to zirconium.

These geochemical simulations consider the strontium fluoride capsule degradation rates and compositions given in Tables 11 and 12. Degradation of waste package materials and contents from waste package failure are shown in Figure 19 for the SrF2Max2275 and SrF_2Min2275 cases. Figure 19 is given to represent all strontium fluoride waste package cases because with the exception of differing initial capsule mass loading, the degradation history of waste package components is identical for all strontium fluoride package simulations. Waste package material degradation is in good agreement with that of the baseline analysis (see Reference 7, Figure 6-12, p. 6-43), with the exception of additional components (e.g., capsule packaging materials) and differences of initial material moles resulting from the use of the short waste package.

Similar to the cesium chloride waste package simulations, the most pronounced system response is that of solution pH. Here also, the evolution of pH is complex and initially controlled by capsule degradation and subsequent oxidation and mineral precipitation. The oxidation of metals rapidly dissolved into a package solution from the strontium fluoride capsules drives down the pH through acid producing reactions, which results in a sudden increase of protons that overwhelms the system's buffering capacity during the first 30 days (approximately) of the simulations. Unlike the cesium chloride capsules, the strontium fluoride capsules do not contain boron and phosphorous. Therefore, boric and phosphoric acid formation does not contribute to low pH conditions during strontium fluoride capsule degradation. Dissolution of chromium, iron, and manganese with subsequent eskolatite (Cr_2O_3), hematite (Fe_2O_3), and pyrolusite (MnO_2) formation are the primary acid-producing precipitation reactions affecting the creation of protons during capsule degradation. Respective minimum pH values of approximately 4.6 and 4.5 for SrF2Min2275 and SrF2Max2275 cases occur prior to capsule exhaustion at about 263 days (7.21×10^{-1} years in Figure 19). As the capsules are exhausted, the pH rises to approximately 6 at 10 years in response to dissolved capsule constituent mineralization, dissolution of soluble corrosion products, and the addition of alkalinity by HLW glass degradation and water flux. At 10 years, the pH gradually declines in response to the relatively slow corrosion of carbon and stainless steel waste package materials, after which the pH remains at approximately 5.5. The different pH responses observed in comparison of SrF2Min2275 and SrF2Max2275 cases resulted from the difference of initial capsule mass and subsequent differences of proton creation in precipitation reactions (Figure 19). After the first few years, the current predicted pH response is in good agreement with the range of pH predicted for the baseline analysis (see Reference 7, Section 6.6.1, Figure 6-27). The bulk solution chemistry of strontium fluoride waste package simulations is in good agreement with the baseline (see Reference 7, Section 6.5). Summary data for range of pH, Eh,

and ionic strength are given as a representative of bulk solution chemistry with maximum and minimum impurity concentrations and strontium isotope concentrations for Year 2006 and Year 2275 cases shown in Tables 19 and 20, respectively. Ionic strength and Eh time series data are also presented in Figures 20 and 21. The ionic strength maxima are observed to correspond with exhaustion of the stainless steel (316L) capsule canister and capsule packaging components at approximately 2,000 years, as shown in Figure 19. Consistent with the baseline, the Eh changes only in response to the pH changes (Figure 21) indicating uniformly oxidizing conditions even during the period of relatively rapid capsule degradation.

Table 20. Year 2275 strontium fluoride waste package results summary for in-package constituent concentrations and bulk chemistry.

Strontium Fluoride WP at Year 2275	Maximum Mass Loading	Minimum Mass Loading
Initial Solution Eh =	7.40E-01	7.40E-01
Max Eh =	9.53E-01	9.45E-01
Max Ionic Strength =	5.56E-01	5.29E-01
Max/initial pH =	8.09	8.09
Min. pH =	4.50	4.62
Element	(mg/L)	(mg/L)
Barium	2.69161E+02	3.37344E-01
Cadmium	1.52722E+01	1.65368E+00
Chromium	1.86380E-04	1.01262E-04
Fluorine	6.58599E+03	9.84326E+02
Lead	1.25431E-01	5.75726E-02
Silver	2.80997E-01	2.32844E-01
Strontium Total	1.07799E+03	4.63650E+02
Strontium-87	1.07799E+03	4.63650E+02
Strontium-90	0.00000E+00	0.00000E+00
U-Total	2.75828E+00	9.33049E-01
Zirconium	6.93312E+03	7.57734E+02

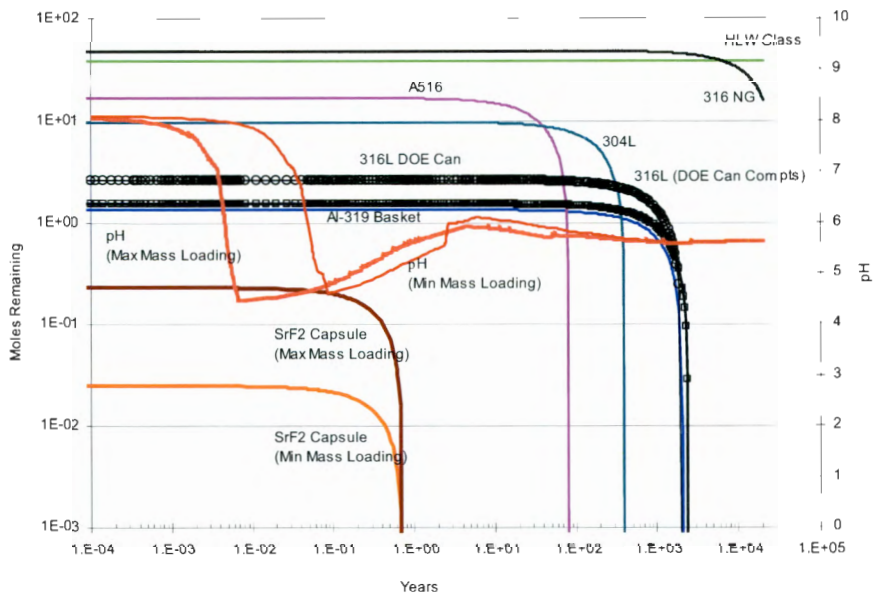

Figure 19. Degradation of waste package materials and content for Year 2275 minimum and maximum strontium fluoride mass loading cases.

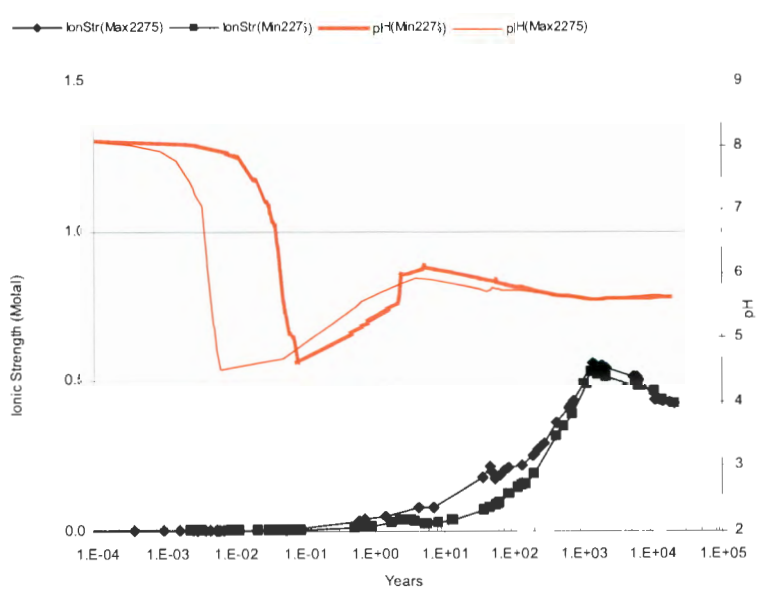

Figure 20. Comparison of pH and ionic strength for the Year 2275 strontium fluoride cases.

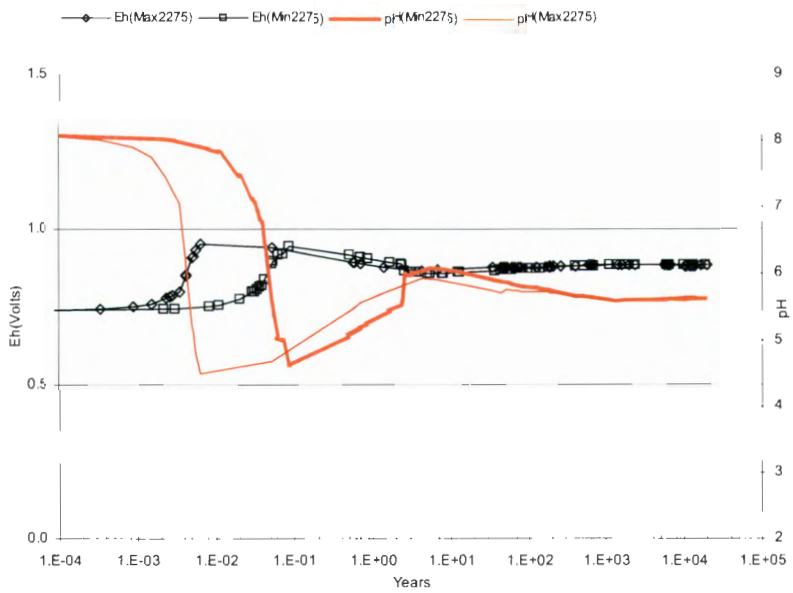

Figure 21. Comparison of pH and Eh for the Year 2275 strontium fluoride cases.

As in the cesium chloride waste package simulations, Year 2275 strontium fluoride waste package simulations are intended to provide most likely capsule constituent concentrations for input to the TSPA. Concentration histories are presented to provide insight into the timing and controls of those concentrations. Figures 22 and 23 show the predicted solution concentrations of the contaminant metals, strontium, and pH histories from waste package failure for SrF2Min2275 and SrF2Max2275 cases, respectively. Maximum solution concentrations of these capsule constituents, given in Tables 20 and 21, are dependent on the solubility of individual constituents and the solubility of mineral phases predicted to form with individual constituents. Capsule constituents predicted to precipitate as solid mineral phases are shown with pH histories for SrF2Min2275 and SrF2Max2275 case in Figures 24 and 25. With the exception of cadmium, mineral phases are predicted to form for all constituents during at least some portion of the simulation period. Those minerals include chlorargyrite (AgCl), barite ($BaSO_4$), eskolatite (Cr_2O_3), celestite ($SrSO_4$), lead phosphate ($PbHPO_4$), and strontium fluoride. No mineral phase(s) is/are predicted for cadmium. Therefore, the timing and maximum solution concentrations of cadmium are determined solely by the strontium fluoride capsule degradation rate and the amount of cadmium initially added to the simulations. With the exception of strontium, maximum solution concentrations are observed to occur within the first year of both Year 2275 mass loading cases (Figures 22 and 23). This timing corresponds with capsule exhaustion (Figure 19) suggesting the maximum solution concentration of all constituents, excluding strontium, is controlled by the prescribed capsule degradation rate with little influence imposed by water flux. Following capsule exhaustion, constituent concentrations are controlled, at least to some degree, by the solubility of mineral phases. Mineral solubility control of solution concentrations is most evident in the chromium and lead-time series data after 1 year (Figures 22 and 23).

Although irreversible, kinetic control is prescribed for strontium fluoride capsule degradation, the thermodynamic control of solubility explicit for EQ3/6 calculations affects the formation of solid phase strontium fluoride as the capsules degrade (Figures 24 and 25). The control of strontium fluoride solubility by the system's chemical thermodynamics produces maximum solution concentrations of strontium occurring on the order of thousands of years later than that of the capsule impurities (Figures 22 and 23). The formation of strontium fluoride and a subsequent delay in maximum strontium concentrations brings into question the applicability of a strontium fluoride capsule degradation rate derived from the laboratory estimation of strontium fluoride surface area for use under the conditions simulated. It follows that Assumption 3.5.4 may not be appropriate for the current strontium fluoride waste package simulations as a change (i.e., reduction) in the strontium fluoride capsule degradation rate would impact the rate of impurity additions to the simulation, thus changing the influence imposed by water flux on solution concentrations. In light of this result, the maximum constituent concentrations given in Tables 19 and 20 may be considered to provide a level of conservatism greater than that of the most likely failure scenario, with respect to a higher estimation of constituent concentrations in the solution.

Major mineral assemblages, excluding capsule constituents, predicted to form in SrF2Min2275 and SrF2Max2275 cases are shown in Figures 26 and 27. Other than slight differences in the timing of formation, mineral assemblages are consistent for both mass-loading cases. This result indicates that differences in pH histories during the first few years of capsule degradation will not influence the later time mineral assemblage. Further, with the exception of mineral phases forming as a direct result of capsule degradation (e.g., chlorargyrite and celestite), a good agreement is found between the current mineral assemblage and that of the baseline analysis (see Reference 7, Section 6.5.1.2, Figure 6-13). This agreement implies that replacement of SNF with strontium fluoride capsules in the waste packages will have a minimal impact on the assemblage of minerals and corrosion products forming by waste package material corrosion.

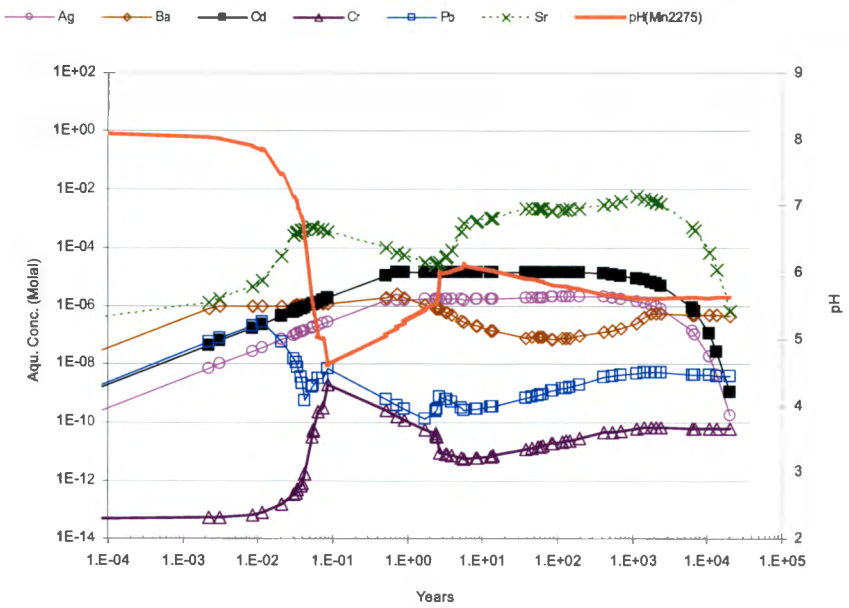

Figure 22. Year 2275 waste package concentrations of capsule constituents for the minimum strontium fluoride mass loading case.

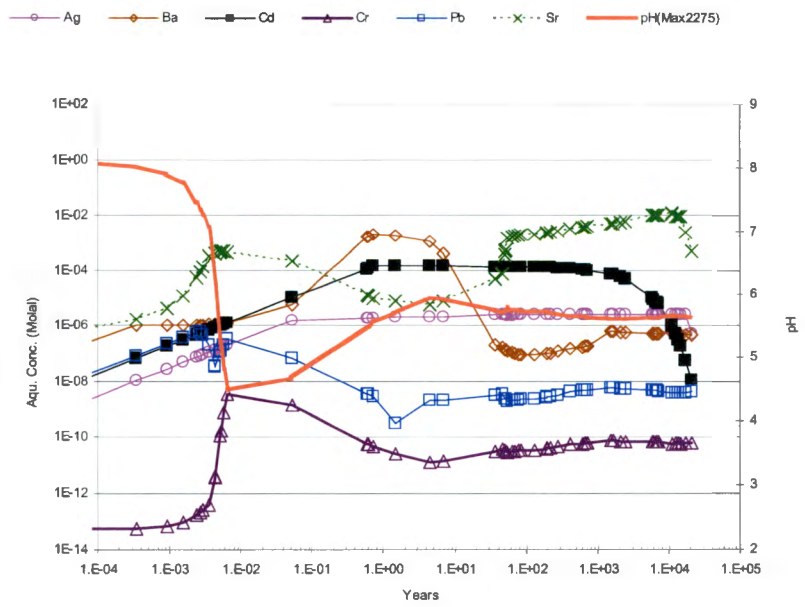

Figure 23. Year 2275 waste package concentrations of capsule constituents for the maximum strontium fluoride mass loading case.

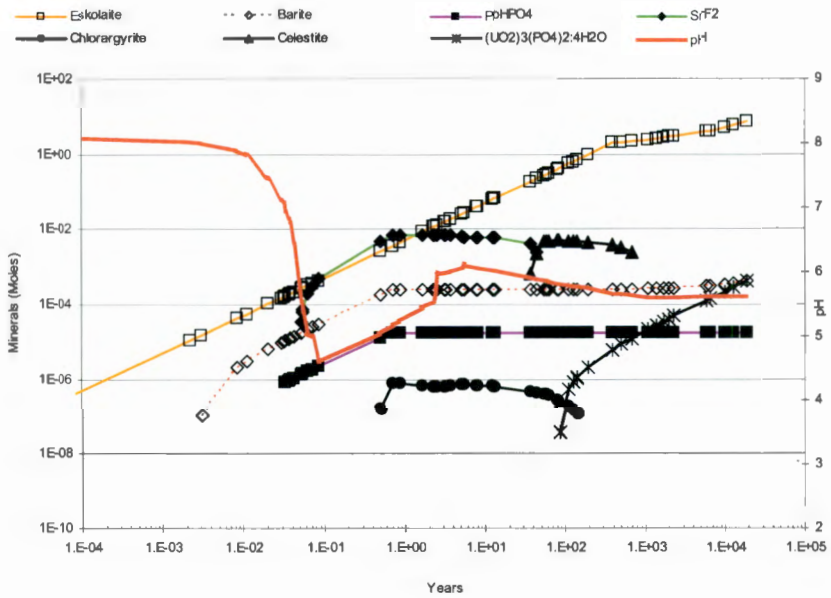

Figure 24. Mineralized capsule constituents for the Year 2275 minimum mass loading strontium fluoride waste package case.

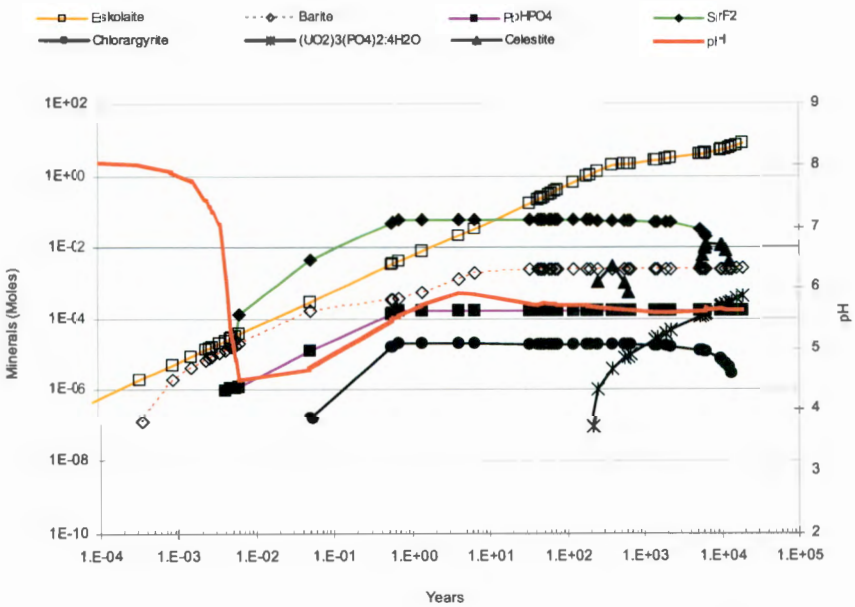

Figure 25. Mineralized capsule constituents for the Year 2275 maximum mass loading strontium fluoride waste package case.

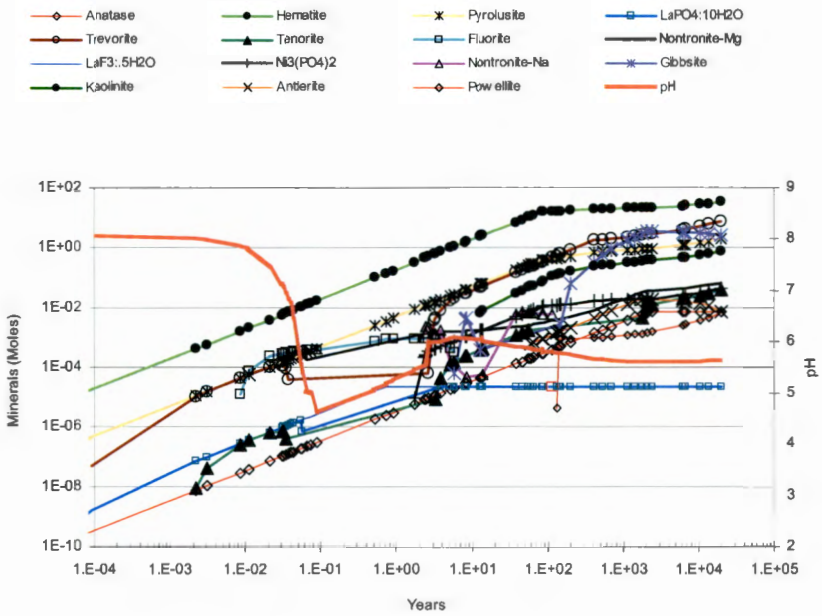

Figure 26. Major minerals forming in the Year 2275 minimum mass loading strontium fluoride waste package case, excluding capsule constituents.

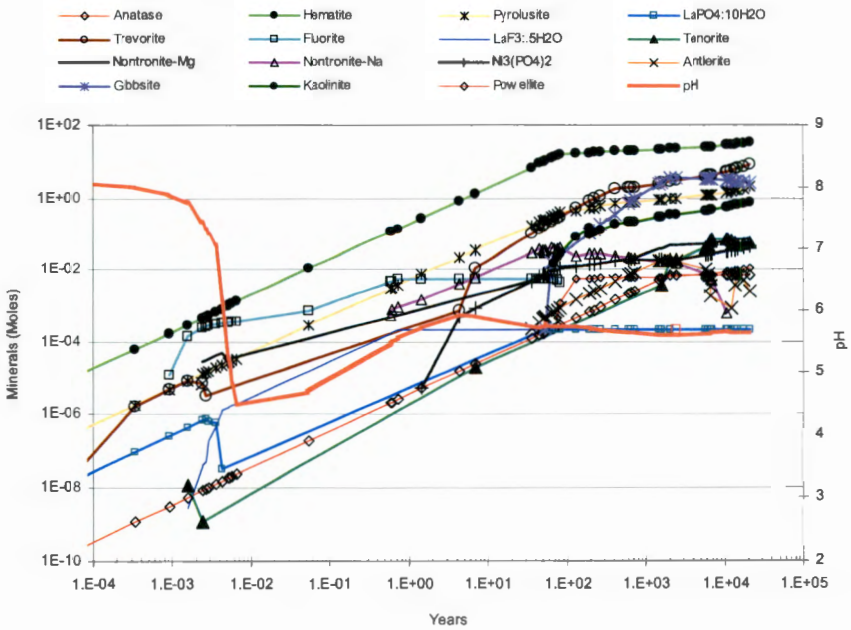

Figure 27. Major minerals forming in the Year 2275 maximum mass loading strontium fluoride waste package case, excluding capsule constituents.

4. TOTAL SYSTEM PERFORMANCE ASSESSMENT

4.1 TSPA Modeling Software

4.1.1 TSPA Background

As part of the repository analysis process, the Yucca Mountain Project developed detailed computer simulations (the TSPA models) to evaluate radionuclide transport through the repository. Figure 28 shows a high-level overview of the complex structure of a TSPA model. Each TSPA model was developed and revised as needed by the specific repository development phase. As activities completed, the models were archived and replacement models were developed. All TSPA models have undergone a screening process to ensure that all relevant features, events, and processes affecting material transport are represented in the specific model. The models have also gone through a process of review, qualification, and validation in accordance with Yucca Mountain quality program procedures.

The TSPA Final Environmental Impact Statement (TSPA-FEIS) model was used for this study. The TSPA-FEIS is the latest completed TSPA model available. More refined models are under development for final licensing work, but are not available for this study. The TSPA-FEIS model is derived from the TSPA Site Recommendation (TSPA-SR) model. The TSPA-SR model was a qualified model (verified and approved under the quality assurance program controls by Yucca Mountain). Changes to the TSPA-SR were made to support the FEIS that was written for the repository. The TSPA-FEIS model was a technically approved model, used during the FEIS process. The TSPA-FEIS, while written and approved by technically knowledgeable personnel at Yucca Mountain, was not required to be qualified under the repository quality control program. The TSPA-FEIS is suitable for use in this study because the study is scoping in nature rather than a formal regulatory analysis. Future studies that may be conducted for formal regulatory consideration should use a formally qualified version of the TSPA model, such as the TSPA License Application model currently being developed.

4.1.2 TSPA-FEIS Validation on NSNFP Computers

As written, the TSPA-FEIS model was run using GoldSim Version 7.17.200. When the model was obtained for use by the NSNFP, the computer hardware and operating systems specified for operation of the model were no longer available. This required the use of next generation hardware and operating system software, which caused some stability and reliability issues while running GoldSim Version 7.17.200. Discussions with the software and model developers indicated that the stability and reliability issues could be overcome by using GoldSim Version 7.51.200 to run the model. To assure that the TSPA-FEIS calculated comparable results in the new software, the model was run using GoldSim 7.51.200 and the model results from both versions of GoldSim were compared. The mean values of these runs are illustrated in Figures 29 and 30. The 7.51.200 version of GoldSim does random sampling differently from the 7.17.200 version, so individual realization results from each version vary slightly. Subject matter experts reviewed the results from these runs and concluded there was no significant difference in statistical results from the different versions. The overall statistics of the multi-realization results from the two GoldSim versions are essentially the same. This comparison demonstrates that the model results validate adequately and that the use of GoldSim 7.51.200 on NSNFP computers for this study provides similar results to use of the model in GoldSim 7.17.200 on the older Yucca Mountain computers.

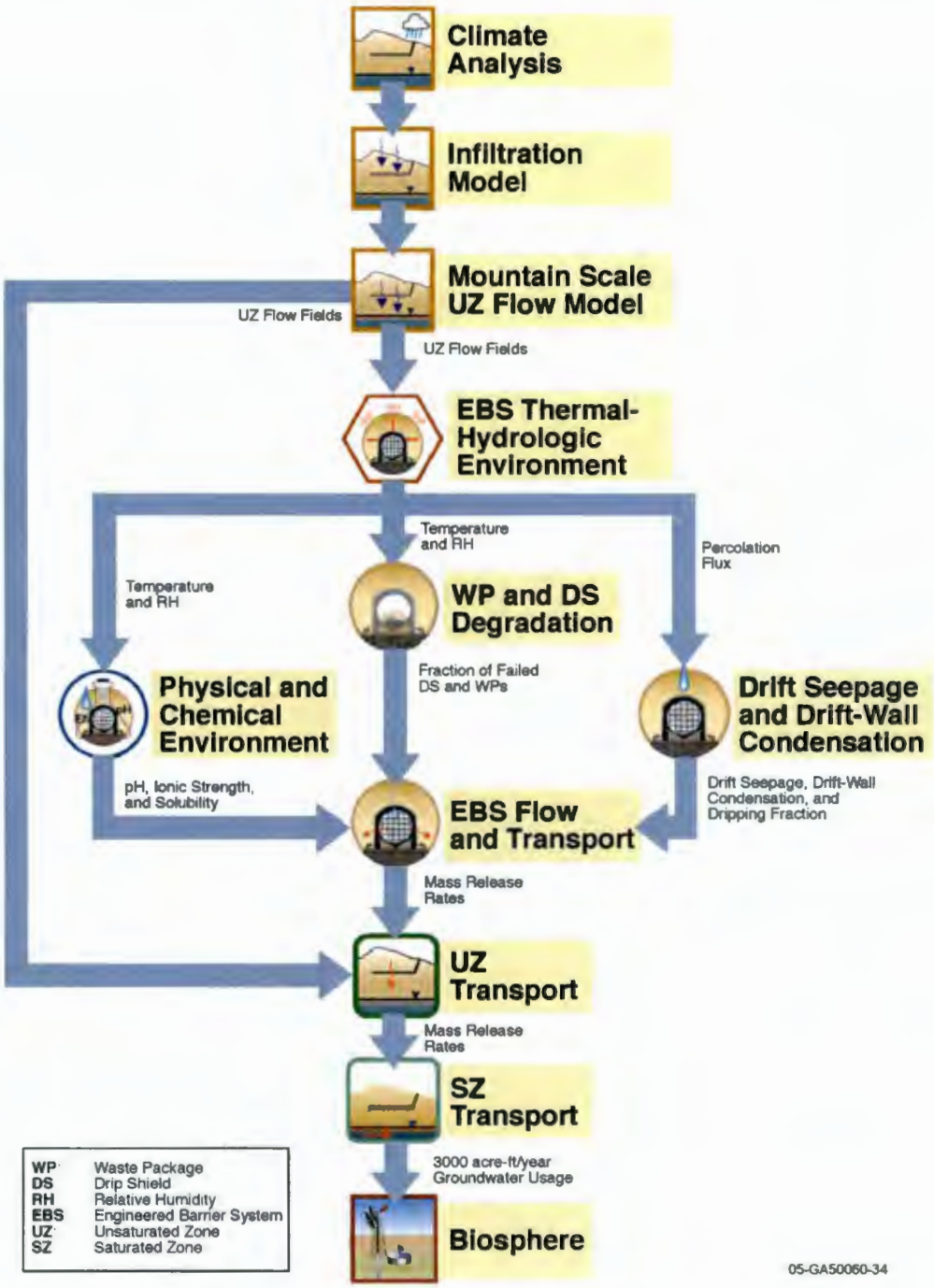

Figure 28. An illustration of the complexity of a TSPA model.

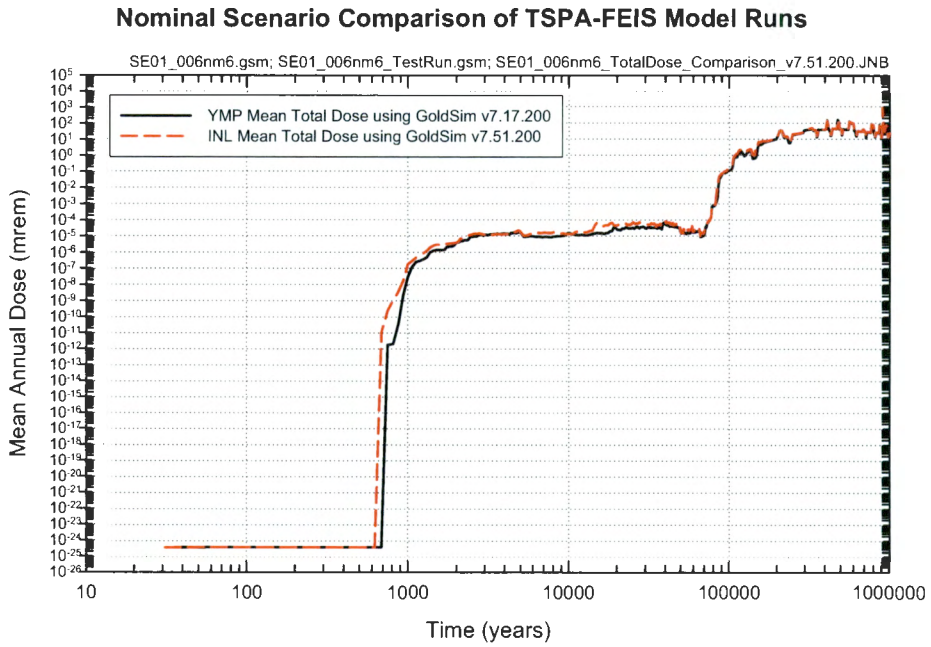

Figure 29. TSPA-FEIS validation comparison between GoldSim software versions using the base case and nominal scenario.

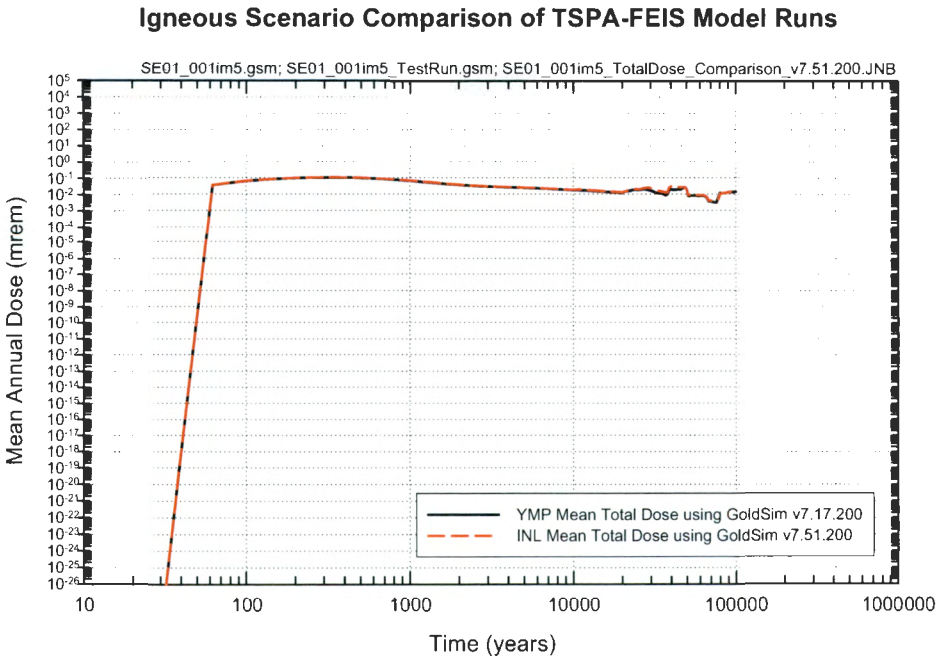

Figure 30. TSPA-FEIS validation comparison between GoldSim software versions using the base case and igneous scenario.

4.2 Stochastic Modeling Use and Interpretation

Uncertainty will exist in any projection of geologic and environmental conditions surrounding the repository in the future. Three different concepts related to uncertainty are involved in the performance assessment for the repository: (1) uncertainty about what will happen in the future; (2) uncertainty about parameters, model components and submodels, and other analysis assumptions; and (3) variability. These uncertainties are handled by constructing a model that expresses uncertain variables as a stochastic element, which is simply a probability distribution for the value of a variable. The TSPA modeling software (GoldSim) propagates the input uncertainties into uncertainties in the results using a Monte Carlo simulation. Monte Carlo simulation is the most commonly employed technique for implementing the probabilistic framework in engineering and scientific analyses. In the Monte Carlo simulation, the entire system is simulated numerous times (e.g., 300 or 5000). Each simulation is assumed to be equally likely, and is referred to as a realization of the system. For each realization, all the uncertain parameters are sampled (i.e., a single random value is selected from the specified distribution describing each parameter). The system is then simulated through time (given the particular set of input parameters) such that the performance of the system can be computed. The stochastic framework used in TSPA model calculations uses this well-established methodology for incorporating the effects of uncertainties in scenarios, conceptual models, and parameters. The benefits of stochastic modeling include obtaining the full range of possible outcomes (and the likelihood of each outcome) to quantify predictive uncertainty and analyzing the relationship between the uncertain inputs and the uncertain outputs to provide insight into the most important parameters.

4.3 TSPA Assumptions

The TSPA-FEIS model is the basis for all TSPA analysis in this report. All underlying assumptions that apply to the TSPA-FEIS model also apply to the TSPA analysis work done here. Additional assumptions made for this analysis are common with the geochemical analysis and are listed in Section 2.4 as common analysis assumptions with the additional assumption that the entire capsule inventory is available for transport after the waste package is breached. This conservative assumption eliminates the need to estimate the degradation rates for the material inside the capsules. Also, the TSPA analysis does not take barrier credit for any packaging other than the waste package. The DOE standard canister and any other capsule packaging are assumed to not impede contaminant transport in any way.

4.4 Effects of Capsule pH Ranges on the TSPA

In the TSPA-FEIS model, solubility of certain radionuclides (U, Pu, Th, and Np species) is a function of pH. Because a new waste package configuration is being used, it is appropriate to use new expected pH ranges. The pH ranges calculated in the geochemistry analysis discussed in Section 3 were compared to the original pH ranges used in the chemistry portion of the TSPA-FEIS model. The TSPA-FEIS model uses a pH range (sampling from a uniform distribution) for various time periods after waste package failure. The pH ranges used in the Base Case TSPA-FEIS model (for HLW glass and DOE SNF) are shown in Table 21. The pH ranges that were used to model radionuclide transport for the cesium and strontium capsules in the waste package (with the HLW glass) are also shown in Table 21. The pH ranges from the 2275 max loading geochemistry cases in Section 3 were used. The new pH ranges used do not fall outside the range of valid use for the TSPA-FEIS model because the equations used to calculate solubility as a function of pH include a cap of the largest concentrations possible. Thus, the TSPA-FEIS

model is valid for use of any pH[10]. The pH ranges for 10,000 years to 1,000,000 years were left unmodified because the data from the geochemistry analyses did not completely address this time period. The pH range for this last time period is high which would tend to yield higher solubilities. This would keep the results conservative.

Table 21. The pH ranges used for TSPA analysis.

Waste Package Configurations	pH Range (0 to 300 Years after waste package fails)	pH Range (300 to 10k Years after waste package fails)	pH Range (10k to 1M Years after waste package fails)
DOE SNF + HLW (Base Case FEIS model)	3.265 to 3.636	5.569 to 7.731	8.76 to 10
Cesium Capsules + HLW	2.5 to 8.09	5.58 to 5.63	unchanged
Strontium Capsules + HLW	4.5 to 8.09	5.61 to 5.66	unchanged

4.5 Radionuclide TSPA Results and Analysis

This section discusses the approach, cases, and results of the TSPA-FEIS analyses of radionuclide transport that were performed in this study.

4.5.1 Radionuclide Specie Modeling Approach

The intent of this part of the study was to evaluate changes in dose caused by representative replacement of the DOE SNF canister in the waste package with a canister containing the radionuclide inventories of cesium and/or strontium. To permit evaluation of the changes in dose from these waste packages, several variables were set in the TSPA for each case:

1. To confine the dose calculations to only the DOE inventory, the commercial SNF waste packages in the simulation were not permitted to fail. The effect of this setting is to define the dose from this source as zero.

2. The dissolution rate was set to instantaneous for the specie being studied in each simulation.

3. The number of waste packages in the simulations was changed to 84 for cesium and 38 for strontium, and the DOE SNF species were zeroed, except for the specie being studied (e.g., cesium-137).

4. The HLW inventory in the waste packages was left intact.

For the simulation of radionuclide transport, the TSPA-FEIS model was run one time for each case. Various cases were analyzed, patterned after previous work at Yucca Mountain. Some used the nominal scenario (1,000,000 year duration) and the others used the igneous scenario (100,000 year duration). Different inventories were used in different simulations depending on the type of simulation being run. Details for each radionuclide cases are shown in Table 22. In all cases, the initial inventory for the radionuclides was the Year 2006 values shown in Tables 2 and 4.

The TSPA-FEIS model data does not include the cesium-135 isotope. For this study, modifications to the model and a few extra runs were made to include the effects of cesium-135 on the dose. This was done by replacing the mass values and half-life values of cesium-137 with those of cesium-135 and re-running certain cases. However, the dose conversion factors for cesium-135 were not substituted into the model due to the complexity of the substitution. Because of this limitation, all calculated doses with cesium-135 shown here have an inherent error, which results in high estimates of dose from this nuclide. These runs should be repeated when the license application TSPA becomes available, since it will more accurately model both the radionuclide doses.

Table 22. Simulation descriptions for the radionuclide analysis.

Case Label	Case Description (See Nomenclature)	Scenario (See Nomenclature)	Simulation Period (years)	Number of Realizations
Base Case	All projected repository inventory, with 7,860 commercial SNF waste packages and 3,910 DOE codisposal waste packages, containing 1 DOE standardized canister with DOE SNF and 5 HLW canisters with HLW glass.	Nominal	1,000,000	300
Base Case 1	Base Case	Igneous	100,000	5,000
Cesium 1	Base Case modified to: • Set the release from commercial waste packages to zero • Modify number of codisposal packages to 84 to match projected cesium waste packages.	Nominal	1,000,000	300
Cesium 2	Cesium 1 case modified to: • Replace each DOE standardized canister	Nominal	1,000,000	300

Case Label	Case Description (See Nomenclature)	Scenario (See Nomenclature)	Simulation Period (years)	Number of Realizations
	containing DOE-SNF with a DOE standardized canister containing the maximum inventory of cesium-137 chloride			
Cesium 3	Cesium 1 case modified to: • Replace each DOE standardized canister containing DOE-SNF with a DOE standardized canister containing the maximum inventory of cesium-135 chloride	Nominal	1,000,000	300
Cesium 4	Base Case modified to: • Add maximum inventory of cesium-135 chloride to each DOE waste package	Nominal	1,000,000	300
Cesium Strontium 1	Base Case modified to: • Add maximum inventories of cesium-137 chloride and strontium-90 fluoride to each DOE waste package	Nominal	1,000,000	300
Cesium Strontium 2	Base Case 1 modified to: • Add maximum inventories of cesium-137 chloride and strontium-90 fluoride to each DOE waste package	Igneous	100,000	5,000
Strontium 1	Base Case modified to: • Set the release from commercial waste packages to zero • Modify number of codisposal packages to 38 to match projected strontium waste packages	Nominal	1,000,000	300

Case Label	Case Description (See Nomenclature)	Scenario (See Nomenclature)	Simulation Period (years)	Number of Realizations
Strontium 2	Strontium 1 case modified to: • Replace each DOE standardized canister containing DOE-SNF with a DOE standardized canister containing the maximum inventory of strontium-90 fluoride	Nominal	1,000,000	300