OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT 1. QA: QA SPECIAL INSTRUCTION SHEET

Page: 1 of: 2

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1. QA: QA Page: 1 of: 119

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 Document Identifier: CAL-EDC-MD-000015 REV00

 Page 2 of 119

CONTENTS

1	Dur	200		Q		
	-					
	Method					
	Assumptions11					
4.	Use o		puter Software and Models			
	4.1		re			
	4.2	Models	S	16		
5.	Calcu	ulation .		17		
	5.1	Calcula	ation Inputs			
		5.1.1	WP Materials and Performance Parameters			
		5.1.2	Physical and Chemical Form of the Enrico Fermi WP			
		5.1.3	Chemical Composition of Incoming Water	24		
		5.1.4	Drip Rate of Incoming Water			
		5.1.5	Densities and Molecular Weights of Solids			
		5.1.6	Atomic Weights			
		5.1.7	Thermodynamic Database			
		5.1.8	Data Conversion			
		5.1.9	Suppressed Minerals			
	5.2	-	alculations			
		5.2.1	Scenarios Considered			
		5.2.2	EQ6 Case Nomenclature	30		
6.	Resu					
	6.1	Summa	ary of Results	32		
		6.1.1	Gd and U Retention: One-stage Runs			
		6.1.2	Gd and U Retention: Two-Stage Runs			
			6.1.2.1 Scenario I Two-stage Runs			
			6.1.2.2 Scenario II Two-stage Runs			
	6.2		e Term: Effluent Concentration of Fissile U			
		6.2.1	Influence of Degradation Rates on Source Term			
		6.2.1	Influence of Degradation Order on Source Term			
		6.2.3	Influence of Higher CO ₂ Partial Pressure on Source Term			
	6.3		vity Analyses			
		6.3.1	GdPO ₄ Degradation Rate and Mass			
			6.3.1.1 Effects of Increasing GdPO ₄ Degradation Rate on Gd Loss			
		())	6.3.1.2 Effects of Increased GdPO ₄ Mass on Gd Loss			
		6.3.2	New Glass Degradation Rate			
			6.3.2.1 Effects on Internal Accumulation			
_			6.3.2.2 Effects on Source Term			
8.	Attac	hments	3	119		

aste Package Project							Ca	lcu
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Waste Package ProjectCalculationTitle: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposal Waste Packages:
Effects of Updated Design and RatesPage 3 of 119Document Identifier: CAL-EDC-MD-000015 REV00Page 3 of 119

FIGURES

1.	Case 1 (nm1x1321): WP Materials, Minerals, and Aqueous U	35
2.	Case 2 (nm1x1331): WP Materials, Minerals, and Aqueous U	38
3.	Case 3 (nm1{xy}1333): WP Materials, Minerals, and Aqueous U	41
4.	Case 4 (nm1x2331): WP Materials, Minerals, and Aqueous U	44
5.	Case 6 (nm1x2432): WP Materials, Minerals, and Aqueous U	48
6.	Case 8 (nm1{xyz}3333): WP Materials, Minerals, and Aqueous U	51
7.	Case 11 (1 st Stage: nm1x1403): WP Materials, Minerals, and Aqueous U	.55
8.	Case 11 (2 nd Stage: nm2{xy}1031): WP Materials, Minerals, and Aqueous U	.58
9.	Case 12 (1 st Stage: nm1x1303): WP Materials, Minerals, and Aqueous U	.61
10	. Case 12 (2 nd Stage: nm2x1332): WP Materials, Minerals, and Aqueous U	.64
11	. Case 14 (1 st Stage: nm1x1033): WP Materials, Minerals, and Aqueous U	.68
12	. Case 14 (2 nd Stage: nm2{xy}1303): WP Materials, Minerals, and Aqueous U	.71
13	. Case 15 (1 st Stage: nm1x1032): WP Materials, Minerals, and Aqueous U	.74
14	. Case 15 (2 nd Stage: nm2x1302): WP Materials, Minerals, and Aqueous U	.77
15	. Case 15 (2 nd Stage: nm2y1302): WP Materials, Minerals, and Aqueous U	.78
16	. Case 16 (nm1x3432): WP Materials, Minerals, and Aqueous U	.83
17	. Case 16 (nm1x3432): Enrichment and U-bearing solids in the WP	.84
18	. Case 17 (nt1x1331): WP Materials, Minerals, and Aqueous U	.86
19	. Case 17 (nt1x1331): Enrichment Fraction and U-bearing Solids in the WP	.87
20	. Case 18 (nt1x1432): WP Materials, Minerals, and Aqueous U	.89
21	. Case 18 (nt1x1432): Enrichment Fraction and U-bearing solids in the WP	.90
22	. Case 19 (1 st Stage: nm1x1031): WP Materials, Minerals, and Aqueous U	.92
23	. Case 19 (2 nd Stage: nm2x1402): WP Materials, Minerals, and Aqueous U	.93
24	. Case 19 (2 nd Stage: nm2x1402): Enrichment Fraction and U bearing solids in the WP	.94
25	. Case 20 (2 nd Stage: nc2x1402): WP Materials, Minerals, and Aqueous U	.96
26	. Case 20 (2 nd Stage: nc2x1402): Enrichment Fraction and U-bearing Solids in the WP	.97

Waste Package Project	Calculation
Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposal	Waste Packages:
Effects of Updated Design and Rates	
Document Identifier: CAL-EDC-MD-000015 REV00	Page 4 of 119

FIGURES (Continued)

27. Cases 8, 23, and 24: GdPO ₄ Degradation, Aqueous Gd, and pH	100
28. Cases 23-26: Gd Solids, Aqueous Gd, and pH	104
29. Case 27 (nm1n1331): WP Materials, Minerals, and Aqueous U	108
30. Case 28 (nm2n1402): WP Materials, Minerals, and Aqueous U	111
31. Case 28 (nm2n1402): Enrichment and U-bearing Solids in the WP	112

Waste Package Project	Calculation
Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisp	osal Waste Packages:
Effects of Updated Design and Rates	
Document Identifier: CAL-EDC-MD-000015 REV00	Page 5 of 122

TABLES

1.	Computer Software Used in this Calculation15
2.	Properties of Materials in Enrico Fermi Codisposal WP20
3.	Steels Composition and Degradation Rates
4.	Simplified Glass Composition and Degradation Rates
5.	Fermi Fuel Composition and Degradation Rates
6.	GdPO ₄ Shot Composition and Degradation Rates23
7.	EQ3NR Input File Constraints for Incoming Water Composition25
8.	EQ6 Input File Elemental Molal Composition for Incoming Water
9.	Drip Rate Values for Input to EQ6
10.	Summary of Gd Retention for One-stage EQ6 Runs
11.	Summary of Intact Fuel and Glass in WP for One-stage EQ6 Runs
12.	Summary of U Retention for One-stage EQ6 Runs
13.	Case 1 (nm1x1321): Composition of Corrosion Products (g), Total Mass, and Density36
14.	Case 1 (nm1x1321): Solution Composition in Molality
15.	Case 2 (nm1x1331): Composition of Corrosion Products (g), Total Mass, and Density39
16.	Case 2 (nm1x1331): Solution Composition in Molality
17.	Case 3 (nm1{xy}1333): Composition of Corrosion Products (g), Total Mass, and Density
18.	Case 3 (nm1{xy}1333): Solution Composition in Molality
19.	Case 4 (nm1x2331): Composition of Corrosion Products (g), Total Mass, and Density46
20.	Case 4 (nm1x2331): Solution Composition in Molality47
21.	Case 6 (nm1x2432): Composition of Corrosion Products (g), Total Mass, and Density49
22.	Case 6 (nm1x2432): Solution Composition in Molality
23.	Case 8 (nm1{xyz}3333): Composition of Corrosion Products (g), Total Mass, and Density
24.	Case 8 (nm1{xyz}3333): Solution Composition in Molality

Waste Package Project	Calculation
Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposal	Waste Packages:
Effects of Updated Design and Rates	
Document Identifier: CAL-EDC-MD-000015 REV00	Page 6 of 119

TABLES (Continued)

.

25. Gd and U Retention for Scenario I Two-Stage EQ6 Runs	54
26. Case 11 (1 st Stage: nm1x1403): Composition of Corrosion Products (g), Total Mass,	
and Density	56
27. Case 11 (1 st Stage: nm1x1403): Solution Composition in Molality	57
 Case 11 (2nd Stage: nm2{xy}1031): Composition of Corrosion Products (g), Total Mass, and Density 	59
29. Case 11 (2 nd Stage: nm2{xy}1031): Solution Composition in Molality	60
30. Case 12 (1 st Stage: nm1x1303): Composition of Corrosion Products (g), Total Mass, and Density	62
31. Case 12 (1 st Stage: nm1x1303): Solution Composition in Molality	63
32. Case 12 (2 nd Stage: nm2x1332): Composition of Corrosion Products (g), Total Mass, and Density	65
33. Case 12 (2 nd Stage: nm2x1332): Solution Composition in Molality	66
34. Gd and U Retention for Scenario II Two-stage EQ6 Runs	67
35. Case 14 (1 st Stage: nm1x1033): Composition of Corrosion Products (g), Total Mass, and Density	69
36. Case 14 (1 st Stage: nm1x1033): Solution Composition in Molality	70
37. Case 14 (2 nd Stage: nm2{xy}1303): Composition of Corrosion Products (g), Total Mass, and Density	72
38. Case 14 (2 nd Stage: nm2{xy}1303): Solution Composition in Molality	73
39. Case 15 (1 st Stage: nm1x1032): Composition of Corrosion Products (g), Total Mass, and Density	75
40. Case 15 (1 st Stage: nm1x1032): Solution Composition in Molality	76
41. Case 15 (2 nd Stage: nm2{xy}1302): Composition of Corrosion Products (g), Total Mass, and Density	79
42. Case 15 (2 nd Stage: nm2{xy}1302): Solution Composition in Molality	
43. Summary of Cases Run for Source Term Calculations	81
44. Isotopic Mole Fractions of HLW Glass and Fermi Fuel	81
45. Results of One Stage Source Term Cases	82

Waste Package Project	Calculation
Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposal	Waste Packages:
Effects of Updated Design and Rates	
Document Identifier: CAL-EDC-MD-000015 REV00	Page 7 of 119

-

TABLES (Continued)

46. Case 16 (nm1x3432): Solution Composition in Molality	85
47. Case 17 (nt1x1331): Solution Composition in Molality	88
48. Case 18 (nt1x1432): Solution Composition in Molality	91
49. Case 19 (2 nd Stage: nm2x1402): Solution Composition in Molality	95
50. Case 20 (2 nd Stage: nc2x1402): Solution Composition in Molality	98
51. Gd and U Retention: Sensitivity of Faster GdPO ₄ Degradation Rates	99
52. Case 23 (nA1x3333): Composition of Corrosion Products (g), Total Mass, and Density	101
53. Case 23 (nA1x3333): Solution Composition in Molality	102
54. Gd and U Retention: Cases with an Increase in GdPO ₄ Mass	103
55. Case 25 (nA1d3333): Comparison of Corrosion Products (kg), Total Mass, and Density	105
56. Case 25 (nA1d3333): Solution Composition in Molality	106
57. Gd and U Retention for Different HLW Glass Degradation Rates	107
58. Case 27 (nm1n1331): Composition of Corrosion Products (kg), Total Mass, and Density	109
59. Case 27 (nm1n1331): Solution Composition in Molality	110
60. Case 28 (nm2n1402): Solution Composition in Molality	113

Waste Package Project	Calculation
Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposal V	Waste Packages:
Effects of Updated Design and Rates	
Document Identifier: CAL-EDC-MD-000015 REV00	Page 8 of 119

1. PURPOSE

The Monitored Geologic Repository (MGR) Waste Package Project of the BSC Management and Operating Contractor for the Department of Energy's Office of Civilian Radioactive Waste Management performed calculations to provide input for disposal of spent nuclear fuel (SNF) from the Enrico Fermi Reactor owned by the DOE (Ref. 9). The Fermi SNF has been considered for disposal at the proposed Yucca Mountain site. Because of the high content of fissile materials in the SNF, the waste package (WP) design required special consideration of the amount and placement of neutron absorbers, and the possible transport of absorbers and fissile materials over geologic time. If there is a breach in the WP, water will enter and infiltrate the WP. This water would be able to moderate neutrons, increasing the likelihood of a criticality event within the WP. Also, infiltrating water may in time gradually leach the fissile components from the WP and separate them from the neutron absorbers. Such phenomena would affect the neutronics of the system.

This study presents calculations of the long-term geochemical behavior of WPs containing one DOE disposal container and five high-level waste (HLW) glass pour canisters (GPCs) arranged according to the codisposal concept (Ref. 14). The specific study objectives were to determine:

- The extent to which criticality control material suggested for this WP design will remain in the WP after corrosion/dissolution of the initial WP configuration (such that it can be effective in preventing criticality).
- The extent to which fissile uranium (U) will be carried out of the degraded WP by infiltrating water (such that internal criticality is no longer possible, but the possibility of external criticality may be enhanced).
- The nominal chemical composition and amounts of minerals and other solids left in the WP. These may be used for the criticality evaluations of the WP design, and to suggest the range of parametric variations for additional evaluations.

The chemical compositions (and subsequent criticality evaluations) of the simulations are calculated for time periods up to \sim 670,000 years. This longer time frame is closer to the one million year time horizon recommended by the National Academy of Sciences to the Environmental Protection Agency for performance assessment related to a nuclear repository (Ref. 31). However, it is important to note that after 100,000 years, most of the materials of interest (fissile and absorber materials) will have either been removed from the WP, reached a steady state, or been transmuted. The sketch of the WP in Attachment II is a potential design of the type considered in this calculation.

Besides fissile materials, the calculation included the element gadolinium (Gd) with a high neutron absorption cross section, which is included in the DOE canister along with the Enrico Fermi fuel to reduce the possibility for criticality. The results of this calculation will be used to ensure that the type and amount of criticality control material used in the WP design will prevent criticality both internally and externally.

The scope of this study is to repeat several cases from a previous calculation (Ref. 32). This requirement is due to updates in the reaction rates of several WP components and the redesign of

Waste Package Project	Calculation
Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposal	Waste Packages:
Effects of Updated Design and Rates	
Document Identifier: CAL-EDC-MD-000015 REV00	Page 9 of 119

the WP to include a 316NG Stainless Steel sleeve inside of the Alloy-22 containment (Attachment II). The case numbers and identifications, which correspond to the previous study, are detailed below in the results.

This calculation also includes calculation of the "source term" for external criticality. The source term provides input for descriptions of the chemistry effluent solutions from the WPs as they degrade. Particular attention is paid to the concentrations of fissile enrichments of U in the effluent. These source terms will then be used in future external transport and accumulation analyses.

This document has been prepared according to Administrative Procedure AP-3.12Q, REV0, ICN 4 (Ref. 29), *Calculations*, and is subject to the Quality Assurance Requirements and Description (QARD) Document (Ref. 30) requirements. This calculation has been prepared in accordance with the *Technical Work Plan for: Department of Energy Spent Nuclear Fuel Work Packages* (Ref.17).

Waste Package Project	Calculation
Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposal	Waste Packages:
Effects of Updated Design and Rates	
Document Identifier: CAL-EDC-MD-000015 REV00	Page 10 of 119

2. METHOD

The method used for this calculation involves the following steps:

- Use of the qualified and modified version of the EQ3/6 reaction-path code (as described in Section 4) for tracing the degradation of the WP. The software estimates the concentrations remaining in the aqueous solution and the composition of the precipitated solids. (EQ3NR is used to determine a starting fluid composition for EQ6 reaction-path calculations.
- Use of "solid-centered flow-through" mode (SCFT) in EQ6; in this mode, an increment of aqueous "feed" solution is added continuously to the WP system, and a like volume of the existing solution is removed, simulating a continuously-stirred tank reactor. This mode is discussed in Section 4.
- Determination of fissile material concentrations in solution as a function of time (from the output of EQ6 simulated reaction times up to ~670,000 years).
- Calculation of the amount of U released from the WP as a function of time (U loss reduces the chance of criticality within the WP).
- Determination of the concentration of the neutron absorber Gd in solution as a function of time (from the output of EQ6 over times up to ~670,000 years).
- Calculation of the amount of neutron absorber retained within the WP as a function of time.
- Determination of composition and amounts of reaction-product solids (precipitated minerals or corrosion products, and unreacted package materials).
- Comparison of the former calculation (Ref. 32) with this calculation that incorporates the new WP design and degradation rates of WP components.
- Determination of fissile U content in solution for source term calculations.

This calculation used version 7.2bLV (Ref. 21) of EQ6. The User's Manual for 7.2bLV (Ref. 36) provides a detailed description of the code. The code retains the solid-centered flow-through (SCFT) mode developed in the previous Addendum to EQ6 (Ref. 37) and is complete, mathematically correct and technically adequate for the application. Further detail on the specific methods employed for each step is available in Section 5 of this calculation.

With regard to the development of this calculation, the control of the electronic management of data was evaluated in accordance with AP-SV.1Q, *Control of the Electronic Management of Information* (Ref. 38). The evaluation (Ref. 17) determined that current work processes and procedures are adequate for the control of electronic management of data for this activity.

3. ASSUMPTIONS

All assumptions are for preliminary design; and are used throughout Section 5 and 6.

- 3.1 It is assumed that the solutions that drip into the WP will have the major ion composition of J-13 well water as given in (Ref. 15 [DTN: MO0006J13WTRCM.000]) for ~670,000 years. The rationale for this assumption is that the groundwater composition is controlled largely by transport through the host rock, over pathways of hundreds of meters, and the host rock composition is not expected to change substantially over 10⁶ years. The assumption that the J-13 well water can approximate the water entering the WP implicitly assumes that any effects of contact with the engineered materials in the drift will be minimal after a few thousand years. For a few thousand years after waste emplacement, the composition may differ because of perturbations resulting from reactions with engineered materials and from the thermal pulse. These are not taken into account in this calculation because the outer shell and inner liner are not expected to breach until after that perturbed period. Therefore, the early perturbation is not relevant to the calculations reported in this document.
- 3.2 It is assumed that an aqueous solution fills all voids within the WP. The rationale for this assumption is that it provides the maximum degradation rates of WP components with the potential for precipitation of radionuclides within the WP or the flushing of radionuclides from the WP, and is therefore conservative. This assumption is justified by recent evaluations of codisposal WPs which show that degradation of the WP materials (specifically, HLW glass and steel) overwhelms the native chemistry of the incoming water. (Ref. 4, Figures 5-3 through 5-20 of show pH values between 3 and 10 in the WP).
- 3.3 It is assumed that the density of the incoming water is 1.0 g/cm³. The rationale for this assumption is that for dilute solutions, the density is extremely close to that of pure water and that any differences are insignificant with respect to other uncertainties in the data and calculations. Moreover, this value is used only initially in EQ3/6 to convert concentrations of dissolved substances from parts per million to molality.
- 3.4 It is assumed that water will circulate freely enough in the partially degraded WP that all degraded solid products will react with each other through the aqueous solution medium. The rationale for this assumption is that it provides the most rapid aqueous degradation and is, therefore, conservative.
- 3.5 It is assumed that 25°C thermodynamic data can be used for the calculations. Though the initial breach of the WP may occur when the contents are at temperatures ≥ 50°C (Ref. 5, Figures 3-20 through 3-22), at times > 25,000 years, the WP temperatures are likely to be close to 25°C.
- 3.6 In general it is assumed that chromium (Cr) and molybdenum (Mo) will oxidize fully to chromate (or dichromate) and molybdate, respectively. This assumption is based on the available thermodynamic data (Ref. 3, "data0.ymp"), which indicate that in the presence of air, the Cr and Mo would both oxidize to the VI valence state. Laboratory observation of the corrosion of Cr and Mo containing steels and alloys, however, indicates that any

Waste Package Project	Calculation
Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codis	posal Waste Packages:
Effects of Updated Design and Rates	
Document Identifier: CAL-EDC-MD-000015 REV00	Page 12 of 119
	· · · · · · · · · · · · · · · · · · ·

such oxidation would be extremely slow. In fact, oxidation to the VI state may not occur at a significant rate with respect to the time frame of interest, or there may exist stable Cr(III) solids that substantially lower aqueous Cr concentration. For the present analyses, the assumption is made that, over the times of concern, oxidation will occur. The rationale for this assumption is that by allowing the Cr and Mo to oxidize, the pH of the system will be lowered, allowing for the removal of neutron absorbers and retention of fissile materials.

- 3.7 It is assumed that gases in the WP solution remain in equilibrium with the ambient atmosphere outside the WP. In other words, contact of WP fluids with the gas phase in the repository is assumed to be sufficient to maintain equilibrium with the carbon dioxide (CO_2) and oxygen (O_2) present, whether or not this is the normal atmosphere in open air or rock gas that seeps out of the adjacent tuff. Moreover, the specific partial pressures of CO_2 and O_2 of the ambient repository atmosphere are set to, respectively, $10^{-3.0}$ and $10^{-0.7}$ atm. The rationale for choosing the O_2 partial pressure is that it is equivalent to that in the atmosphere (Ref. 40, p. F-210). The rationale for choosing the CO_2 partial pressure is to reflect the observation that J-13 well water appears to be in equilibrium with above-atmospheric CO_2 levels (Ref. 39, Table 7).
- 3.8 It is assumed that precipitated solids that are deposited remain in place, and are not mechanically eroded or entrained as colloids in the advected water. The rationale for this assumption is that it conservatively maximizes the amount of fissile material deposited inside the WP.
- 3.9 It is assumed that the corrosion rates used in this calculation encompass rates for microbially assisted degradation, and that the degradation rates will not be controlled principally by microbes (Ref. 5, p. 3-84). The rationale for this assumption is (1) corrosion rates measured under environmental conditions inherently include exposure to microbes, and (2) the lack of organic nutrients available for microbial corrosion will limit the involvement of microbes. Microbes can act as catalysts but this catalytic effect is not expected to significantly change the types of solids formed in the WP.
- 3.10 It is assumed that sufficient decay heat is retained within the WP over times of interest to cause convective circulation and mixing of the water inside the WP. The rationale for this assumption is the analysis in Reference 8, Attachment VI.
- 3.11 It is assumed that the rate of entry of water into, as well as the rate of egress from, a WP is equal to the rate at which water drips onto the WP. The rationale for this assumption is that for most of the time frame of interest, i.e., long after the outer barriers become largely degraded, it is more reasonable to assume all or most of the dripping water will enter the degraded WP than to assume a significant portion will instead be diverted around the remains. However, the calculations include scenarios with very low drip rates, which effectively simulate diversion of the bulk of the water striking the WP.
- 3.12 It is assumed that the most insoluble solids for a fissile radionuclide will form, i.e., equilibrium will be reached. The rationale for this assumption is conservatism; the

Waste Package Project	Calculation
Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisp	oosal Waste Packages:
Effects of Updated Design and Rates	
Document Identifier: CAL-EDC-MD-000015 REV00	Page 13 of 119

highest chance of internal criticality occurs when the fissile solids have lowest solubility, and are thus retained in the WP.

- 3.13 For any WP components that were described as "304" stainless steel, without indication of the carbon grade, the alloy was assumed to be the low-carbon equivalent (see Section 5.1.1 for nomenclature). The rationale of this assumption is that, in general, the carbon in the steel is totally insignificant compared to the carbon supplied by the fixed CO_2 fugacity of the EQ3/6 calculation, and to the constant influx of carbonate via the incoming water.
- 3.14 It is assumed that the reported alkalinity in analyses of J-13 well water corresponds to bicarbonate (HCO₃⁻) alkalinity. Contributors to alkalinity in J-13 well water, in addition to bicarbonate, potentially include borate, phosphate, and silicate. However, at pH less than 9, the contribution of silicate will be small, and in any case the concentrations of all three of these components in J-13 well water are small. Fluoride or nitrate do not contribute to alkalinity unless a sufficiently low pH is reached. The rationale for this assumption is the observation that the calculated electrical neutrality, using the assumption, is zero within the analytical uncertainty, as it should be. The same assumption is implicitly made in Reference 15 (DTN: MO0006J13WTRCM.000).
- 3.15 A number of minor assumptions have been made about the geometry of the Enrico Fermi codisposal WP. These assumptions are outlined and referenced in the spreadsheet "Fermi_Fuel_kz.xls" (Ref. 1), and are also discussed in Section 5.1. The bases for these assumptions are to represent the WP geometry with the greatest accuracy and where inadequate information is available to choose among competing representations of WP geometry, the choice that appears to lead to greatest conservatism is always chosen.
- 3.16 It is assumed that the high-level waste glass composition is as given in Reference 16, Attachment I, p. I-7, and that the density of the HLW glass is 2.85 g/cm³ (Ref. 43, p. 2.2.1.1-4). The rationale for this assumption is that the references cited above are the most recent and comprehensive sources available to provide this information.
- 3.17 Zircaloy and Zr corrosion kinetics studies (Ref. 6) revealed these materials to be resistant against chemical and biological corrosion. These studies on corrosion of Zircaloy-clad SNF indicate growth of oxide films for a time span of a million years to be about 7.6E-03 millimeter (0.3 mil). It was also assumed that the Zr cladding would breach soon after it comes in contact with water. The basis for this assumption is justified since it is conservative and accounts for any cladding that is damaged during storage, shipping, or packing.
- 3.18 It is assumed that the molecular weight of all "special reactants" (steel, glass, etc) is equal to 100g/mole. The rationale for this assumption is that it simplifies conversion of WP material compositions (often available in weight percent) to moles for EQ6 input files. By using this molecular weight for all special reactants, calculation of masses in WPs is simple and straightforward.
- 3.19 It is generally assumed that only the inside surface area of the 316NG liner is greatly exposed to degradation within the WP. The basis for this assumption is that after breach,

Waste Package Project	Calculation
Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codispo	osal Waste Packages:
Effects of Updated Design and Rates	-
Document Identifier: CAL-EDC-MD-000015 REV00	Page 14 of 119

water is expected to fill the inside of the WP. This is also more conservative for internal criticality since more U is retained within the WP if only the inner surface area is taken into account.

- 3.20 If the outer shell of the WP comes into contact with water within the WP, it will react so slowly that it will have an insignificant effect on the chemistry of the WP solution. The basis for this assumption is that Alloy 22 corrodes very slowly compared to other reactants in the WP (Ref. 13). At the rate which soluble corrosion products are likely to be flushed from the WP, any input from the outer shell would have negligible effects on the chemistry.
- 3.21 The general composition and density of GdPO₄ was taken to be the same as that for the mineral monazite ((Ce,La,Nd,Th)PO₄). The rationale is that since there is no data on GdPO₄, monazite properties could be used to bound characteristics of GdPO₄ since Gd is also a lanthinide and should have similar properties to the actinide and lanthinides occurring in monazite.
- 3.22 It is assumed that the degradation rate of $GdPO_4$ is the same as that for quartz. The rationale for this assumption is that little is known about $GdPO_4$ degradation, only that it is relatively slow. For the purposes of this study, quartz dissolution rate is used since it is also known to be slow and is also well documented (Ex. Refs. 58 and 59).

Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposal Waste Packages: Effects of Updated Design and Rates

Document Identifier: CAL-EDC-MD-000015 REV00

4. **USE OF COMPUTER SOFTWARE AND MODELS**

SOFTWARE 4.1

This section describes the computer software used in the calculation.

Software Name	Version	Software Tracking Number (Qualification Status)	Description and Components Used		nd Output Files ^a I in Attachment I)
EQ3/6	7.2b	Qualified LLNL:UCRL-MA-110662 EQ3/6, Ref. 42	EQ3NR: a speciation- solubility code	input: pickup: output:	*.3i *.3p *.3o
			EQPT: a data file preprocessor	input: output:	data0.* data1.*
EQ6	7.2bLV	Qualified 10075-7.2bLV-00 EQ6, Ref. 21	EQ6: a reaction path code which models water/rock interaction or fluid mixing in either a pure reaction progress mode or a time mode	input: pickup: output:	*.6i *.6p *.6o *.elem_aqu.txt *.elem_min.txt *.elem_tot.txt *.min_info.txt *.bin
ASPRIN	1.0	Qualified 10487-1.0-00 ASPRIN, Ref. 45	ASPRIN: performs post- processing of numerical information (from an output data file created by EQ6), to calculate isotopic inventories for elements of interest	input: output:	*.bin (from EQ6) *.txt
MS EXCEL	Version 97 SR-2	Commercial off-the-shelf software: Exempt in accordance with AP-SI.1Q (Ref. 25), Section 2.1.	Excel: used in this document for graphical representation and arithmetical manipulations	input: output:	*.elem_*.txt *.xls
PP	NA	Ref. 2. Used solely for visual display or graphical representation: Exempt in accordance with AP-SI.1Q (Ref. 25), Section 2.1.2.	PP: a plotting tool used for graphical representation	input: output:	*.bin (from EQ6) *.wmf

Table 1. Computer Softwa	are Used in this Calculation
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^a Files are explained in more detail in Attachment I.

The software products were run on a standard PC and all applicable products were obtained from Software Configuration Management (SCM). The software was appropriate for the application and was used within the range of validation in accordance with AP.SI-1Q.

The EQ6 software was used within its range of validation. However, some runs simulated periods of high ionic strength (1 to \sim 4). While EO6 is capable of handling high ionic strengths. there is no qualified Yucca Mountain Project (YMP) thermodynamic database with corrections for high ionic strength. To address this issue, several sensitivity tests were performed using

Waste Package Project	Calculation
Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codispos	al Waste Packages:
Effects of Updated Design and Rates	
Document Identifier: CAL-EDC-MD-000015 REV00	Page 16 of 119

other thermodynamic databases that have corrections for high ionic strength (Ref. 24, Sec. 5.1.2). The results show that calculations at high ionic strength, using the "data0.ymp" database (Ref. 3), overestimate the solubility of Pu and U, which is conservative with respect to external accumulations of these elements.

4.2 MODELS

The mathematical model *Defense High Level Waste Glass Degradation* was used for degradation rate expressions for dissolution of glass immersed in water. Both the earlier version of the model (Ref. 28, Equations 7 and 8) and the most recent version of the model (Ref. 46, Equations 7 and 8) were used in the calculations. The earlier version of the model was used in Sections 6.1 and 6.2 of this document. Two sensitivity cases were performed with the more recent model to check the effects of the new rate on U retention and source term calculations. The results are presented in Section 6.3.

The model does not have a Model Warehouse Data Tracking Number. The use of the model in the current calculation is justified, since the purpose of the model is to describe the degradation of HLW glass in a flooded WP.

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Waste Package Project

Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposal Waste Packages: Effects of Updated Design and Rates

Document Identifier: CAL-EDC-MD-000015 REV00

Page 17 of 119

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5. CALCULATION

The calculations begin with selection of data for compositions, amounts, surface areas, and reaction rates of the various components of Fermi WPs. These quantities are converted to the form required for entry into EQ6. For example, weight percentages of elements or component oxides are converted to moles of elements per 100g of WP component; degradation rates in μ m/y are converted to moles/(cm²·s), etc. The final part of the input to EQ6 consists of the composition of incoming water (Section 5.1.3) together with a rate of influx to the WP that corresponds to suitably chosen percolation rates into a drift and drip rate (Section 5.1.4) into a WP. The EQ6 output provides the results of the chemical degradation calculations for the WP or components thereof. In selected cases, the degradation of the WP is divided into phases. In the first of these cases, degradation of HLW glass takes place before breach of the DOE canister and subsequent exposure of the Fermi fuel to water. The second scenario assumes that all WP components are breached except for the GPCs. The results include the compositions and amounts of solid products and of elements dissolved in solution. Details of the results are presented in Section 6.

When "time" or "years" are discussed in the calculation, this refers to the time or years after the WP has been breached, allowing water to enter. In all tables from this document, the number of digits reported does not necessarily reflect the accuracy or precision of the calculation. In most tables, two to four digits after the decimal place have been retained to prevent round-off errors in subsequent calculations.

5.1 CALCULATION INPUTS

5.1.1 WP Materials and Performance Parameters

This section (Section 5) provides a brief overview of the physical and chemical characteristics of Fermi WPs, and describes how the WP is represented in the EQ6 inputs. With the exception of the addition of the 316NG stainless steel inner sleeve, all the WP internals in this calculation are the same as the previous calculation (Ref. 32). The conversion of the WP physical description into parameters suitable for the EQ6 input files is performed by the spreadsheets "Fermi-IA-2001.xls" and "UenrichFermi.xls" (Attachment III). Additional details of the description may be found in Reference 9 (Section 3.1) and the references cited therein.

Material nomenclature used throughout this document includes: UNS N06625 and SA-240 S30403 (hereafter referred to as 304L), SA-516 (hereafter referred to as A516), SA-240 S31603 (hereafter referred to as 316L), and SA-240 S31603 nuclear grade stainless steel (hereafter referred to as 316NG stainless steel).

5.1.2 Physical and Chemical Form of the Enrico Fermi WP

It is convenient to consider the Enrico Fermi WP as several structural components:

- The outer shell constructed of Alloy 22.
- The inner sleeve (also called liner) constructed of 316NG stainless steel.

Waste Package Project	Calculation
Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposal	Waste Packages:
Effects of Updated Design and Rates	
Document Identifier: CAL-EDC-MD-000015 REV00	Page 18 of 119

- The "outer web", a carbon steel (A516) structural basket designed to hold the HLW glass pour canisters (GPCs) in place.
- The 5 GPCs, which consist of 304L canisters, filled with solidified HLW glass.
- A centrally located 316L stainless steel DOE canister with an internal 316L stainless steel basket.
- Filler material: A516 carbon steel and GdPO₄ shot
- The individual fuel assemblies
- The Al alloy shipping canisters.

The normalized moles (defined as 100 grams/mole for all components) and the normalized surface area of the 316NG inner sleeve were calculated in file "Fermi-IA-2001.xls" sheet "EDA2" (Attachment III). The term "normalized" means that the total moles and surface area for each component are divided by a normalization factor, which is the void volume of the WP. The normalization is necessary because EQ6 calculations are based on 1 liter of aqueous solution. The void volume was calculated to be 4102 liters (Ref. 47, Table 5-4). The normalized moles and surface area of the remaining components were calculated in file "Fermi-IA-2001.xls", sheet "normal" (Attachment III). Some of these initial values come from Reference 9 (Section 3.1) and spreadsheet "Fermi_Fuel_Kz.xls" in Reference 1, which is the electronic media for Reference 32.

Table 2 provides the normalized moles, surface areas, and densities for all of the major components in the Enrico Fermi codisposal WPs.

Table 3 provides a summary of the compositions of the principal alloys used in the calculations, along with a range of degradation rates. In the new calculation, the degradation rate for the A516 carbon steel is set to an average number for all runs. This average rate lies in between the average and high rates of the previous calculation. The "low" and "average" rates for the stainless steels are comparable to the "average" and "high" rates used in the earlier calculations (Ref. 32) (with corrections made for a molecular weight of 100g/mole in the current calculation). The "high" rates added to this calculation come from the *Waste Package Degradation Process Model Report* (Ref. 19, Fig. 3-15) and are much higher than the highest rate of 1 μ m/y used in the previous calculation (new rates are converted to EQ6 input format in Attachment III of Ref. 50).

Table 4 gives the simplified molar composition of the HLW glass used in the calculations. Several minor changes were made to these basic compositions to increase the efficiency of the calculations and to decrease the EQ6 run time. Principally, minor elements in the HLW glass, and other package materials compositions were removed or merged with chemically similar elements (e.g., Li was merged with Na in the glass composition). If the HLW glass composition is simplified, it can be entered as a "psuedo–mineral", GlassSRL, in the database. Entering the glass as a mineral reactant allows EQ6 to apply a pH-dependent degradation rate using the Transition State Theory formalism (Ref. 35, Section 3.3.3). Since neptunium (Np) and plutonium (Pu) made up only 1.1% of the total actinide content of the HLW glass, they were combined with

Waste Package Project	Calculation
Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposa	1 Waste Packages:
Effects of Updated Design and Rates	
Document Identifier: CAL-EDC-MD-000015 REV00	Page 19 of 119

U to further simplify the composition. EQ6 estimates of Pu and U loss from the WP are not greatly affected by the changes made to the elemental compositions of the HLW glass.

A pH-dependent rate for HLW glass degradation was derived from Reference 28 and Reference 46, Section 6.2.3.3, Equations 7 and 8. The glass rate based on Reference 28 is taken from Table 3 of Reference 20. The glass rate based on Reference 46 was normalized in "HLWglass-2001.xls" (Attachment III). The first rate mechanism (described with k_1) in Table 4 is dominant at pH values above 7, while the second rate mechanism (described with k_2) is dominant at pH values below 7. The high glass degradation rate constants in Table 4 are those predicted at 50°C, while the moderate rate constants are those derived for degradation at 25°C (Refs. 28 and 46, Sec. 6.2.3.3, Eq. 7 and 8).

All "rates" given in Table 3 through Table 6 are rate constants ($mol/cm^2 \cdot s$) which EQ6 multiplies by the normalized surface area (in cm^2) to derive a rate in moles per second for each WP component. Therefore, the true degradation rate of all WP components is highly dependent on surface area.

Table 5 summarizes the composition of the fuel used in this calculation. New rates come from Reference 48, Section 3.2.2 (converted to EQ6 format in "Fermi-IA-2001.xls", Attachment III).

Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposal Waste Packages: Effects of Updated Design and Rates

Document Identifier: CAL-EDC-MD-000015 REV00

Page 20 of 119

EQ6 Parameter	V	ρ	m;	sk
Reactant	Molar Volume (cm ³ /mol) ⁿ	Density (g/cm³)	Initial Moles °	Surface Area ^p (cm ²)
HLW Glass	35.09	2.85 ⁹	21.82 ^d	1228.5 ^b
Fresh U-Mo	5.739	17.242 ^j	1.227186 ^a	75.123 ^f
GdPO₄ Shot	20.00	5.00 ¹ 0.035135 ^e (0.07027) ^e		84.2552° (168.5104)°
A516 Shot	12.739	7.85 ^h	1.783567° (1.67655)°	2724.2515 [°] (2639.996) [°]
A516 Outer Web	12.739	7.85 ^h	9.269 ^d	120.0 ^d
A516 Impact Plates	12.739	7.85 ^h	0.2110 ^d	1.615 ^d
304L Glass Pour Canister	12.59	7.94 ⁱ	5.494 ^d	141.5 ^d
316L DOE SNF Canister	12.53	7.98 ⁱ	0.8592 ^d	22.67 ^d
316L Basket	12.53	7.98 ⁱ	0.9226 ^a	55.440 ^f
316NG Inner Shell	12.53	7.98 ⁱ	27.51 [°]	57.305346°
AI Alloy Shipping Canister	36.90	2.71 ^k	0.209885 ^a	55.4971 ^f
J-13 Water	N/A	1.0 ^m	N/A	N/A

Table 2. Properties of Materials in Enrico Fermi Codisposal WP

Source: ^a Ref. 1, spreadsheet "Fermi Fuel kz.xls", recalculated for molecular weight of 100g/mol in spreadsheet "Fermi-IA 2001.xls" (Attachment III).

b A HLW glass fracture factor of 21 (Ref. 49, p. 6-79) was used to adjust the values of HLW glass surface area from Ref. 47, Table 5-4 in spreadsheet "Fermi-IA-2001.xls" (Attachment III).

- Calculated in "Fermi-IA-2001.xls", sheet "EDA2" (Attachment III) from SK0200 REV 04 (Attachment II).
- Ref. 47, Table 5-4
- Calculated in "Fermi-IA-2001.xls" (Attachment III), parentheses are for values when the GdPO₄ content is doubled in Section 6.3.1.1
- Ref. 1, spreadsheet "Fermi Fuel kz.xls"
- ⁹ Ref. 43 (Based on range of HLW glass densities, p. 2.2.1.1-4)
- Ref. 33 (p. 9) Ref. 23 (p.7, Table XI) i
- j. Ref. 32, Table 5-4
- k Ref. 32, Table 5-2
- 1 Ref. 57, p. 413 (average density of monazite, See Assumption 3-21)

NOTES: ^m The density of a dilute solution is assumed to be 1.0 (Assumption 3.3).

- ⁿ Molar volume calculated by dividing the molecular weight (100g/mole) by density. ° To determine mass (g) of each reactant, multiply the normalized moles by 100
- g/mole and multiply by the normalization factor of 4102 liters.
- To determine the true surface area (cm²) of each reactant, multiply the normalized area by the normalization factor of 4102 liters.

Waste Package Project

Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposal Waste Packages: Effects of Updated Design and Rates

Document Identifier: CAL-EDC-MD-000015 REV00

Page 21 of 119

		i Carbon Steel	1	Stainless Steel		Stainless teel		i Stainless Steel	Al	Alloy
Element	wt% ^a	Moles/ 100g ^h	wt% ^b	Moles/ 100g ^h	wt% ^c	Moles/ 100g ^h	wt% ^d	Moles/ 100g ^h	wt%'	Moles/ 100g ^m
С	0.28	0.0233	0.03	0.002498	0.03	0.00250	0.02 ^j	0.001665	0	0
Mn	1.045	0.0190	2.00	0.036405	2.00	0.03640	2.00	0.036405	0.15	0.00273
Р	0.035	0.00113	0.045	0.001453	0.045	0.00145	0.045	0.001453	0	0
S	0.035	0.00109	0.03	0.000936	0.03	0.00094	0.03	0.000936	0	0
Si	0.29	0.0103	0.75	0.026704	1.00	0.03560	1.00	0.035606	0.6	0.02136
Cr	0	0	19.00	0.36541	17.00	0.32694	17.00	0.326948	0.195	0.00375
Ni	0	0	10.00	0.17039	12.00	0.20446	12.00	0.204464	0	0
Мо	0	0	0	0	2.50	0.02606	2.50	0.026058	0	0
N	0	0	0.10	0.007139	0.10	0.00714	0.08 ^j	0.005712	0	0
Fe	98.3	1.76	68.045	1.2184	65.295	1.16924	65.325	1.169756	0.7	0.01253
Zn	0	0	0	0	0	0	0	0	0.25	0.00382
Cu	0	0	0	0	0	0	0	0	0.275	0.00433
Mg	0	0	0	0	0	0	0	0	1.00	0.04114
Ti	0	0	0	0	0	0	0	0	0.15	0.00313
AI	0	0	0	0	0	0	0	0	96.68	3.58319
Total	100	1.8148	100	1.8294	100	1.8107	100	1.8090	100	3.6716
Rate	μm/y	Moles/ (cm²⋅s) ^k	μm/y	Moles/ (cm²⋅s) ^k	μ	m/y	Moles	s/ (cm²⋅s) ^k	Moles	/ (cm²⋅s) ⁱ
Low	Same as Avg	Same as Average	0.1 ^f	2.52E-14	0.1 ^f 2.53E-14		Same a	s Average		
Avg	72 ^e	1.79E-11	1 ⁿ	2.52E-13		1 ⁿ	2.	53E-13	2.5	4E-13
High	Same as Avg	Same as Average	34 ^g	8.656E-12		2 ⁹	5.0	56E-13	Same a	s average

Table 3. Steels Composition and Degradation Rates

Source: ^a Ref. 44 (p. 321, Table 1)

^b Ref. 34. (p. 3, Table 1)

^c Ref. 41 (p. 2, Table 1)

^d Ref. 41 (p.2, Table 1, 316 stainless steel base for 316NG)

^a Ref. 27 (pp. 2.2-96 through 2.2-98)

Ref. 26 (pp. 11-13)

^g Ref. 19 (Eq. 3-14 derived from Figure 3-15, 50th percentile value)

h Ref. 50 (Attachment III)

Ref. 18 (p. 603), converted to EQ6 format in Ref. 20 (Table 4)

^j Ref. 52 (p. 931)

Converted to values appropriate for input into EQ6 in Ref. 50 (Table 5-2)

Ref. 51 (p. 373)

^m Converted to values appropriate for input into EQ6 in "Fermi-IA-2001.xls" (Attachment III)

NOTE: ⁿ The average steel degradation rate was taken as 10 times the low rate.

Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposal Waste Packages: Effects of Updated Design and Rates Document Identifier: CAL-EDC-MD-000015 REV00

Page 22 of 119

Element	Moles/ 100g ^a			Comment		
0	2.7038					
U	0.0078					
Np	0	Mer	ged with U (~0.1% of a	actinides)		
Pu	0	Mer	ged with U (Pu ~1% a	ctinides)		
Ва	0.0011					
AI	0.0863					
S	0.0040					
Са	0.0162					
Р	0.0005					
Cr	0	Mer	ged with AI (overwhelr	ned by steel Cr; (Cr ₂ O ₃ similar to Al ₂ O ₃)	
Ni	0	Mer	ged with Fe			
Pb	0	Mer	ged with Ba (both form	n insoluble CrO₄ ⁼	compounds in EQ6 runs)	
Si	0.7765					
Ti	0	Mer	ged with Si (TiO ₂ simil	ar to SiO ₂)		
В	0.2912		_			
Li	0	Mer	ged with Na			
F	0.0017					
Cu	0	Mer	ged with Fe			
Fe	0.1722					
K.	0.0752					
Mg	0.0333					
Mn	0	Ме	rged with Fe			
Na	0.5767					
Cl	0	Removed (overwhelmed by CI in in-dripping water)				
	Total De	grad	ation Rate = k ₁ [H+] ^{-0.0}	⁴ + k ₂ [H+] ^{0.6} (mo	les/cm²⋅s)	
Low Rate	Constant (I	k1)	liter/(cm2·s)	8.858E-19 ^b	8.858E-19 ^c	
High Rate	e Constant (k1)	liter/(cm2⋅s)	1.076E-17 ^b	1.076E-17 ^c	
Low Rate	Constant (I	k ₂)	liter/(cm2·s)	7.976E-13 ^b	1.115E-11 ^c	
High Rate	e Constant (k2)	liter/(cm2-s)	4.874E-12 ^b	1.354E-10 ^c	

Table 4. Simplified Glass Composition and Degradation Rates

Source: ^a Simplified composition based on Ref. 16 (Attachment I, p. I-7). This is the composition added to the "data0.ymd" for the pseudo-mineral GlassSRL. One mole = 100g HLW glass.

^b Ref. 28; (Section 6.2.3, Equations 7 and 8); Converted to inputs for EQ6 in Ref. 20 (Table 3)

c Ref. 46: (Section 6.2.3, Equations 7 and 8); Converted to inputs for EQ6 in spreadsheet "HLWglass-2001.xis" (Attachment III)

Element		Composition				
Liement	wt% ^a	Moles/100g				
U	89.74	0.37701008				
Мо	10.26	0.1069492				
Rate	moles/(cm²⋅s) ^b	Basis				
Low	3.4601E-17	Extrapolation of temperature dependent rate regression of Ref. 48 to 25°C				
High	3.4601E-13	10,000 times low rate (according to Ref. 48)				

Table 5. Fermi Fuel Composition and Degradation Rates

NOTE: ^a Ref. 32, Table 5-4

^b Ref. 48, Section 3.2.2, recalculated in "Fermi-IA-2001.xls", sheet "rates" (Attachment III)

For the Enrico-Fermi fuel type, the Gd is added to the WP as $GdPO_4$ shot which is mixed with A516 carbon steel shot inside the 316L stainless steel basket structure within the DOE canister. Table 6 gives the composition of the $GdPO_4$ shot used in this calculation.

Table 6.	GdPO₄	Shot Com	position	and Degra	adation Rates

Element	Wt% ^a	Moles/100g ^b		
Р	12.280	0.3964772		
0	25.374	1.5859082		
Gd	62.346	0.3964771		
Rate	Moles/(cm ² ·s)	Basis		
Low	1.40E-16 ^c	Quartz degradation rate		
Medium	2.52E-14 ^d	304L stainless steel degradation rate		
High	1,798E-11 ^d	A516 carbon steel degradation rate		

Source: ^a Taken as similar to composition of monazite ((Ce,La,Nd,Th)PO₄), Ref. 57 (p. 413)

^b Calculated in "Fermi-IA-2001.xls", sheet "compositions"

^c Ref. 58 (Figure 2) and Ref. 59 (Tables I and III), converted to values appropriate for use in EQ6 in "Fermi-IA-2001 xls", Sheet "rates" (Attachment III) (See Assumption 3-22).

NOTE: ^d Due to the uncertainty in the degradation rate of GdPO₄, the low rate (based on quartz) was used in all EQ6 runs. The medium and high rates were used in sensitivity cases to test how dependent Gd retention is on the degradation rate.

Waste Package Project	Calculation
Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisp	oosal Waste Packages:
Effects of Updated Design and Rates	
Document Identifier: CAL-EDC-MD-000015 REV00	Page 24 of 119

5.1.3 Chemical Composition of Incoming Water

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1. 1. 1.

It was assumed that the water composition entering the WP would be the same as that for water from well J-13 (Assumption 3.1). This water has been analyzed repeatedly over a span of at least 20 years (Ref. 15, DTN: MO0006J13WTRCM.000). The composition of J-13 well water as used in this calculation has been adjusted slightly (see Assumptions 3.7 and 3.15). The concentration of Si (as listed in Ref. 15) had to be converted into a concentration in terms of $SiO_2(aq)$ for input into EQ3NR. The conversion was accomplished by the following:

 $[SiO_2(aq)] = [Si] \times M_{SiO_1} / M_{Si}$

where the square brackets indicate concentration (mg/liter), M indicates molecular weight, and the subscripts indicate the particular species.Based on the molecular weights of Si and O in Reference 12 and the concentration of Si in Reference 15, the concentration for $SiO_2(aq)$ is:

 $(28.5 \text{ mg/liter}) \times (28.0855 + 2 \times 15.9994) / (28.0855) = 60.97 \text{ mg/L}$

Table 7 and Table 8 contain the EQ3NR input file constraints for J-13 well water composition and the EQ6 input file elemental molal composition for J-13 well water used for this calculation.

The "Basis Species" column of Table 7 lists the chemical species names recognized by EQ3NR and EQ6. Since some of the components of J-13 well water, as analyzed (Ref. 15, DTN: MO0006J13WTRCM.000) are in a different chemical form than the species listed in this column, these components must be substituted or "switched" with the basis species for input into EQ6 and are listed in the "Basis Switch" column. Basis species listed as "Trace" in the "Basis Switch" column are not found in J-13 well water, as analyzed (Ref. 15), but are in the composition of other WP components and must be input at a trace concentration for numerical stability in EQ6 calculations.

Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposal Waste Packages: Effects of Updated Design and Rates

Document Identifier: CAL-EDC-MD-000015 REV00

Page 25 of 119

Basis Species	Basis Switch	Concentration ^a	Units
redox		-0.7 °	log fO ₂
Na+		45.8	mg/L
SiO ₂ (aq)		60.97	mg/L
Ca++		13.0	mg/L
K+		5.04	mg/L
Mg++		2.01	mg/L
H+		8.1 ^b	рН
HCO3-	CO ₂ (g)	-3°	log fCO ₂
F-		2.18	mg/L
CI-		7.14	mg/L
NO3-	NH ₃ (aq)	8.78	mg/L
SO4		18.4	mg/L
Al+++	Trace	1.000E-16	Molality
Mn++	Trace	1.000E-16	Molality
Fe++	Trace	1.000E-16	Molality
B(OH)₃(aq)	Trace	1.000E-16	Molality
HPO₄	Trace	1.000E-16	Molality
Ba++	Trace	1.000E-16	Molality
CrO ₄	Trace	1.000E-16	Molality
Cu++	Trace	1.000E-16	Molality
Gd+++	Trace	1.000E-16	Molality
MoO4	Trace	1.000E-16	Molality
Ni++	Trace	1.000E-16	Molality
Pu++++	Trace	1.000E-16	Molality
Ti(OH)₄(aq)	Trace	1.000E-16	Molality
UO ₂ ++	Trace	1.000E-16	Molality
Zn++	Trace	1.000E-16	Molality

Table 7. EQ3NR Input File Constraints for Incoming Water Composition

Source: ^a Ref. 15 (A trace concentration (1.000E-16 molal) is added for elements that are not in J-13 well water as analyzed, but are in the composition of the WP components, to ensure numerical stability in EQ3/6 runs.)

NOTES: ^b If log (fCO2) = -3, then EQ3NR calculates pH = 8.1 (Ref. 39, Table 7). See Assumption 3.7. ^c (Ref. 40, p. F-210) See Assumption 3.7.

The values in Table 7 were run through EQ3 to provide the values to be used in the EQ6 file (Table 8).

Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposal Waste Packages: Effects of Updated Design and Rates Document Identifier: CAL-EDC-MD-000015 REV00

Page 26 of 119

Element	Mole/Kg	Element	Mole/Kg
0	5.55E+01	Mg	8.27E-05
AI	1.00E-16	Mn	1.00E-16
В	1.00E-16	Мо	1.00E-16
Ва	1.00E-16	N	1.42E-04
Ca	3.24E-04	Na	1.99E-03
CI	2.01E-04	Ni	1.00E-16
Cr	1.00E-16	S	1.92E-04
F	1.15E-04	Si	1.02E-03
Fe	1.00E-16	U	1.00E-16
С	2.07E-03	к	1.29E-04
Н	1.11E+02	Gd	1.00E-16
Р	1.00E-16		

Table 8. EQ6 Input File Elemental Molal Composition for Incoming Water

NOTE: ^a These values are output from EQ3NR for input into EQ6 input files.

5.1.4 Drip Rate of Incoming Water

It is assumed (Assumption 3.11) that the drip rate onto a WP is the same as the rate at which water flows through the WP. The drip rate is taken from a correlation between percolation flux and drip rate, also called mean seep flow rate (Ref. 10, Figure 3.2-15). A range of drip rates was chosen. Specifically, values of 0.0015, 0.015, and 0.15 m³/year were used for most cases, corresponding to percolation fluxes ranging from about 10 mm/year to 80 mm/year. The value of 10 mm/year corresponds to a high infiltration rate for the present-day climate and 80 mm/year corresponds to about twice the high infiltration rate for the glacial-transition climate (Ref. 10, Table 3.2-2). [Table 3.2-2 of Ref. 10 gives values of net infiltration rate, rather than percolation flux; however, they are equal at the potential repository level (Ref. 10, Section 3.2.3.4, p. 3-33)].

Drip Rate (m³/year)	Drip Rate (normalized for EQ6 input) (moles/s) ^a
0.0015	1.16E-11
0.015	1.16E-10
0.15	1.16E-09

Table 9. I	Drip	Rate	Values	for	Input	to	EQ6
------------	------	------	--------	-----	-------	----	-----

NOTE: ^a The values of drip rate in units of m³/year are multiplied by 1000 liters/m³, divided by 1 liter/mole, divided by 365.25 days/year, divided by 86,400 s/day, and divided by 4102 liters of void volume in the WP.

Waste Package Project	Calculation
Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposal	Waste Packages:
Effects of Updated Design and Rates	•
Document Identifier: CAL-EDC-MD-000015 REV00	Page 27 of 119

5.1.5 Densities and Molecular Weights of Solids

EQ6 calculates total mineral volumes, using the molar volume values (V0PrTr) embedded in the EQ3/6 data0 file ("data0.ymd", Attachment III). The mineral volumes are printed to EQ6 output files with endings such as "elem_min.txt" and "min_info.txt". The mineral volumes are used to calculate corrosion product density ("S+A.xls" and "S+A sensitivity.xls", Attachment III) for Section 6 of this report. For many solids that are in the EQ6 database, the molar volumes are not available. These solids are flagged in the database with fictitious molar volumes of "500". Version 7.2bLV of EQ6 ignores the minerals with a molar volume of "500" when it calculates the total mineral volume. For the current study, the data0 file contains valid molar volume entries for the solids that comprise the vast bulk of the volume, such as hematite, nontronite, trevorite, and pyrolusite. Molar volumes have also been added for several minerals as outlined in Section 5.1.7; therefore, the error in the density calculations due to a lack of molar volumes for the minor minerals is minimal.

5.1.6 Atomic Weights

Atomic weights were taken from Reference 11 and Reference 12.

5.1.7 Thermodynamic Database

The thermodynamic database used for the EQ6 calculations, "data0.ymd", (Attachment III) is a slightly altered version of the qualified database "data0.ymp" (Ref. 3). Adjustments made to the database do not negatively impact the calculations. For further explanation of changes to the database, see Reference 50, Section 5.1.7, and Reference 53, Section 5.1.7.

The database used in Reference 32 was "data0.nuc". Several changes have been made to the qualified database (Ref. 3), which were not in the "nuc" database. Some of these include changes to U bearing minerals such that those with questionable thermodynamic data were removed. The Log K was also changed for several minerals including soddyite. This has the net effect of allowing different U minerals to form in the WP for the current calculation than those formed in Reference 32.

5.1.8 Data Conversion

The data presented in Section 6 are transformed into EQ3/6 format by converting weight percents into moles per 100g; normalizing surface areas, volumes, and moles to one liter reactive water in the system; and converting rate constants to moles/(cm²·s). In Section 6, the "moles" in plots are for the sub-sampled (one liter fluid) EQ6 system for all EQ6 solid special reactants. To obtain the actual mass (g) of a reactant in the WP, multiply *plotted* moles by (100 g/mole)·(4102 liters void space in the WP). To obtain the actual mass of a mineral in the WP, multiply *plotted* moles by (mineral molecular weight)·(4102 liters void space in the WP). The mineral molecular weights are given in the EQ3/6 database ("data0.ymd"), which is included in the electronic file distribution for this document (Attachment III).

· · · · ·

Document Identifier: CAL-EDC-MD-000015 REV00

Page 28 of 119

5.1.9 Suppressed Minerals

The following minerals were suppressed (not allowed to form) in <u>all</u> EQ6 runs:

Quartz	Celadonite	Dolomite-ord
Tridymite	Dolomite	Annite
Muscovite	Dolomite-dis	Phlogopite
BaZrO ₃	CaZrO ₃	

The micas (muscovite, annite, and phlogopite) and celadonite are high temperature minerals that, although thermodynamically favored to form at the low 25°C temperature expected for the proposed repository, rarely do. Dolomite growth is also rarely seen at 25°C, so it was also suppressed. The more stable quartz and tridymite were suppressed because repository waters are often supersaturated with respect to quartz, suggesting that if it is growing near the repository horizon, it is doing so slowly. The Zr minerals are carryovers from the previous calculation (Ref. 32). BaZrO₃ was removed from the current database due to suspicions about data quality. CaZrO₃ remains in the database but is still suppressed because it is not known to form at low temperatures

In several runs, the iron (Fe) mineral hematite (Fe_2O_3) was suppressed to observe the effects that the precipitation of the most thermodynamically stable Fe mineral has on the loss of materials from the WP.

5.2 EQ6 CALCULATIONS

5.2.1 Scenarios Considered

The rationale for selection of scenarios in EQ6 simulations is to provide conservative criticality assessments of solubility and transport of fissile materials (i.e., U compounds) and criticality control materials (Gd, the neutron absorber) from the WP. An internal criticality event is possible if fissile material remains behind in the WP while neutron absorbers are flushed out.

The "Disposal Criticality Analysis Methodology Topical Report" document defines the internal and external degradation scenarios for disposal criticality analysis (Ref. 22, pp. 3-8 through 3-16). The internal degradation configurations are based on the assumption that groundwater drips onto the upper surface of the WP and penetrates it. Groundwater accumulates inside the WP, which could dissolve and flush the SNF from the WP. The following is a summary of three groups of degradation configurations from Reference 22:

• WP internals degrade faster than the waste forms

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- WP internals degrade at the same rate as the waste form
- WP internals degrade slower than the waste forms.

The WP internals include all components within the WP, except SNF. The waste forms refer to Enrico Fermi SNF and HLW glass. The above configurations set the framework in which EQ6

Waste Package Project	Calculation
Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codispos	sal Waste Packages:
Effects of Updated Design and Rates	
Document Identifier: CAL-EDC-MD-000015 REV00	Page 29 of 119

scenarios could be developed.

The proposed criticality control material (Gd) is incorporated into GdPO₄ shot. Degradation of the GdPO₄ shot is expected to yield varied amounts of (1) aqueous (dissolved) Gd and (2) a solid Gd phosphate, possibly GdPO₄·10H₂O. Gadolinium phosphate is sparingly soluble in neutral solutions, though the solubility does increase at low and high pH (Ref. 4, Section 5.3.1). Formation of GdPO₄·10H₂O is expected to be the controlling solid phase because of the amount of phosphate from degrading stainless steel and HLW glass. Dissolution of solid Gd carbonates and phosphates, at high pH, is also enhanced by dissolved carbonate. Uranium is also quite soluble in the alkaline, carbonate-rich solutions produced when HLW glass degrades. Thus the matrix of EQ6 calculations should include scenarios that may yield both low pH and high pH conditions, particularly high pH with high dissolved carbonate.

Low-pH conditions are likely to occur when the stainless steel of the inner sleeve degrades separately from the HLW glass. To obtain sustained, low-pH conditions it is generally necessary to break the degradation process into two stages. The first stage involves an early breach of the 304L stainless steel canisters holding the HLW glass, followed by fast degradation of the HLW glass and removal of the alkaline components during a period of relatively high drip rate. In the second stage, the 316L DOE canister holding the fuel assemblies is allowed to breach, exposing some portion of the fuel to acid conditions. To keep the pH low, the drip rate must be reduced for the second stage.

Another way to sustain a low pH is to assume that the DOE canister is breached and the 304L GPCs are not. The first stage involves early breach of the DOE SNF canister. The degradation of the stainless steels causes the pH to drop below neutral. During the second stage, the 304L GPCs breach and the degradation of the HLW glass causes the pH to rise.

Thus, the reaction scenarios can be divided into two general categories:

Single-Stage Cases – in these calculations, all reactants (steels, HLW glass, and fissile materials) are *exposed* simultaneously to the water in the WP. Because the reaction rates of the materials in the WP may vary greatly, all materials do not necessarily *degrade* simultaneously. These cases correspond to an extreme where the fuel is exposed to degradation immediately. These cases result in the highest dissolved radionuclide levels, and might provide the most conservative estimate of fissile material loss.

Two-Stage Cases – Involve breaking up the case into stages where different components are degraded separately from one another.

<u>Scenario I</u> – In the first stage, the A516 outer web (basket) and the GPCs (HLW glass and 304L steel) are first exposed to water, until the HLW glass is completely degraded and its alkalinity largely flushed out of the system. The first stage is actually run twice; once up to approximately three times as long as is required to degrade the HLW glass, in order to locate the true pH minimum; and it is run a second time, just to the commencement of the low-pH plateau, to create an EQ6 pickup file for the second stage. This repetitive process ensures that the maximum acidity will be achieved in the second stage. In the second stage, the contents of the DOE canister are added as reactants. The aim of the Type I two-stage runs is to force a "conservative" condition of high acidity, by degrading the HLW glass rapidly, before all the acid-producing

Waste Package Project	Calculation
Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codispo	sal Waste Packages:
Effects of Updated Design and Rates	
Document Identifier: CAL-EDC-MD-000015 REV00	Page 30 of 119

steel is degraded. The early HLW glass degradation and flushing requires very high HLW glass degradation rates; the total effective rate of the HLW glass is further increased by considering cracks as part of the total surface area. These high HLW glass degradation rates, if used with a slow flush rate, can produce unreasonably high ionic strengths (>1); such high ionic strengths are beyond the applicability of EQ3/6's "B-Dot" activity coefficient corrections.

<u>Scenario II</u> - In the first stage all of the WP components are exposed to degradation except for the HLW glass. Once the GPCs are approximately 2/3 consumed, stage two begins with the addition of the HLW glass to the system. The aim of the Scenario II cases is to force a condition of high acidity by excluding the HLW glass from the system in stage one. The high acidity causes most of the U in the system to precipitate out of solution into minerals. When stage two begins and the glass starts to degrade, the pH of the system will rise to basic levels causing the U minerals to dissolve. Since most of the U in solution is from the fuel, the enrichment fraction of the solution during this time period should be very high. In the extremely acidic condition (pH of 3 to 4) during the first stage, Gd minerals are unstable, and dissolve causing loss of Gd from the WP.

5.2.2 EQ6 Case Nomenclature

This study included 20 single-stage cases (including 3 source term cases) and 8 two-stage cases (including 3 source term cases), with varied combinations of steel, HLW glass, and fuel degradation rates with differing water fluxes. The names for the EQ6 input files, corresponding to each run, consists of the file name with the extension ".6i". For example, the EQ6 input file name for Case 1 is nm1x1321.6i. These input files are included in Attachment III. Each EQ6 run has associated tab-delimited text files, also included in Attachment III. Most of the important run conditions could be inferred from the root-file name. For most cases, the root-filename is evaluated from left to right, as follows:

The first character "n" indicates Enrico Fermi DOE Owned Fuel

The second character has different meanings:

- "c" indicates that the log $fCO_2 = -2$ (log $fCO_2 = -3$ in all other cases)
- "m" for minor constituents of J-13 water taken as trace (for all cases that have another symbol for the second character, minor constituents are still set to trace)
- "g" indicates that hematite has been suppressed.
- "t" indicates that the total surface area of the 316NG liner was exposed to degradation instead of the usual assumption that only the inside is significantly exposed to degradation.
- "A" indicates the GdPO₄ degradation rate is the same as A516 carbon steel
- "L" indicates the GdPO₄ degradation rate is the same as 304L stainless steel

The <u>third</u> character is "1" for one-stage runs and first stage of a two-stage run. "2" indicates the second stage of two-stage runs.

Waste Package Project	Calculation
Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposal	Waste Packages:
Effects of Updated Design and Rates	_
Document Identifier: CAL-EDC-MD-000015 REV00	Page 31 of 119

The <u>fourth</u> character has different meanings:

- "n" indicates that the new glass rate from Reference 46 has been used (all other cases use the glass rate indicated in Reference 28).
- "d" indicates that the mass of the GdPO₄ in the WP was doubled.
- Because of the size of some files, the runs had to be divided among several input files to obtain a time of 6.34E+05 years. The fourth character indicates the subdivision by:
 - "x" first part
 - "y" second part
 - "z" third part

The <u>fifth</u> character is "1", "2", or "3" corresponding to "low", "average", and "high" steel degradation rates respectively.

The <u>sixth</u> character is "3" or "4" indicating a "low" or "high" pH-dependent glass degradation rate respectively. No glass exposed to the system is indicated with a "0".

The <u>seventh</u> character is indicative of the degradation rate of the fuel. "2" indicates the "low" degradation rate given in Table 5, and "3" indicates the "high" rate. No fuel exposed to the system is indicated with a "0".

The <u>eighth</u> character in the block indicates the choice of water flush rate, with "1", "2", and "3" indicating $0.0015 \text{ m}^3/\text{y}$, $0.015 \text{ m}^3/\text{y}$, and $0.15 \text{ m}^3/\text{ respectively}$.

Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposal Waste Packages: Effects of Updated Design and Rates

Document Identifier: CAL-EDC-MD-000015 REV00

Page 32 of 119

6. **RESULTS**

6.1 SUMMARY OF RESULTS

Technical product input information requiring confirmation may affect this document. Subsequent revisions will reflect any document changes occurring as a result of completing confirmation activities. A review of the DIRS database will confirm the status of the technical product input information.

6.1.1 Gd and U Retention: One-stage Runs

Table 10 through Table 12 summarize the total percentage of Gd and U moles retained at the end of the one-stage EQ6 runs and compare cases that are similar to those in Reference 32. Several new cases (e.g., those with fast steel rates) have no equivalent in the older calculation (Ref. 32).

Case	File Name	File Name (Previous Study) ^c	Gd Retention ~250,000 Years (Previous Study) ^c	Gd Retention ~250,000 Years ^d	Length of Run (Years)	Gd Retention at End of Run ^ª
1	nm1x1321	^b			634,350	100.00%
2	nm1x1331	N07_1111	99.50%	99.80%	634,370	99.77%
3	nm1(xy)1333	N06_1113	99.53%	97.20%	411,730	96.55%
4	nm1x2331	N10_2111	97.70%	99.60%	669,380	99.56%
5	nm1x2422				633,780	99.66%
6	nm1x2432	N12_2212	99.97%	99.50%	633,780	99.34%
7	nm1{xyz}3323				633,780	95.53%
8	nm1{xyz}3333		****		622,460	94.64%
9	nm1{xyz}3433				618,580	95.98%
10	ng1{xyz}3323	*****			633,780	95.42%

Table 10. Summary of Gd Retention ^e for One-stage	e EQ6 Runs
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NOTES: ^a Gd retention calculated at ~634,000 years in "fermi-losses.xls" (Attachment III).

^b All blank spaces represent no applicable data or not directly correlative.

^c From Ref. 32 (Table 5-9).

^d Calculated in "losses-oldtime.xls" (Attachment III).

* Retention of Gd is presented in percentage of total initial moles retained within the WP.

All cases run for this calculation predicted more than 94.5% Gd retention in the WP. As the drip rate increases, the loss of Gd also increases, but only slightly (up to 5%). For more information on effects of reactant rates on Gd loss, see Reference 53 (Section 6.2.8.1). The increased phosphorus (P) from the inner sleeve allows Gd retention even at lower pH values due to the formation of GdPO₄·10H₂O, a very low solubility compound. In comparable cases, Gd retention (at 250,000 years) closely parallels the older runs in Reference 32, Table 5-9. Since the cases from the older calculation were run out to only 250,000 years, it is unclear as to whether the levels of Gd in the WP would have remained high, or more losses would have been predicted over a longer time frame.

Waste Package Project	Calculation
Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisp	osal Waste Packages:
Effects of Updated Design and Rates	
Document Identifier: CAL-EDC-MD-000015 REV00	Page 33 of 119

When the "data0.nuc" database was used in Reference 32, the major Gd mineral to form during the degradation of the GdPO₄ shot was less hydrated than the Gd mineral that forms when "data0.ymd" (Ref. 3) is used (GdPO₄·H₂O versus GdPO₄·10H₂O). Reference 54, Section 6.8.3 shows that this difference in GdPO₄ hydration has no effect on Gd retention within the WP.

Case	File Name	Length of Run (Years)	% Fuel Left in the WP at End of Run ^a	% of Total U moles in the Fuelª	% of Glass in the WP at End of Run ^a
1	nm1x1321	634,350	95.76%	70.01%	46.33%
2	nm1x1331	634,370	0.00%	0.00%	48.36%
3	nm1(xy)1333	411,730	0.00%	0.00%	0.00%
4	nm1x2331	669,380	0.00%	0.00%	0.00%
5	nm1x2422	633,780	95.76%	70.01%	0.00%
6	nm1x2432	633,780	0.00%	0.00%	0.00%
7	nm1{xyz}3323	633,780	95.76%	70.01%	0.00%
8	nm1{xyz}3333	622,460	0.00%	0.00%	0.00%
9	nm1{xyz}3433	618,580	0.00%	0.00%	0.00%
10	ng1{xyz}3323	633,780	95.76%	70.01%	0.00%

Table 11. Summary of Intact Fuel and Glass in WP for One-stage EQ6 Runs

NOTES: ^a Calculated in spreadsheet "fermi-losses.xls" (Attachment III).

Table 12.	Summary of U Retention ^e for One-stage EQ6 Runs
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Case	File Name	File Name (Previous Study) ^c	U Retention ~250,000 Years (Previous Study) ^c	U Retention ∼250,000 Years ^d	Length of Run (Years)	U Retention at End of Run ^a
1	nm1x1321	b			634,350	99.82%
2	nm1x1331	N07_1111	86.03%	99.83%	634,370	99.60%
3	nm1(xy)1333	N06_1113	7.43%	75.43%	411,730	69.68%
4	nm1x2331	N10_2111	7.40%	0.00%	669,380	0.00%
5	nm1x2422				633,780	70.61%
6	nm1x2432	N12_2212	39.00%	0.00%	633,780	0.00%
7	nm1{xyz}3323				633,780	70.01%
8	nm1{xyz}3333				622,460	46.97%
9	nm1{xyz}3433				618,580	0.00%
10	ng1{xyz}3323				633,780	71.07%

NOTES: ^a U retention calculated in "fermi-losses.xls" (Attachment III). ^b All blank spaces represent no applicable data or not directly correlative.

^c From Ref. 32 (Table 5-9).

^d Calculated in "losses-oldtime.xls" (Attachment III).

* Retention of U is presented in percentage of total initial moles retained within the WP.

Waste Package Project	Calculation
Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codi	sposal Waste Packages:
Effects of Updated Design and Rates	
Document Identifier: CAL-EDC-MD-000015 REV00	Page 34 of 119

Retention of U ranges from 99.82% to 0.00 (at the end of the one-stage runs). Uranium retention stems primarily from the formation of 5 major U-bearing minerals including: $(UO_2)_3(PO_4)_2.6H_2O$; α -uranophane (Ca(UO_2SiO_3OH)_2.5H_2O); CaUO_4; schoepite (UO_3.2H_2O); and Na-boltwoodite (NaUO_2SiO_3OH.1.5H_2O). In the previous study (Ref. 32), soddyite $((UO_2)_2SiO_4.2H_2O)$ is the only major U bearing mineral reported in the calculation, though haiweeite (Ca(UO)_2(Si_2O_5)_3.5H_2O), and Na_4UO_2(CO_3)_3 were probably also present as minor U minerals (Ref. 32, Section 5.1.7). The differences in U retention in the U-bearing minerals formed have to do with 3 changes made from the previous calculation. The first, and probably most important, change is the addition of the 316NG liner which significantly affects the chemistry (most notably, pH) of the system, especially at slower steel degradation rates, compared to the previous calculation. The second change is the database used in this calculation ("data0.ymd") which is a slightly altered version of the qualified database "data0.ymp" (Ref. 3). The previous calculation used the unqualified database "data0.nuc" (Attachment III). A third change worth mentioning is that the new calculation uses a pH dependent glass degradation rates.

Due to the large number of cases prepared for this calculation, only figures and tables for representative cases are presented in this calculation. The times used in all tables are indicative of periods of interest due to low or high pH, significant changes in aqueous U or Gd concentration, or when major components are completely degraded.

The results of Case 1 (nm1x1321), shown in Figure 1 and Table 13 and Table 14, demonstrate the consequences of WP degradation with a slow steel rate, slow pH dependant glass rate, slow fuel rate, and $0.0015 \text{ m}^3/\text{y}$ drip rate. The consequences include: changes in pH, variations in the dissolved U content of the water flushed from the WP, and the formation of solubility-controlling and space-filling materials and solid solutions. The pH of the system decreases with steel degradation followed by a slight increase when the 316L from the DOE canister and basket as well as the 304L from the GPCs are exhausted. Since the HLW glass is degrading slowly, the alkalinity from the glass is insufficient to neutralize the pH until all the steel is consumed at around 600,000 years when the 316NG liner is exhausted. The Mg and Ca carbonate minerals formed from the dissolution of HLW glass do not fully neutralize the acid produced from steel corrosion until this point. The steel degradation causes lower pH conditions due to the oxidation of the Cr and Mo released upon steel degradation. Since pH remains low for an extended time, much of the HLW glass (46.33%) remains intact.

Figure 1 also shows the concentration of aqueous U and the prominent mineral phases of this element. Phosphates, associated with increased phosphorus from the degradation of the 316NG liner, dominate in this case. Uranium retention is high (99.82%) because not only are conditions conducive to U-mineral formation, but 95.75% of the fuel (70% total U) and 46% of the glass (12.5% total U) remains intact. This accounts for 82.5% of the total U in the WP.

Waste Package Project

Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposal Waste Packages: Effects of Updated Design and Rates

Document Identifier: CAL-EDC-MD-000015 REV00

Page 35 of 119

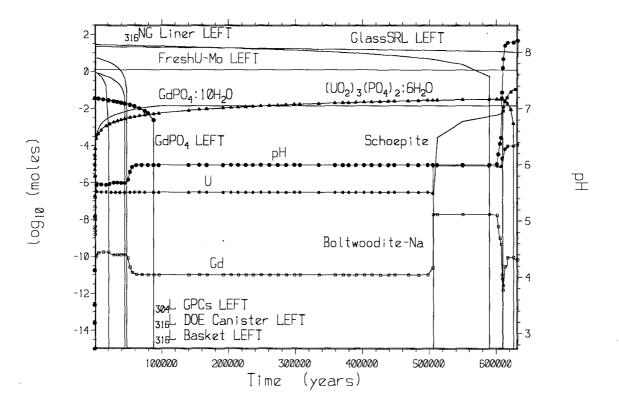


Figure 1. Case 1 (nm1x1321): WP Materials, Minerals, and Aqueous U

Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposal Waste Packages: Effects of Updated Design and Rates

Document Identifier: CAL-EDC-MD-000015 REV00

Page 36 of 119

Floment	Years				
Element	20844	505630	550280	610290	634350
0	6.79E+02	1.81E+03	1.91E+03	2.03E+03	2.08E+03
Al	2.13E+01	3.99E+01	4.16E+01	4.40E+01	4.75E+01
В	4.91E-15	6.55E-14	2.31E-13	0.00E+00	1.31E-09
Ва	6.40E-02	1.26E+00	1.37E+00	1.52E+00	1.75E+00
Са	3.54E-01	7.03E+00	7.65E+00	8.46E+00	9.58E+00
CI	0.00E+00	0.00E+00	0.00E+00	3.11E-15	0.00E+00
Cr	2.42E-02	4.78E-01	5.20E-01	1.80E-11	0.00E+00
Cu	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
F	0.00E+00	0.00E+00	0.00E+00	6.14E-03	7.47E-02
Fe	1.42E+03	3.19E+03	3.33E+03	3.49E+03	3.51E+03
Gd	4.84E-01	2.19E+00	2.19E+00	2.19E+00	2.19E+00
Н	1.94E+00	6.19E+00	6.58E+00	8.22E+00	7.83E+00
С	1.26E-13	0.00E+00	0.00E+00	1.33E-01	1.53E-01
Р	6.67E-01	2.11E+00	2.22E+00	2.34E+00	1.91E+00
К	0.00E+00	5.67E+00	6.20E+00	7.19E+00	1.10E+01
Mg	7.37E-02	5.55E+00	6.06E+00	6.79E+00	7.94E+00
Mn	2.10E+01	7.26E+01	7.67E+01	8.14E+01	8.14E+01
Мо	8.47E-01	1.68E+01	1.83E+01	1.98E+01	1.17E+01
N	0.00E+00	0.00E+00	0.00E+00	4.16E-16	0.00E+00
Na	0.00E+00	7.37E-01	7.98E-01	2.42E+00	1.70E+01
Ni	5.85E+00	1.44E+02	1.57E+02	1.72E+02	1.72E+02
S	0.00E+00	0.00E+00	0.00E+00	3.33E-13	0.00E+00
Si	1.70E+01	2.22E+02	2.40E+02	2.65E+02	2.98E+02
Ti	3.15E-02	3.15E-02	3.15E-02	3.15E-02	3.15E-02
U	9.51E-01	1.94E+01	2.10E+01	2.33E+01	2.61E+01
Zn	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Total (Kg)	529	1353	1420	1504	1532
Density (g/cm³)	5.04	4.71	4.70	4.67	4.62

Table 13. Case 1 (nm1x1321): Composition of Corrosion Products (g), Total Mass, and Density

NOTE: Mass (g) of each element is based on 1 liter aqueous fluid. To obtain total grams of each element in the WP, multiply by WP void volume of 4102 liters.

Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposal Waste Packages: Effects of Updated Design and Rates

Document Identifier: CAL-EDC-MD-000015 REV00

Page 37 of 119

	Years				
Element	20844	505630	550280	610290	634350
AI	1.03E-05	2.23E-06	2.16E-06	3.26E-08	1.14E-07
В	1.51E-02	1.31E-02	1.30E-02	1.80E-02	5.28E-02
Ва	8.96E-07	4.65E-07	4.65E-07	6.48E-08	5.81E-09
Са	9.29E-05	1.14E-04	1.14E-04	5.63E-04	1.69E-05
CI	2.01E-04	2.01E-04	2.01E-04	2.01E-04	2.01E-04
Cr	2.09E-01	4.09E-02	4.09E-02	9.73E-03	3.15E-07
Cu	2.84E-07	1.00E-16	1.00E-16	1.00E-16	1.00E-16
F	2.03E-04	1.91E-04	1.91E-04	1.39E-13	2.35E-14
Fe	1.01E-11	4.42E-12	4.42E-12	1.17E-12	1.16E-12
Gd	1.69E-10	2.37E-11	1.84E-08	1.46E-12	6.72E-11
С	4.03E-05	5.28E-05	5.36E-05	8.70E-04	3.43E-03
Р	1.59E-05	1.28E-05	3.44E-08	1.87E-05	1.44E-03
К	4.02E-03	2.66E-03	2.66E-03	1.83E-03	2.03E-03
Mg	2.08E-03	2.81E-04	2.81E-04	1.33E-04	4.59E-04
Mn	1.34E-10	1.61E-11	1.61E-11	6.14E-15	7.43E-16
Мо	6.66E-03	2.35E-03	2.35E-03	3.98E-04	9.29E-03
N	4.27E-03	8.56E-04	8.56E-04	1.62E-04	1.42E-04
Na	3.18E-02	2.77E-02	2.77E-02	1.93E-02	2.96E-02
Ni	1.00E-01	1.20E-02	1.20E-02	4.53E-06	3.75E-07
S	9.66E-04	4.88E-04	4.88E-04	4.49E-04	9.17E-04
Si	5.66E-05	5.66E-05	5.66E-05	4.22E-05	3.96E-05
Ti	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
U	2.89E-07	2.53E-07	7.73E-06	1.16E-05	1.08E-04
Zn	1.81E-07	1.00E-16	1.00E-16	1.00E-16	1.00E-16
рН	5.64	6.00	6.00	7.65	8.21

Table 14. Case 1 (nm1x1321): Solution Composition in Molality

Waste Package Project	Calculation
Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Cod	lisposal Waste Packages:
Effects of Updated Design and Rates	
Document Identifier: CAL-EDC-MD-000015 REV00	Page 38 of 119

Case 2 (nm1x1331), shown in Figure 2 and Table 15 and Table 16, demonstrates the consequences of WP component degradation when the conditions of Case 1 are combined with a fast fuel degradation rate. There is little effect on pH and the retention of Gd and U change very little. The major difference is that the density of the "sludge" formed in the WP increases slightly due to the increased amount of heavy elements added to the system by the completely degraded fuel. Once again, nearly half of the HLW glass remains intact due to the sustained low pH during most of the run.

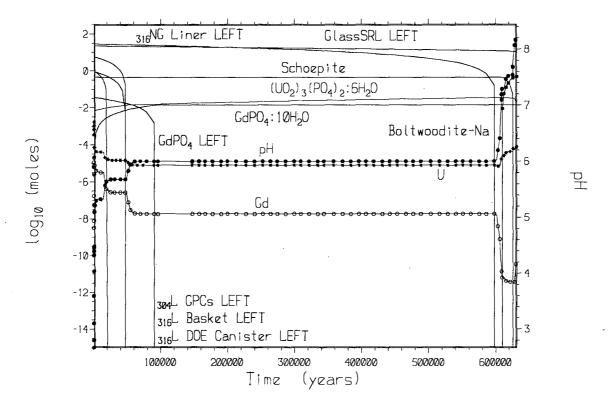


Figure 2. Case 2 (nm1x1331): WP Materials, Minerals, and Aqueous U

Uranium retention for Case 2 (at 250,000 years) is 13% (total U) higher than Case 3 (N07_1111) of Reference 32. This is due to the early rise in pH to almost 9 at 100,000 years in old Case 3. Since U minerals are highly soluble at higher pH values, more U (in the form of stable carbonate and hydroxyl complexes in solution) is lost from the WP. The addition of the 316NG liner in the current calculation keeps the pH low (around 6) until late in the run. Because of this lower pH, more U-bearing minerals are able to form and the U is retained in the WP.

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Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposal Waste Packages: Effects of Updated Design and Rates

Document Identifier: CAL-EDC-MD-000015 REV00

Page 39 of 119

Element	Years					
Element	28306	91461	628190	634370		
0	7.61E+02	9.81E+02	2.09E+03	2.10E+03		
AI	2.18E+01	2.43E+01	4.56E+01	4.65E+01		
В	2.86E-13	6.92E-13	1.40E-11	0.00E+00		
Ba	9.57E-02	2.58E-01	1.63E+00	1.69E+00		
Ca	5.39E-01	1.42E+00	9.03E+00	9.30E+00		
CI	0.00E+00	0.00E+00	0.00E+00	1.16E-12		
Cr	3.62E-02	9.76E-02	0.00E+00	8.05E-14		
Cu	0.00E+00	0.00E+00	0.00E+00	0.00E+00		
F	0.00E+00	0.00E+00	4.03E-02	5.75E-02		
Fe	1.51E+03	1.89E+03	3.50E+03	3.50E+03		
Gd	6.53E-01	2.12E+00	2.19E+00	2.19E+00		
н	3.60E+00	4.39E+00	1.02E+01	9.79E+00		
С	0.00E+00	0.00E+00	1.42E-01	1.47E-01		
Р	8.00E-01	1.35E+00	2.56E+00	2.49E+00		
К	0.00E+00	7.97E-01	9.00E+00	9.94E+00		
Mg	8.77E-03	7.78E-01	7.31E+00	7.61E+00		
Mn	2.36E+01	3.47E+01	8.14E+01	8.14E+01		
Мо	1.29E+00	3.41E+00	1.88E+01	1.73E+01		
N	0.00E+00	0.00E+00	0.00E+00	8.43E-15		
Na	0.00E+00	2.29E-01	1.02E+01	1.42E+01		
Ni	2.89E+00	1.91E+01	1.68E+02	1.68E+02		
S	0.00E+00	0.00E+00	0.00E+00	2.02E-10		
Si	2.29E+01	5.21E+01	2.80E+02	2.89E+02		
Ti	3.15E-02	3.15E-02	3.15E-02	3.15E-02		
U	1.11E+02	1.13E+02	1.30E+02	1.30E+02		
Zn	0.00E+00	0.00E+00	0.00E+00	0.00E+00		
Total (Kg)	600	762	1552	1559		
Density (g/cm ³)	5.02	4.95	4.65	4.64		

Table 15. Case 2 (nm1x1331): Composition of Corrosion Products (g), Total Mass, and Density

NOTE: Mass (g) of each element is based on 1 liter aqueous fluid. To obtain total grams of each element in the WP, multiply by WP void volume of 4102 liters.

Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposal Waste Packages: Effects of Updated Design and Rates

Document Identifier: CAL-EDC-MD-000015 REV00

Page 40 of 119

Flowert	Years					
Element	28306	91461	628190	634370		
AI	8.48E-06	2.16E-06	5.45E-08	1.00E-07		
В	1.48E-02	1.31E-02	3.12E-02	4.84E-02		
Ba	8.16E-07	4.64E-07	1.49E-08	6.65E-09		
Ca	1.43E-04	1.15E-04	5.70E-05	2.02E-05		
CI	2.01E-04	2.01E-04	2.01E-04	2.01E-04		
Cr	1.72E-01	4.09E-02	8.77E-06	7.34E-07		
Cu	1.49E-08	1.00E-16	1.00E-16	1.00E-16		
F	2.01E-04	1.91E-04	3.08E-12	2.04E-14		
Fe	9.10E-12	4.42E-12	1.14E-12	1.15E-12		
Gd	2.54E-07	1.84E-08	1.85E-12	3.32E-11		
С	4.22E-05	5.36E-05	1.51E-03	2.91E-03		
Р	2.41E-08	3.44E-08	1.95E-05	8.88E-04		
К	3.96E-03	2.66E-03	9.10E-04	1.98E-03		
Mg	1.56E-03	2.81E-04	3.34E-05	2.11E-04		
Mn	1.05E-10	1.60E-11	1.52E-15	7.97E-16		
Мо	3.87E-03	2.32E-03	1.05E-03	6.16E-03		
Ν	3.45E-03	8.56E-04	1.42E-04	1.42E-04		
Na	3.13E-02	2.77E-02	5.68E-03	2.10E-02		
Ni	7.88E-02	1.20E-02	1.03E-06	4.36E-07		
S	8.53E-04	4.88E-04	6.20E-04	8.57E-04		
Si	5.68E-05	5.66E-05	4.25E-05	4.01E-05		
Ti	0.00E+00	0.00E+00	0.00E+00	0.00E+00		
U	1.40E-05	7.73E-06	5.25E-05	7.54E-05		
Zn	1.32E-08	1.00E-16	1.00E-16	1.00E-16		
рН	5.68	6.00	7.91	8.16		

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Table 16. Case 2 (nm1x1331): Solution Composition in Molality

Waste Package Project	Calculation
Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codispo	sal Waste Packages:
Effects of Updated Design and Rates	
Document Identifier: CAL-EDC-MD-000015 REV00	Page 41 of 119

Case 3 (nm1(xy)1333), shown in Figure 3 and in Table 17 and Table 18, demonstrates WP component degradation for the same conditions as Case 2, except with a drip rate 100 times faster. There is a strong effect on pH and U retention. When drip rate increases, pH rises since the acid released during the degradation of the steel will be flushed out of the WP. As the pH increases, the degradation of the HLW glass also increases allowing for a slightly basic (rather than slightly acidic) solution inside the WP. The higher pH in this case (~8.1) compared to that of Case 2 (~6.4) allows the loss of 30% more total U from the WP. The effect on Gd retention is minor. The GdPO₄·10H₂O, although very stable, undergoes slightly more dissolution as the fluid within the WP changes from acidic to alkaline conditions at around 50,000 years. The result is 3% more loss of the total Gd in the package.

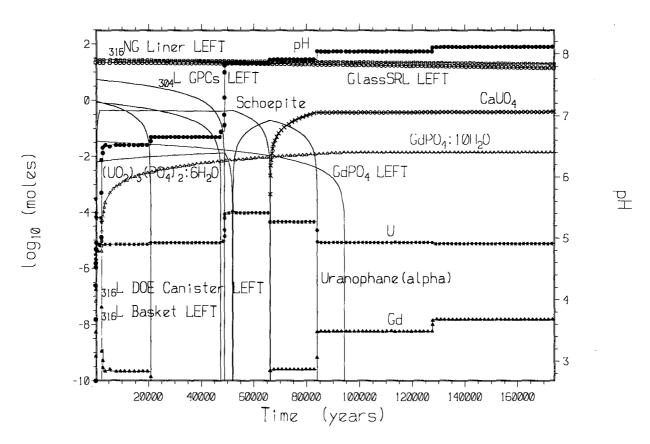


Figure 3. Case 3 (nm1{xy}1333): WP Materials, Minerals, and Aqueous U

Uranium retention for Case 3 (at 250,000 years) is 68%, total U, higher than Case 2 (N06_1113) of Reference 32 due primarily to the early rise in pH to 8.4 at approximately 50,000 years in old Case 2. The slightly lower pH (8.1) for Case 3 of the current calculation allows more U to remain in minerals, thus, more U is retained within the WP. The slightly lower pH is due to the presence

Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposal Waste Pac	kages:
Effects of Updated Design and Rates	
Document Identifier: CAL-EDC-MD-000015 REV00Page 42	of 119

of the degrading 316NG liner. Like the other stainless steels, the oxidation of Cr and Mo released from the 316NG liner helps keep the pH slightly lower, even with the high flush rate.

Element	Years					
Liement	2905	23280	52034	174160	411730	
0	5.88E+02	7.68E+02	9.79E+02	1.56E+03	2.71E+03	
AI	2.04E+01	2.13E+01	2.28E+01	3.89E+01	7.10E+01	
В	0.00E+00	6.41E-15	0.00E+00	5.46E-14	0.00E+00	
Ва	4.59E-15	0.00E+00	2.28E-02	1.06E+00	3.14E+00	
Са	1.07E+00	2.63E+00	6.78E+00	3.70E+01	6.52E+01	
CI	9.85E-14	0.00E+00	0.00E+00	0.00E+00	8.67E-16	
Cr	2.17E-09	0.00E+00	0.00E+00	0.00E+00	1.52E-12	
Cu	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	
F	9.39E-13	0.00E+00	1.68E-01	2.40E-01	3.84E-01	
Fe	1.15E+03	1.45E+03	1.76E+03	2.20E+03	3.04E+03	
Gd	1.79E-02	4.91E-01	1.16E+00	2.14E+00	2.12E+00	
Н	4.23E+00	4.69E+00	5.34E+00	8.01E+00	1.92E+01	
С	9.73E-12	0.00E+00	2.00E-03	9.30E-02	2.75E-01	
Р	4.27E-01	7.21E-01	1.05E+00	1.59E+00	2.30E+00	
К	2.64E-13	0.00E+00	3.18E-18	0.00E+00	1.90E-15	
Mg	1.07E-02	0.00E+00	3.54E-01	4.77E+00	7.79E+00	
Mn	1.31E+01	2.19E+01	3.11E+01	4.23E+01	6.40E+01	
Мо	1.22E+00	0.00E+00	0.00E+00	0.00E+00	2.40E-16	
N	1.84E-13	0.00E+00	1.14E-18	0.00E+00	8.04E-16	
Na	1.27E-12	0.00E+00	8.53E-02	2.43E+00	2.42E-14	
Ni	2.75E-01	2.36E+01	5.63E+01	1.23E+02	2.53E+02	
S	1.38E-11	0.00E+00	1.74E-18	0.00E+00	1.60E-13	
Si	9.04E+00	4.10E+01	8.73E+01	3.66E+02	8.98E+02	
Ti	3.15E-02	3.15E-02	3.15E-02	3.15E-02	3.15E-02	
U	1.09E+02	1.08E+02	1.05E+02	9.27E+01	1.05E+02	
Zn	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	
Total (Kg)	463	595	746	1090	1764	
Density (g/cm³)	4.99	4.90	4.81	4.34	3.97	

Table 17. Case 3 (nm1{xy}1333): Composition of Corrosion Products (g), Total Mass, and Density

NOTE: Mass (g) of each element is based on 1 liter aqueous fluid. To obtain total grams of each element in the WP, multiply by WP void volume of 4102 liters.

Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposal Waste Packages: Effects of Updated Design and Rates

Document Identifier: CAL-EDC-MD-000015 REV00

Page 43 of 119

F 1	Years					
Element	2905	23280	52034	174160	411730	
Al	3.17E-08	1.64E-08	5.17E-08	6.44E-08	1.03E-15	
В	1.41E-04	1.52E-04	3.94E-04	4.81E-04	1.00E-16	
Ва	5.34E-07	5.72E-07	1.37E-08	5.33E-09	1.16E-08	
Са	3.36E-04	2.65E-04	1.50E-05	2.60E-04	3.53E-04	
CI	2.01E-04	2.01E-04	2.01E-04	2.01E-04	2.01E-04	
Cr	2.09E-03	1.70E-03	4.09E-04	4.09E-04	4.09E-04	
Cu	1.00E-16	1.00E-16	1.00E-16	1.00E-16	1.00E-16	
F	1.16E-04	1.16E-04	1.16E-04	1.17E-04	1.14E-04	
Fe	1.92E-12	1.70E-12	1.14E-12	1.15E-12	1.14E-12	
Gd	2.18E-10	9.29E-11	3.00E-11	1.53E-08	7.29E-09	
С	9.19E-05	1.12E-04	1.47E-03	2.24E-03	1.49E-03	
Р	8.30E-08	1.12E-07	4.46E-07	2.55E-09	2.31E-09	
К	1.65E-04	1.68E-04	2.31E-04	2.53E-04	1.29E-04	
Mg	1.49E-04	1.00E-04	7.77E-06	1.35E-04	1.84E-04	
Mn	8.09E-13	4.24E-13	1.42E-15	6.79E-16	1.23E-15	
Mo	1.99E-04	4.55E-05	3.26E-05	3.26E-05	3.26E-05	
N	1.83E-04	1.74E-04	1.49E-04	1.49E-04	1.49E-04	
Na	2.27E-03	2.29E-03	2.93E-03	2.97E-03	1.99E-03	
Ni	6.05E-04	3.17E-04	9.80E-07	3.78E-07	8.28E-07	
S	1.99E-04	1.98E-04	1.98E-04	1.99E-04	1.93E-04	
Si	5.12E-05	5.02E-05	4.49E-05	3.94E-05	1.92E-04	
Ti	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	
υ	7.17E-06	8.19E-06	1.12E-04	7.50E-06	2.32E-06	
Zn	1.00E-16	1.00E-16	1.00E-16	1.00E-16	1.00E-16	
рН	6.52	6.66	7.90	8.12	7.94	

 Table 18. Case 3 (nm1{xy}1333): Solution Composition in Molality

Waste Package Project	Calculation
Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposa	1 Waste Packages:
Effects of Updated Design and Rates	
Document Identifier: CAL-EDC-MD-000015 REV00	Page 44 of 119

Case 4 (nm1x2331), shown in Figure 4 and in Table 19 and Table 20, demonstrates the general consequences of applying an average steel degradation rate to Case 2. In the EQ6 scenarios, higher steel and glass degradation rates must be combined with faster flushing rates or high ionic strengths can occur which are outside the valid range for the qualified EQ6 database (Ref. 3). Case 4 has a maximum ionic strength of 3.15 at around 5000 years, which is above the maximum valid ionic strength of 1.00. Sensitivity tests (Ref. 24, Section 5.1.2) have shown that at ionic strengths between 1.00 and 4.00, the "data0.ymp" (Ref. 3) database overestimates the solubility of Pu and U, which is conservative for external criticality. Cases that simulate ionic strength above 4.00 should not be used.

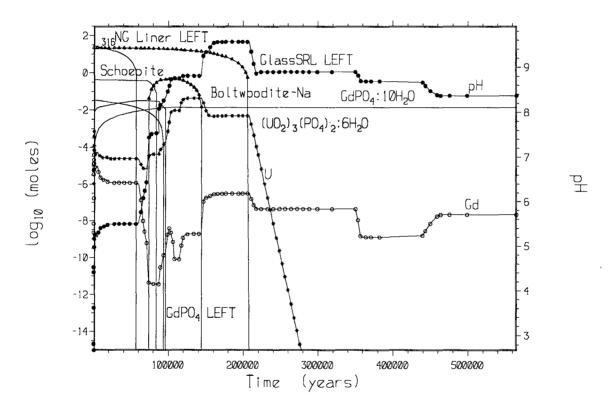


Figure 4. Case 4 (nm1x2331): WP Materials, Minerals, and Aqueous U

In cases such as this, where the steel degrades quickly and the glass slowly, the pH of the system becomes acidic until all steel within the WP is exhausted. Afterwards, the pH becomes basic and peaks while the glass is degrading. Since the pH peaks at around 9.6 for several thousand years, all U is lost from the WP. Some U is retained in runs having slow glass degradation and high drip rates since both parameters help keep the pH from exceeding 8.5.

Uranium retention for Case 4 (at 250,000 years) is 0.00% compared to 7.40% in Case 6 (N10_2111) of Reference 32. Both cases show a marked rise in pH at around 10,000 years when

Waste Package Project	Calculation
Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposal	Waste Packages:
Effects of Updated Design and Rates	
Document Identifier: CAL-EDC-MD-000015 REV00	Page 45 of 119
1 0	Page 45 of 119

the stainless steels are fully degraded. However, Case 6 (Ref. 32) has a constant HLW glass degradation rate compared to the pH dependant rate used in Case 4 of the current calculation. As mentioned before, when the pH increases, the rate of glass degradation also increases. For this reason, the pH in Case 4 peaks at 9.6 at 164,000 years. The pH in old Case 6 doesn't reach 9.0 until 250,000 years. Before this point, it remained at 8.4 for almost 90,000 years. The earlier high pH value in Case 4 causes more U to be lost from the WP earlier than the equivalent case (N10_2111) in Reference 32.

Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposal Waste Packages: Effects of Updated Design and Rates

Document Identifier: CAL-EDC-MD-000015 REV00

Page 46 of 119

Element	Years				
Element	87597	115700	357970	669380	
0	1.72E+03	1.81E+03	2.39E+03	2.39E+03	
AI	2.51E+01	3.10E+01	7.11E+01	7.11E+01	
В	1.35E-10	0.00E+00	0.00E+00	0.00E+00	
Ва	3.11E-01	6.89E-01	3.29E+00	3.29E+00	
Са	1.73E+00	3.49E+00	1.58E+01	1.70E+01	
CI	0.00E+00	4.97E-13	4.55E-16	0.00E+00	
Cr	0.00E+00	2.59E-19	0.00E+00	0.00E+00	
Cu	0.00E+00	0.00E+00	0.00E+00	0.00E+00	
F	3.27E-02	1.04E-01	1.57E-01	1.57E-01	
Fe	3.41E+03	3.44E+03	3.60E+03	3.60E+03	
Gd	2.03E+00	2.18E+00	2.18E+00	2.18E+00	
н	5.72E+00	5.29E+00	1.22E+01	1.17E+01	
С	2.72E-02	5.02E+00	2.88E-01	1.66E+00	
Р	2.39E+00	9.37E-01	1.20E+00	1.20E+00	
к	2.71E+00	9.53E+00	5.13E+01	4.54E+01	
Mg	1.33E+00	3.33E+00	1.74E+01	1.74E+01	
Mn	8.14E+01	8.14E+01	8.14E+01	8.14E+01	
Мо	1.55E+00	2.82E-17	0.00E+00	0.00E+00	
N	0.00E+00	2.09E-17	1.14E-18	0.00E+00	
Na	9.31E+00	2.82E+01	1.36E+01	7.14E+00	
Ni	2.41E+01	2.41E+01	2.41E+01	2.41E+01	
S	0.00E+00	8.27E-11	1.94E-14	0.00E+00	
Si	8.32E+01	1.38E+02	5.16E+02	5.19E+02	
Ti	3.15E-02	3.15E-02	3.15E-02	3.15E-02	
U	1.14E+02	1.05E+02	0.00E+00	0.00E+00	
Zn	0.00E+00	0.00E+00	0.00E+00	4.95E-13	
Total (Kg)	1337	1387	1658	1656	
Density (g/cm ³)	4.99	4.96	4.28	4.29	

Table 19. Case 4 (nm1x2331): Composition of Corrosion Products (g), Total Mass, and Density

NOTE: Mass (g) of each element is based on 1 liter aqueous fluid. To obtain total grams of each element in the WP, multiply by WP void volume of 4102 liters.

Waste Package Project	Calculation
Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposal	Waste Packages:
Effects of Updated Design and Rates	
Document Identifier: CAL-EDC-MD-000015 REV00	Page 47 of 119

Given that the pH reached 9 in the previous Case 6, the U present at 250,000 years should escape the WP in a few more thousand years. Therefore, the outcome of the two cases is identical, but the time it takes to reach 100% loss of U is different.

Element	Years				
Liement	87597	115700	357970	669380	
AI	2.45E-08	4.27E-07	2.06E-07	9.62E-08	
В	2.90E-02	8.69E-02	1.00E-16	1.00E-16	
Ва	8.45E-08	8.18E-10	4.61E-10	1.70E-09	
Са	2.62E-05	6.52E-07	3.72E-06	8.57E-05	
CI	2.01E-04	2.01E-04	2.01E-04	2.01E-04	
Cr	8.67E-06	1.14E-10	1.00E-16	1.00E-16	
Cu	1.00E-16	1.00E-16	1.00E-16	1.00E-16	
F	4.58E-06	5.81E-04	1.15E-04	1.15E-04	
Fe	1.18E-12	1.29E-12	1.24E-12	1.17E-12	
Gd	3.71E-12	8.03E-11	1.30E-09	2.16E-08	
С	6.56E-04	4.03E-02	8.68E-03	3.99E-03	
Р	1.85E-06	1.09E-04	1.10E-06	7.67E-09	
к	6.31E-04	1.15E-03	8.31E-04	1.70E-03	
Mg	1.52E-05	6.94E-05	2.93E-05	1.07E-04	
Mn	8.17E-15	9.56E-16	6.96E-16	4.65E-16	
Мо	2.30E-03	9.63E-07	1.00E-16	1.00E-16	
Ν	1.42E-04	1.42E-04	1.42E-04	1.42E-04	
Na	6.67E-03	7.99E-02	8.87E-03	2.78E-03	
Ni	5.98E-06	4.24E-08	3.02E-08	1.18E-07	
S	5.90E-04	1.38E-03	1.92E-04	1.92E-04	
Si	4.67E-05	5.14E-05	4.45E-05	3.96E-05	
Ti	0.00E+00	0.00E+00	0.00E+00	0.00E+00	
U	4.26E-05	9.23E-03	1.00E-16	1.00E-16	
Zn	1.00E-16	00E-16 1.00E-16 1.01E-15		1.27E-18	
Hq	7.54	8.75	8.69	8.37	

Table 20. Case 4 (nm1x2331): Solution Composition in Molality

Case 6 (nm1x2432), shown in Figure 5 and in Table 21 and Table 22, demonstrates the consequences of WP degradation with an average steel, fast fuel, and average drip rate combined with a high pH-dependent HLW glass degradation rate.

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Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposal Waste Packages: Effects of Updated Design and Rates

Document Identifier: CAL-EDC-MD-000015 REV00

Page 48 of 119

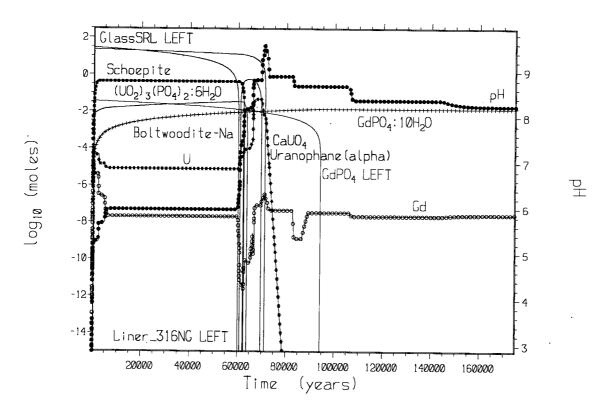


Figure 5. Case 6 (nm1x2432): WP Materials, Minerals, and Aqueous U

Once again, the pH is slightly acidic until all of the steel is degraded at 60,000 years. After this point, the pH increases from ~6.0 to ~9.6 over a period of 10,000 years. At this point, all of the HLW glass is degraded and, eventually, all U is lost from the WP due to the high solubility of U-minerals at the higher pH values.

Case 6 and Case 8 (Ref. 32) differ greatly. Case 6 from the current calculation loses all U from the WP within 80,000 years. On the other hand, Case 8 retains 39% of the U after 250,000 years. Again, the pH dependent versus independent rates of HLW glass degradation become a factor. For Case 6, all the fuel is degraded before the pH peak. At this pH peak, the HLW glass is also fully degraded. Prior to this point, all the U was in U-bearing minerals which are unstable at high pH values. As soon as the pH rose to around 8.8 the minerals dissolved and all the U was flushed from the WP. The constant glass rate in Case 8 (N12_1212, Ref. 32) also caused a pH high of 9.6, however, this occurred at only 1000 years into the run. After this point the pH drops rapidly to below 8 where U minerals can form. At the point where the pH drops, the fuel is still degrading, so about 1/3 of the U is retained within the WP.

Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposal Waste Packages: Effects of Updated Design and Rates

Document Identifier: CAL-EDC-MD-000015 REV00

Page 49 of 119

Element	Years					
Element	9360	62473	83355	107530	354250	633780
0	9.72E+02	2.05E+03	2.43E+03	2.43E+03	2.45E+03	2.49E+03
AI	2.38E+01	4.35E+01	7.11E+01	7.11E+01	7.11E+01	7.11E+01
В	3.52E-13	1.28E-15	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Ва	2.23E-01	1.49E+00	3.28E+00	3.28E+00	3.28E+00	3.28E+00
Ca	1.30E+00	8.47E+00	1.71E+01	1.81E+01	2.27E+01	2.59E+01
CI	0.00E+00	0.00E+00	4.05E-16	1.63E-17	0.00E+00	1.92E-18
Cr	8.46E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Cu	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
F	0.00E+00	3.70E-02	2.22E-01	2.22E-01	2.22E-01	2.22E-01
Fe	1.89E+03	3.49E+03	3.60E+03	3.60E+03	3.60E+03	3.60E+03
Gd	2.10E-01	1.44E+00	1.93E+00	2.18E+00	2.18E+00	2.18E+00
Н	4.04E+00	9.71E+00	1.25E+01	1.26E+01	1.29E+01	1.32E+01
С	0.00E+00	1.31E-01	2.87E-01	7.06E-01	2.87E-01	2.87E-01
Р	9.79E-01	2.40E+00	1.46E+00	1.51E+00	1.51E+00	1.51E+00
к	6.63E-01	8.32E+00	3.59E+01	3.33E+01	0.00E+00	0.00E+00
Mg	6.71E-01	6.82E+00	1.64E+01	1.65E+01	1.55E+01	1.40E+01
Mn	3.49E+01	8.14E+01	8.14E+01	8.14E+01	8.14E+01	8.14E+01
Мо	3.11E+00	1.78E+01	0.00E+00	0.00E+00	0.00E+00	0.00E+00
N	0.00E+00	0.00E+00	1.14E-18	3.80E-18	0.00E+00	0.00E+00
Na	1.69E-01	9.96E+00	2.20E+01	8.71E+00	7.95E+00	7.14E+00
Ni	1.54E+01	1.52E+02	1.52E+02	1.52E+02	1.52E+02	1.52E+02
S	0.00E+00	0.00E+00	1.71E-14	2.13E-15	0.00E+00	4.35E-18
Si	4.74E+01	2.61E+02	5.21E+02	5.23E+02	5.48E+02	5.76E+02
Ti	3.15E-02	3.15E-02	3.15E-02	3.15E-02	3.15E-02	3.15E-02
U	1.13E+02	1.28E+02	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Zn	0.00E+00	0.00E+00	0.00E+00	4.35E-13	0.00E+00	0.00E+00
Total (Kg)	758	1530	1699	1697	1701	1717
Density (g/cm³)	4.96	4.67	4.29	4.30	4.30	4.28

Table 21. Case 6 (nm1x2432): Composition of Corrosion Products (g), Total Mass, and Density

NOTE: Mass (g) of each element is based on 1 liter aqueous fluid. To obtain total grams of each element in the WP, multiply by WP void volume of 4102 liters.

Calculation

Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposal Waste Packages: Effects of Updated Design and Rates

Document Identifier: CAL-EDC-MD-000015 REV00

Page 50 of 119

Flowert	Years					
Element	9360	62473	83355	107530	354250	633780
AI	2.18E-06	5.28E-08	2.06E-07	9.61E-08	7.16E-08	7.16E-08
В	1.21E-02	3.65E-02	1.00E-16	1.00E-16	1.00E-16	1.00E-16
Ва	4.82E-07	1.61E-08	4.61E-10	1.70E-09	5.56E-09	5.56E-09
Ca	1.12E-04	6.23E-05	3.72E-06	8.56E-05	2.47E-04	2.47E-04
CI	2.01E-04	2.01E-04	2.01E-04	2.01E-04	2.01E-04	2.01E-04
Cr	4.09E-02	4.28E-05	1.00E-16	1.00E-16	1.00E-16	1.00E-16
Си	1.00E-16	1.00E-16	1.00E-16	1.00E-16	1.00E-16	1.00E-16
F	1.85E-04	2.99E-12	1.15E-04	1.15E-04	1.15E-04	1.15E-04
Fe	4.56E-12	1.14E-12	1.24E-12	1.17E-12	1.14E-12	1.14E-12
Gd	2.03E-08	1.83E-12	1.30E-09	2.16E-08	1.54E-08	1.54E-08
С	5.28E-05	1.46E-03	8.68E-03	3.99E-03	2.11E-03	2.11E-03
Р	3.35E-08	1.84E-05	1.10E-06	7.67E-09	2.21E-09	2.21E-09
к	2.48E-03	9.42E-04	8.31E-04	1.70E-03	1.29E-04	1.29E-04
Mg	2.43E-04	3.63E-05	2.93E-05	1.07E-04	1.43E-04	1.43E-04
Mn	1.74E-11	1.62E-15	6.96E-16	4.65E-16	6.93E-16	6.93E-16
Мо	2.38E-03	9.90E-04	1.00E-16	1.00E-16	1.00E-16	1.00E-16
N	8.56E-04	1.42E-04	1.42E-04	1.42E-04	1.42E-04	1.42E-04
Na	2.58E-02	5.88E-03	8.87E-03	2.78E-03	2.03E-03	2.03E-03
Ni	1.30E-02	1.11E-06	3.02E-08	1.18E-07	3.95E-07	3.95E-07
S	4.74E-04	6.93E-04	1.92E-04	1.92E-04	1.92E-04	1.92E-04
Si	5.72E-05	4.24E-05	4.45E-05	3.96E-05	3.86E-05	3.86E-05
Ti	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
U	7.80E-06	4.97E-05	1.00E-16	1.00E-16	1.00E-16	1.00E-16
Zn	1.00E-16	1.00E-16	7.89E-16	3.63E-18	1.00E-16	1.00E-16
рН	5.98	7.90	8.69	8.37	8.10	8.10

Table 22. Case 6 (nm1x2432): Solution Composition in Molality

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Waste Package Project	Calculation
Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codispos	al Waste Packages:
Effects of Updated Design and Rates	
Document Identifier: CAL-EDC-MD-000015 REV00	Page 51 of 119

Case 8 (nm1{xyz}3333), shown in Figure 6 and Table 23 and Table 24, demonstrates the effects of WP component degradation using the highest steel degradation rate, slow pH-dependent glass degradation rate, fast fuel rate, and fast flushing rate.

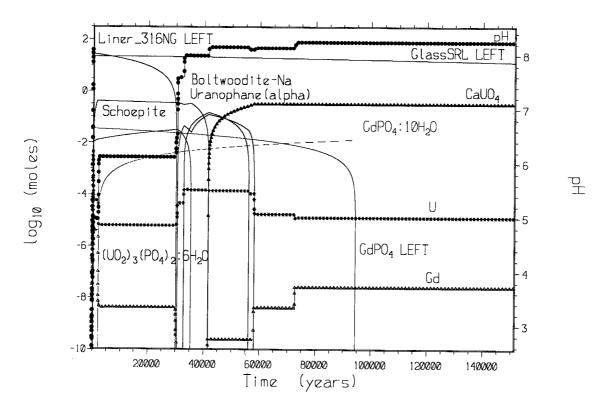


Figure 6. Case 8 (nm1{xyz}3333): WP Materials, Minerals, and Aqueous U

The pH levels for Case 8 are similar to those described for Case 3. However, retention of U and Gd are slightly different. Case 8 predicts only 47% U retention compared to Case 3 where 69.7% U retention was predicted. This may be due to the earlier rise of pH to above 8 at approximately 30,000 years in Case 8 whereas the pH did not rise to this level in Case 3 until almost 50,000 years. Therefore, more U is lost from the WP earlier in Case 8 than in Case 3 due to the early rise in pH.

Though the difference between the other cases presented is slight, Case 8 had the largest Gd loss (6.36%) among all the single stage runs.

Since the high steel degradation rates are new to this calculation there is no corresponding case to Case 8 in the previous calculation (Ref. 32).

1997 - 19

Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposal Waste Packages: Effects of Updated Design and Rates

Document Identifier: CAL-EDC-MD-000015 REV00

Page 52 of 119

Flowers		<u></u> ,	Ye	ars		
Element	2134	3065	32806	41643	72654	151520
0	8.43E+02	8.73E+02	1.69E+03	1.72E+03	1.82E+03	2.12E+03
AI	1.97E+01	1.97E+01	2.10E+01	2.21E+01	2.66E+01	3.91E+01
В	4.69E-18	5.86E-19	1.32E-14	9.96E-18	0.00E+00	0.00E+00
Ва	0.00E+00	0.00E+00	1.27E-02	8.48E-02	3.75E-01	1.19E+00
Са	8.42E-01	1.02E+00	7.77E+00	1.22E+01	2.57E+01	4.61E+01
CI	0.00E+00	0.00E+00	0.00E+00	9.61E-19	1.92E-18	9.61E-19
Cr	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Cu	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
F	0.00E+00	5.15E-19	1.89E-01	3.96E-01	4.01E-01	4.19E-01
Fe	1.72E+03	1.78E+03	3.40E+03	3.41E+03	3.42E+03	3.48E+03
Gd	1.98E-03	2.36E-02	7.13E-01	9.18E-01	1.64E+00	2.13E+00
Н	3.44E+00	3.37E+00	5.19E+00	5.59E+00	4.55E+00	8.11E+00
С	0.00E+00	1.13E-12	1.11E-03	7.42E-03	3.28E-02	4.43E+00
Р	8.06E-01	8.53E-01	2.10E+00	2.12E+00	2.29E+00	2.47E+00
к	0.00E+00	3.18E-18	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Mg	0.00E+00	0.00E+00	7.30E-01	1.73E+00	4.70E+00	7.69E+00
Mn	3.01E+01	3.20E+01	8.14E+01	8.14E+01	8.14E+01	8.14E+01
Мо	2.02E+00	2.44E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
N	0.00E+00	0.00E+00	0.00E+00	7.59E-19	7.59E-19	1.14E-18
Na	0.00E+00	0.00E+00	3.29E-04	3.38E+00	3.81E+00	2.33E+00
Ni	3.95E-04	4.85E-01	1.06E+01	1.05E+01	1.05E+01	1.05E+01
S	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Si	1.57E+01	1.79E+01	8.35E+01	1.03E+02	1.76E+02	3.72E+02
Ti	3.15E-02	3.15E-02	3.15E-02	3.15E-02	3.15E-02	3.15E-02
U	1.06E+02	1.06E+02	1.04E+02	9.39E+01	7.60E+01	7.69E+01
Zn	0.00E+00	0.00E+00	0.00E+00	0.00E+00	6.02E-16	1.55E-11
Total (Kg)	669	692	1320	1333	1378	1525
Density (g/cm ³)	5.07	5.07	5.00	4.96	4.85	4.54

Table 23. Case 8 (nm1{xyz}3333): Composition of Corrosion Products (g), Total Mass, and Density

NOTE: Mass (g) of each element is based on 1 liter aqueous fluid. To obtain total grams of each element in the WP, multiply by WP void volume of 4102 liters.

Calculation

Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposal Waste Packages: Effects of Updated Design and Rates

Document Identifier: CAL-EDC-MD-000015 REV00

Page 53 of 119

Element	Years					
Element	2134	3065	32806	41643	72654	151520
AI	5.42E-07	3.68E-07	5.61E-08	8.86E-08	6.80E-08	6.82E-08
В	1.49E-04	1.29E-04	3.52E-04	4.61E-04	5.10E-04	5.44E-04
Ва	5.62E-07	4.88E-07	1.13E-08	4.59E-09	3.23E-09	2.96E-09
Са	1.46E-04	2.11E-04	1.11E-05	1.68E-05	1.93E-04	1.78E-04
CI	2.01E-04	2.01E-04	2.01E-04	2.01E-04	2.01E-04	2.01E-04
Cr	1.14E-02	8.17E-03	1.00E-16	1.00E-16	1.00E-16	1.00E-16
Cu	1.00E-16	1.00E-16	1.00E-16	1.00E-16	1.00E-16	1.00E-16
F	1.16E-04	1.16E-04	3.30E-08	1.17E-04	1.17E-04	1.18E-04
Fe	3.79E-12	3.35E-12	1.14E-12	1.15E-12	1.15E-12	1.15E-12
Gd	7.14E-09	4.11E-09	2.75E-12	2.46E-10	2.64E-08	2.68E-08
С	5.46E-05	5.78E-05	1.61E-03	2.62E-03	2.86E-03	2.99E-03
Р	3.52E-08	3.88E-08	8.10E-06	1.64E-07	2.59E-09	2.86E-09
к	1.67E-04	1.62E-04	2.20E-04	2.48E-04	2.61E-04	2.69E-04
Mg	9.97E-05	9.75E-05	6.45E-06	9.74E-06	1.11E-04	1.02E-04
Mn	9.51E-12	6.46E-12	1.20E-15	6.18E-16	5.23E-16	5.07E-16
Мо	8.98E-04	5.31E-04	2.80E-04	1.00E-16	1.00E-16	1.00E-16
N	3.55E-04	2.84E-04	1.42E-04	1.42E-04	1.42E-04	1.42E-04
Na	2.29E-03	2.25E-03	2.68E-03	3.26E-03	2.90E-03	3.09E-03
Ni	7.13E-03	4.84E-03	8.11E-07	3.25E-07	2.28E-07	2.09E-07
S	2.26E-04	2.17E-04	1.96E-04	1.98E-04	1.99E-04	1.99E-04
Si	5.68E-05	5.68E-05	4.50E-05	4.31E-05	3.99E-05	4.02E-05
Ti	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
U	6.50E-06	6.29E-06	1.27E-04	1.39E-04	1.13E-05	1.33E-05
Zn	1.00E-16	1.00E-16	1.00E-16	1.00E-16	9.08E-17	1.78E-17
pН	6.05	6.12	7.94	8.14	8.22	8.24

Table 24. Case 8 (nm1{xyz}3333): Solution Composition in Molality

Waste Package Project	Calculation
Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codispo	sal Waste Packages:
Effects of Updated Design and Rates	
Document Identifier: CAL-EDC-MD-000015 REV00	Page 54 of 119

6.1.2 Gd and U Retention: Two-Stage Runs

For the two-stage runs, the glass and the fuel are degraded separately from one another. In cases 11 and 12, the first stage simulates all the WP components being exposed to degradation except what is inside the DOE canister. The second stage begins when the DOE canister is allowed to breach. In the Scenario I two-stage runs, this corresponds to a pH low. For Cases 13 through 15, the first stage assumes that all package components except the glass pour canisters are breached and exposed to degradation to account for the possibility that the DOE canister was damaged during loading. The second stage then begins when the GPCs are 2/3 degraded and assumed to be breached. All values in section 6.1.2 are calculated in "fermi-losses.xls" (Attachment III)

6.1.2.1 Scenario I Two-stage Runs

Table 25 summarizes the retention values for Scenario I two-stage cases. Retention of U ranges from 27.20% to 94.21%. Like the one-stage runs, the retention of U in the WP stems from the formation of $(UO_2)_3(PO_4)_2 \cdot 6H_2O$, schoepite $(UO_3 \cdot 2H_2O)$, Na-boltwoodite $(NaUO_2SiO_3OH \cdot 1.5H_2O)$, α -uranophane $(Ca(UO_2SiO_3OH)_2 \cdot 5H_2O)$, and $CaUO_4$. Soddyite $((UO_2)_2SiO_4 \cdot 2H_2O)$ was once again the most abundant U mineral reported in the two-stage runs of Reference 32.

Gd retention is very high, 99.99% to 100%. The only Gd mineral formed is $GdPO_4 \cdot 10H_2O$.

Case	Case ID	Length of Run (Years)	Gd Retention ^a	U Retention ^a
	nm1x1403	33,979		0.00%
11	nm2{xy}1031	635,630	100.00%	72.80%
40	nm1x1303	33,999		99.99%
12	nm2x1332	633,860	96.89%	94.21%
Case ^b	Case ID ^b	Length of Run (Years) ^b	Gd Retention ^b	U Retention ^b
40	N17A1203	5,002		0.00%
16	N17{B,C}1011	500,050	99.93%	72.62%
47	N18A1103	5,005		99.28%
17	N18{B,C,D}1012	106,340	99.65%	80.91%

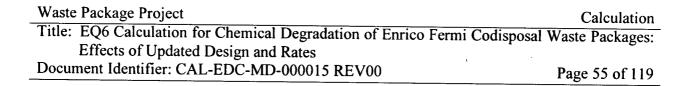
Table 25. Gd and U Retention^c for Scenario I Two-Stage EQ6 Runs

Sources: ^a Calculated in "fermi-losses.xls" (Attachment III)

^b Ref. 32, Table 5-9, values re-calculated in "oldfermi-recalc.xls" (Attachment III)

^c Retention of Gd and U is presented in percentage of total initial moles retained within the WP.

Figure 7 and Table 26 and Table 27 show the results of the first stage of Case 11 (nm1x1403). The pH of the system increases to above 8.8 in the first few years of degradation due to the fast glass degradation rate. This plateau continues for approximately 15,000 years until the glass is completely exhausted. At this point the pH slowly drops to 6.61 over a period of 19,000 years as the steel within the WP continues to degrade. During the initial plateau of high pH, all of the U from the degraded HLW glass is lost from the WP.



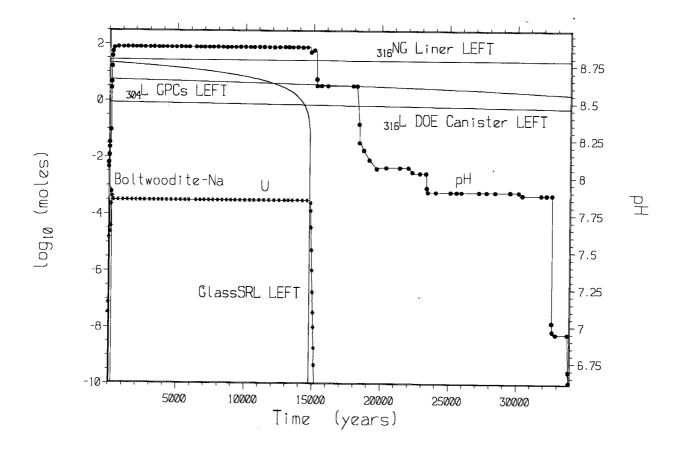


Figure 7. Case 11 (1st Stage: nm1x1403): WP Materials, Minerals, and Aqueous U

This is very close to what is seen in the first stage of Case 16 (Ref. 32). In old Case 16, the pH plateau is shorter-lived than in Case 11 of this calculation, only \sim 900 years, but the end result is the same. All U, from degraded HLW glass, in the first stage of old Case 16, is lost from the WP. This is when the first stage of Case 16 was ended. Case 11 of the current calculation is carried to a pH minimum at 34,000 years.

Calculation

Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposal Waste Packages: Effects of Updated Design and Rates

Document Identifier: CAL-EDC-MD-000015 REV00

Page 56 of 119

 Table 26. Case 11 (1st Stage: nm1x1403): Composition of Corrosion Products (g), Total Mass, and Density

F lamant		Yea	ars	
Element	226	15072	15889	33979
0	4.10E+02	1.31E+03	1.32E+03	1.41E+03
AI	4.76E-01	5.08E+01	5.08E+01	5.08E+01
В	1.91E-11	3.19E-18	0.00E+00	0.00E+00
Ba	3.09E-02	3.30E+00	3.30E+00	3.29E+00
Ca	2.47E-01	2.09E+01	2.12E+01	1.04E+01
CI	0.00E+00	0.00E+00	2.88E-18	0.00E+00
Cr	0.00E+00	0.00E+00	0.00E+00	1.20E+00
Cu	0.00E+00	0.00E+00	0.00E+00	0.00E+00
F	1.81E-02	1.09E-01	1.10E-01	1.38E-01
Fe	9.16E+02	1.29E+03	1.30E+03	1.50E+03
Gd	0.00E+00	0.00E+00	0.00E+00	0.00E+00
н	1.13E-01	9.80E+00	1.03E+01	1.08E+01
С	2.10E-02	7.76E+00	6.96E+00	0.00E+00
Р	8.83E-02	5.33E-01	5.39E-01	6.75E-01
К	1.91E-01	2.14E+01	2.03E+01	0.00E+00
Mg	1.73E-01	1.85E+01	1.85E+01	1.47E+01
Mn	9.76E+00	1.47E+01	1.50E+01	2.11E+01
Мо	0.00E+00	3.25E-18	6.50E-19	0.00E+00
N	0.00E+00	0.00E+00	3.80E-19	0.00E+00
Na	2.94E-01	2.73E+01	2.06E+01	0.00E+00
Ni	4.03E-01	2.69E+01	2.83E+01	6.02E+01
S	0.00E+00	0.00E+00	8.69E-19	2.93E-02
Si	7.39E+00	4.95E+02	4.96E+02	5.17E+02
Ti	4.44E-14	2.64E-12	2.79E-12	5.95E-12
U	6.36E-10	4.09E-17	0.00E+00	0.00E+00
Zn	1.64E-14	3.55E-12	3.74E-12	0.00E+00
Total (Kg)	328	805	807	879
Density (g/cm ³)	5.20	3.68	3.68	3.83

NOTE: Mass (g) of each element is based on 1 liter aqueous fluid. To obtain total grams of each element in the WP, multiply by WP void volume of 4102 liters.

Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposal Waste Packages: Effects of Updated Design and Rates Document Identifier: CAL-EDC-MD-000015 REV00

Page 57 of 119

Element	Years				
Element	226	15072	15889	33979	
AI	1.49E-15	1.18E-07	8.35E-08	1.98E-08	
В	9.81E-03	4.96E-07	1.00E-16	1.00E-16	
Ва	4.17E-10	2.62E-10	6.70E-10	1.02E-06	
Са	3.94E-05	1.95E-05	4.72E-05	2.39E-04	
CI	2.01E-04	2.01E-04	2.01E-04	2.01E-04	
Cr	1.61E-03	1.61E-03	1.61E-03	1.61E-03	
Cu	1.00E-16	1.00E-16	1.00E-16	1.00E-16	
F	1.46E-04	1.13E-04	1.13E-04	1.13E-04	
Fe	1.28E-12	1.31E-12	1.22E-12	1.77E-12	
Gd	1.00E-16	1.00E-16	1.00E-16	1.00E-16	
С	1.29E-02	1.34E-02	7.41E-03	1.01E-04	
Р	4.58E-08	1.23E-07	3.11E-08	4.03E-07	
к	1.82E-03	1.56E-03	9.95E-04	1.29E-04	
Mg	7.15E-06	1.73E-05	4.09E-05	1.08E-04	
Mn	8.58E-16	1.02E-15	6.20E-16	5.34E-13	
Мо	3.90E-05	3.90E-05	3.90E-05	3.90E-05	
N	1.72E-04	1.72E-04	1.72E-04	1.72E-04	
Na	1.94E-02	1.66E-02	1.06E-02	1.99E-03	
Ni	2.58E-08	1.62E-08	4.47E-08	3.98E-04	
S	3.84E-04	1.96E-04	1.96E-04	2.02E-04	
Si	2.51E-04	5.12E-05	4.68E-05	5.09E-05	
Ti	0.00E+00	0.00E+00	0.00E+00	0.00E+00	
U	6.01E-04	1.33E-08	1.00E-16	1.00E-16	
Zn	1.32E-18	5.68E-19	1.11E-18	1.00E-16	
pН	8.77	8.85	8.61	6.61	

Table 27. Case 11 (1st Stage: nm1x1403): Solution Composition in Molality

Waste Package Project	Calculation
Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codispos	al Waste Packages:
Effects of Updated Design and Rates	
Document Identifier: CAL-EDC-MD-000015 REV00	Page 58 of 119

Figure 8 and Table 28 and Table 29 show the results of the second stage of Case 11 (nm2{xy}1031). Since the HLW glass is completely degraded at this point, and its alkalinity largely washed from the WP, the pH of the solution within the WP remains low for the remainder of the run. Since the pH remains low, all of the U within the package during this stage (from Fermi fuel) is retained as the U minerals described earlier. There is no effect on the retention of Gd and 100% remains in the WP as GdPO₄·10H₂O.

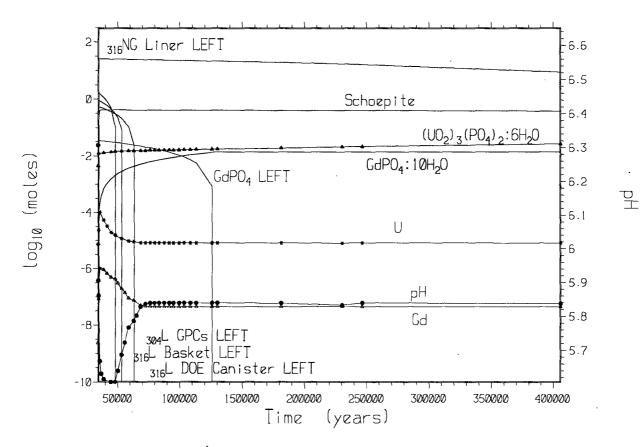


Figure 8. Case 11 (2nd Stage: nm2{xy}1031): WP Materials, Minerals, and Aqueous U

Even though the second stage of Case 16 from Reference 32 begins much sooner than that for current Case 11, the results are basically the same. After the beginning of the second stage, the pH drops rapidly so that most of the U is retained within the WP. Both Case 11 and old Case 16 retain slightly more than 72% of the total U (which, in both cases, is solely from the degraded U/Mo Fermi fuel).

Calculation

Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposal Waste Packages: Effects of Updated Design and Rates

Document Identifier: CAL-EDC-MD-000015 REV00

Page 59 of 119

Table 28. Case 11 (2 nd Stage: nm2{xy}1031): Composition of Corrosion Products (g),	Total Mass, and
Density	

Element	Years			
Liement	33979	635630		
0	1.42E+03	1.72E+03	2.24E+03	2.47E+03
AI	5.08E+01	7.11E+01	7.10E+01	7.10E+01
В	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Ва	3.29E+00	3.29E+00	3.27E+00	3.26E+00
Са	1.04E+01	1.05E+01	1.18E+01	1.25E+01
CI	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Cr	1.19E+00	1.24E+00	1.24E+00	1.15E+00
Cu	0.00E+00	0.00E+00	0.00E+00	0.00E+00
F	1.39E-01	0.00E+00	0.00E+00	0.00E+00
Fe	1.52E+03	2.04E+03	3.13E+03	3.60E+03
Gd	2.33E-06	1.03E+00	2.19E+00	2.19E+00
Н	1.08E+01	1.38E+01	1.42E+01	1.49E+01
С	0.00E+00	3.31E-12	1.89E-12	0.00E+00
Р	6.80E-01	1.18E+00	2.16E+00	2.49E+00
К	2.12E-18	0.00E+00	0.00E+00	0.00E+00
Mg	1.47E+01	1.49E+01	1.51E+01	1.52E+01
Mn	2.12E+01	3.35E+01	6.69E+01	8.14E+01
Мо	0.00E+00	8.34E+00	8.75E+00	7.44E+00
N	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Na	9.97E-18	0.00E+00	0.00E+00	0.00E+00
Ni	6.02E+01	5.49E+01	5.07E+01	4.84E+01
S	3.49E-02	0.00E+00	0.00E+00	5.37E-02
Si	5.17E+02	5.23E+02	5.43E+02	5.52E+02
Ti	6.71E-06	3.15E-02	3.15E-02	3.15E-02
U	7.33E-03	1.10E+02	1.10E+02	1.10E+02
Zn	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Total (Kg)	884	1124	1528	1705
Density (g/cm³)	3.84	4.02	4.26	4.33

NOTE: Mass (g) of each element is based on 1 liter aqueous fluid. To obtain total grams of each element in the WP, multiply by WP void volume of 4102 liters.

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Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposal Waste Packages: Effects of Updated Design and Rates

Document Identifier: CAL-EDC-MD-000015 REV00

Page 60 of 119

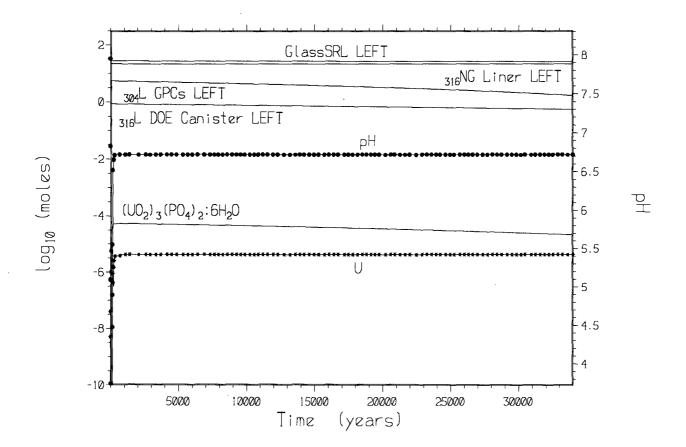
Floment		Yea	ars	
Element	33979	78235	442710	635630
AI	1.43E-08	1.32E-06	1.03E-06	4.54E-08
В	1.00E-16	1.00E-16	1.00E-16	1.00E-16
Ba	1.04E-06	6.92E-07	7.78E-07	1.03E-05
Ca	3.91E-05	7.87E-05	9.55E-05	3.33E-05
CI	2.01E-04	2.01E-04	2.01E-04	2.01E-04
Cr	1.79E-03	4.10E-02	4.11E-02	1.81E-04
Cu	1.93E-07	1.72E-11	1.00E-16	1.00E-16
F	6.64E-05	1.15E-04	1.15E-04	1.15E-04
Fe	2.01E-12	5.98E-12	6.55E-12	2.04E-12
Gd	1.60E-12	4.52E-08	4.14E-08	2.96E-10
С	8.35E-05	4.71E-05	5.47E-05	8.39E-05
Р	1.69E-05	2.75E-08	3.21E-08	7.11E-08
К	1.29E-04	1.29E-04	1.29E-04	1.29E-04
Mg	1.78E-05	2.88E-05	3.51E-05	1.89E-05
Mn	9.86E-13	3.48E-11	3.52E-11	1.05E-12
Мо	4.81E-05	3.23E-03	3.25E-03	1.51E-03
N	1.73E-04	8.57E-04	8.56E-04	1.42E-04
Na	1.99E-03	1.99E-03	1.99E-03	1.99E-03
Ni	7.36E-04	2.62E-02	2.64E-02	7.90E-04
S	1.97E-04	3.09E-04	3.09E-04	2.05E-05
Si	5.68E-05	6.58E-05	7.48E-05	5.68E-05
Ti	0.00E+00	0.00E+00	0.00E+00	0.00E+00
U	2.94E-07	8.21E-06	8.84E-06	6.80E-06
Zn	1.71E-07	1.17E-11	1.00E-16	1.00E-16
рН	6.47	5.84	5.86	6.46

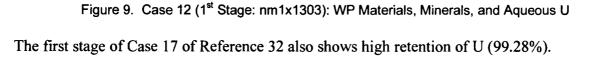
Table 29. Case 11 (2nd Stage: nm2{xy}1031): Solution Composition in Molality

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Waste Package Project	Calculation
Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codispo	osal Waste Packages:
Effects of Updated Design and Rates	
Document Identifier: CAL-EDC-MD-000015 REV00	Page 61 of 119

Figure 9 and Table 30 and Table 31 show the results of the first stage of Case 12 (nm1x1303). Case 12 has the same parameters as Case 11 except that the glass now has a slow pH dependant degradation rate. In the first stage, the pH remains slightly below neutral (~6.7) for most of the run. Since the pH remains low, most of the U (96.89%) is kept inside the WP due to U mineral formation and the intact portion of the HLW glass remaining in the WP. As shown in Section 6.1.1 of this report, the fast drip rate allows some U to escape from the WP, but most is retained.





Calculation

Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposal Waste Packages: Effects of Updated Design and Rates

Document Identifier: CAL-EDC-MD-000015 REV00

Page 62 of 119

Table 30. Case 12 (1 st Stage: nm1x1303): Composition of Corrosion Products (g), Total Mass, and	
Density	

Element		Years	······································
Element	136	968	33999
0	4.02E+02	4.08E+02	6.46E+02
AI	4.79E-02	8.78E-02	1.60E+00
В	0.00E+00	7.07E-14	3.31E-14
Ва	3.25E-03	2.06E-03	0.00E+00
Са	0.00E+00	1.01E-01	1.76E+00
CI	0.00E+00	0.00E+00	0.00E+00
Cr	0.00E+00	7.81E-04	0.00E+00
Cu	0.00E+00	0.00E+00	0.00E+00
F	0.00E+00	3.38E-03	5.49E-02
Fe	9.13E+02	9.23E+02	1.30E+03
Gd	0.00E+00	0.00E+00	0.00E+00
н	1.32E-02 2.05E-02		3.62E-01
С	1.18E-13	0.00E+00	0.00E+00
Р	2.80E-03	1.99E-02	2.70E-01
К	0.00E+00	0.00E+00	0.00E+00
Mg	0.00E+00	0.00E+00	0.00E+00
Mn	9.73E+00	1.00E+01	2.11E+01
Мо	5.33E-03	0.00E+00	0.00E+00
N	0.00E+00	0.00E+00	0.00E+00
Na	0.00E+00	0.00E+00	0.00E+00
Ni	0.00E+00	1.01E+00	4.31E+01
S	7.59E-04	0.00E+00	0.00E+00
Si	3.33E+00	4.52E+00	5.13E+01
Ti	2.86E-14	1.74E-13	5.96E-12
U	3.22E-02	3.91E-02	1.52E-02
Zn	0.00E+00	0.00E+00	0.00E+00
Total (Kg)	324	328	504
Density (g/cm³)	5.26	5.23	4.98

NOTE: Mass (g) of each element is based on 1 liter aqueous fluid. To obtain total grams of each element in the WP, multiply by WP void volume of 4102 liters.

Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposal Waste Packages: Effects of Updated Design and Rates Document Identifier: CAL-EDC-MD-000015 REV00

Page 63 of 119

-		Years	
Element	136	968	33999
Al	2.67E-05	4.52E-15	4.51E-15
В	1.43E-03	1.56E-04	1.57E-04
Ва	1.23E-07	9.26E-07	5.92E-07
Ca	4.05E-04	2.99E-04	2.99E-04
CI	2.01E-04	2.01E-04	2.01E-04
Cr	1.60E-03	1.61E-03	1.61E-03
Cu	1.00E-16	1.00E-16	1.00E-16
F	1.23E-04	1.13E-04	1.13E-04
Fe	1.51E-09	1.61E-12	1.61E-12
Gd	1.00E-16	1.00E-16	1.00E-16
С	3.40E-05	1.22E-04	1.23E-04
Р	2.08E-03	2.40E-07	2.39E-07
К	4.99E-04	1.69E-04	1.69E-04
Mg	2.47E-04	1.01E-04	1.01E-04
Mn	3.77E-07	3.17E-13	3.16E-13
Мо	2.52E-05	3.90E-05	3.90E-05
N	1.72E-04	1.72E-04	1.72E-04
Na	4.83E-03	2.30E-03	2.30E-03
Ni	8.26E-04	2.37E-04	2.36E-04
S	2.23E-03	1.98E-04	1.98E-04
Si	1.87E-04	1.87E-04	1.87E-04
Ti	0.00E+00	0.00E+00	0.00E+00
U	7.39E-06	4.27E-06	4.27E-06
Zn	1.00E-16	1.00E-16	1.00E-16
рН	3.72	6.72	6.72

Table 31. Case 12 (1st Stage: nm1x1303): Solution Composition in Molality

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Waste Package Project	Calculation
Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisp	osal Waste Packages:
Effects of Updated Design and Rates	
Document Identifier: CAL-EDC-MD-000015 REV00	Page 64 of 119

Figure 10 and Table 32 and Table 33 show the results of the second stage of Case 12 (nm2x1332). The pH dips for a short time from the addition of the new steels within the DOE canister, but recovers again to a level of approximately 6.5. The pH remains at this level until all of the steel is gone at 600,000. For the next 34,000 years, the pH rises to above 8.25. During this period, 2.5% more (total U) is washed from the WP.

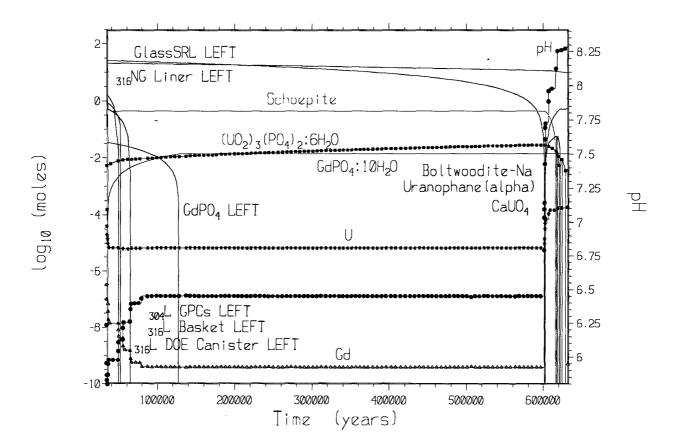


Figure 10. Case 12 (2nd Stage: nm2x1332): WP Materials, Minerals, and Aqueous U

The second stage of Case 17 of Reference 32 shows much greater losses of U than Case 12 (19% loss versus 6% loss). Because of the constant HLW glass degradation rate, the pH is able to rise above 7.8 in old Case 17. This is not enough to wash much of the U from the WP, but fewer and less stable U minerals exist at this pH level, allowing more U complexes to exist in solution so that more U can be flushed from the WP

Gadolinium retention remains high for both cases since both GdPO₄·10H₂O (from "data0.ymd") and GdPO₄·H₂O (from "data0.nuc") are both very stable minerals.

Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposal Waste Packages: Effects of Updated Design and Rates

Document Identifier: CAL-EDC-MD-000015 REV00

Page 65 of 119

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Table 32. Case 12 (2nd Stage: nm2x1332): Composition of Corrosion Products (g), Total Mass, and Density

Element	Years			
Element	34000 80732 608930 633			
0	6.57E+02	1.01E+03	2.19E+03	2.25E+03
AI	1.60E+00	2.37E+01	4.53E+01	4.91E+01
В	5.86E-19	6.92E-14	3.18E-12	0.00E+00
Ва	1.98E-05	1.02E-01	1.35E+00	1.59E+00
Са	1.78E+00	3.47E+00	1.27E+01	1.49E+01
CI	9.61E-19	0.00E+00	0.00E+00	7.25E-14
Cr	0.00E+00	3.88E-02	0.00E+00	0.00E+00
Cu	0.00E+00	0.00E+00	0.00E+00	0.00E+00
F	5.58E-02	0.00E+00	7.23E-02	2.99E-01
Fe	1.32E+03	1.85E+03	3.50E+03	3.51E+03
Gd	3.70E-06	1.08E+00	2.19E+00	2.19E+00
н	3.63E-01	5.45E+00	1.11E+01	1.12E+01
С	8.33E-13	0.00E+00	1.18E-01	1.39E-01
Р	2.76E-01	8.02E-01	2.23E+00	1.89E+00
К	0.00E+00	0.00E+00	4.37E-01	3.91E+00
Mg	2.35E-03	9.49E-01	7.20E+00	8.66E+00
Mn	2.13E+01	3.37E+01	8.14E+01	8.14E+01
Мо	6.50E-19	5.36E-03	0.00E+00	0.00E+00
N	0.00E+00	0.00E+00	0.00E+00	2.49E-15
Na	9.97E-18	0.00E+00	3.03E+00	1.98E+01
Ni	4.31E+01	4.51E+01	2.29E+02	2.29E+02
S	4.62E-06	0.00E+00	0.00E+00	4.72E-12
Si	5.14E+01	7.84E+01	3.57E+02	3.95E+02
Ti	1.06E-05	3.15E-02	3.15E-02	3.15E-02
U	2.79E-02	1.11E+02	1.25E+02	1.24E+02
Zn	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Total (Kg)	512	772	1600	1635
Density (g/cm³)	4.98	4.85	4.57	4.50

NOTE: Mass (g) of each element is based on 1 liter aqueous fluid. To obtain total grams of each element in the WP, multiply by WP void volume of 4102 liters.

Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposal Waste Packages: Effects of Updated Design and Rates

Document Identifier: CAL-EDC-MD-000015 REV00

Page 66 of 119

Flowert	Years			
Element	34000	80732	608930	633860
AI	3.96E-14	5.38E-08	6.10E-08	1.24E-07
В	1.57E-04	1.37E-03	4.29E-03	5.67E-03
Ва	4.50E-07	6.02E-07	9.48E-09	2.60E-09
Ca	1.48E-05	2.86E-04	9.37E-06	1.52E-05
CI	2.01E-04	2.01E-04	2.01E-04	2.01E-04
Cr	1.63E-03	4.09E-03	2.28E-15	1.00E-16
Cu	3.07E-07	1.00E-16	1.00E-16	1.00E-16
F	6.28E-05	1.23E-04	3.59E-08	1.45E-04
Fe	2.04E-12	2.09E-12	1.14E-12	1.16E-12
Gd	1.15E-12	3.92E-10	2.78E-12	6.03E-10
С	8.25E-05	8.42E-05	1.77E-03	3.81E-03
Р	9.08E-05	7.21E-08	9.43E-06	1.63E-07
К	1.70E-04	4.83E-04	3.91E-04	4.77E-04
Mg	6.98E-06	1.11E-04	5.48E-06	8.73E-06
Mn	1.06E-12	1.22E-12	1.03E-15	4.97E-16
Мо	5.35E-05	3.11E-04	1.82E-07	1.00E-16
N	1.73E-04	2.13E-04	1.42E-04	1.42E-04
Na	2.30E-03	4.71E-03	2.45E-03	5.07E-03
Ni	7.85E-04	9.13E-04	6.74E-07	1.80E-07
S	4.67E-04	2.22E-04	2.50E-04	2.69E-04
Si	1.87E-04	5.28E-05	4.51E-05	4.33E-05
Ti	0.00E+00	0.00E+00	0.00E+00	0.00E+00
U	4.08E-07	6.84E-06	1.45E-04	1.89E-04
Zn	2.71E-07	1.00E-16	1.00E-16	1.00E-16
рН	6.46	6.45	7.98	8.29

Table 33. Case 12 (2nd Stage: nm2x1332): Solution Composition in Molality

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Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposa	1 Waste Packages
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Effects of Updated Design and Rates	
Document Identifier: CAL-EDC-MD-000015 REV00	Page 67 of 119

6.1.2.2 Scenario II Two-stage Runs

Table 34 summarizes the retention values for Scenario II two-stage runs. There are no equivalent cases in Reference 32.

Case	Case ID	Length of Run (Years)	Gd Retention	U Retention
40	nm1x1023	59,892		99.71%
13	nm2{xyz}1323	633,370	98.32%	82.97%
	nm1x1033	59,897	*****	95.08%
14	nm2{xy}1303	431,980	95.89%	68.08%
45	nm1x1032	59,928		98.11%
15	nm2{xy}1302	633,780	87.01%	93.30%

Table 34. Gd and U Retention for Scenario II Two-stage EQ6 Runs

NOTE: Retention of Gd and U is presented in percentage of total initial moles retained within the WP.

Cases 13 and 14 are exactly the same except that Case 13 has a slow fuel degradation rate and Case 14 has a fast fuel degradation rate. We have seen previously (Section 6.1.1) that the U retention for cases with the slow fuel degradation rate will be higher than those for the fast fuel rate since most (>95%) of the fuel remains intact. Gadolinium retention remains high for both cases. The "corrosion products" and "WP solution composition" tables are also very similar. For this reason, since the case with a fast fuel degradation rate would be more reactive in terms of criticality, only tables and figures for Cases 14 and 15 are presented in this section

Figure 11 and Table 35 and Table 36 show the results of the first stage of Case 14 (nm1x1033). During the first 2,800 years, the pH remains below 5. During this period, the amount of Gd in solution is high and a 3% (total Gd) loss occurs. After this point, the pH rises and hovers around neutral until the end of the run. It is only at this point that the mineral $GdPO_4 \cdot 10H_2O$ is able to form. Although $GdPO_4 \cdot 10H_2O$ is a very stable mineral, its stability decreases with decreasing pH and it is not able to form until the pH reaches a level above 6.0. Uranium is just the opposite, being more unstable in minerals at higher pH values. Though the pH has not risen above 8.5, the level is high enough to keep some of the U in solution and a 5% loss of U is seen over the next 56,000 years.

Calculation

Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposal Waste Packages: Effects of Updated Design and Rates

Document Identifier: CAL-EDC-MD-000015 REV00

Page 68 of 119

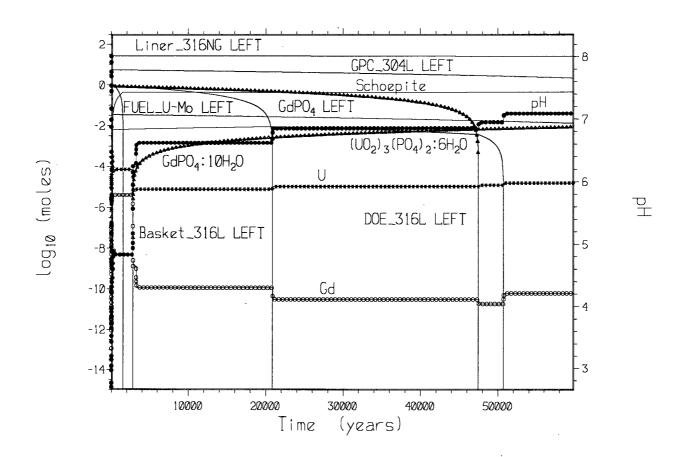


Figure 11. Case 14 (1st Stage: nm1x1033): WP Materials, Minerals, and Aqueous U

Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposal Waste Packages: Effects of Updated Design and Rates

Document Identifier: CAL-EDC-MD-000015 REV00

Page 69 of 119

Element	Years						
	2795	3434	21294	47864	59897		
0	5.76E+02	5.83E+02	6.99E+02	8.38E+02	8.94E+02		
Al	2.02E+01	2.02E+01	2.02E+01	2.02E+01	2.02E+01		
В	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00		
Ва	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00		
Са	1.04E+00	1.18E+00	1.79E+00	4.71E+00	6.10E+00		
CI	3.84E-18	6.05E-14	0.00E+00	0.00E+00	0.00E+00		
Cr	1.34E-15	9.56E-10	0.00E+00	0.00E+00	1.13E-17		
Cu	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00		
F	2.32E-18	4.53E-13	1.41E-03	1.01E-01	1.53E-01		
Fe	1.14E+03	1.14E+03	1.34E+03	1.55E+03	1.63E+03		
Gd	9.34E-04	1.58E-02	4.30E-01	1.05E+00	1.33E+00		
Н	3.86E+00	4.16E+00	4.40E+00	4.72E+00	4.86E+00		
С	4.74E-13	6.02E-12	5.58E-13	0.00E+00	2.95E-13		
Р	4.21E-01	4.29E-01	6.40E-01	8.99E-01	1.01E+00		
к	0.00E+00	1.39E-13	0.00E+00	0.00E+00	1.06E-18		
Mg	8.09E-04	2.50E-12	0.00E+00	0.00E+00	0.00E+00		
Mn	1.27E+01	1.29E+01	1.88E+01	2.51E+01	2.76E+01		
Мо	2.50E+00	1.71E+00	0.00E+00	0.00E+00	2.60E-18		
Ν	7.59E-19	9.37E-14	0.00E+00	0.00E+00	7.59E-19		
Na	0.00E+00	7.61E-13	0.00E+00	0.00E+00	0.00E+00		
Ni	0.00E+00	2.35E-01	1.93E+01	4.74E+01	5.95E+01		
S	3.48E-18	9.34E-12	0.00E+00	0.00E+00	1.74E-18		
Si	6.59E+00	7.32E+00	2.77E+01	5.69E+01	6.99E+01		
Ti	3.15E-02	3.15E-02	3.15E-02	3.15E-02	3.15E-02		
U	1.08E+02	1.08E+02	1.07E+02	1.04E+02	1.03E+02		
Zn	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00		
Total (Kg)	456	459	545	647	687		
Density (g/cm ³)	5.02	5.00	4.94	4.88	4.85		

Table 35. Case 14 (1st Stage: nm1x1033): Composition of Corrosion Products (g), Total Mass, and Density

> NOTE: Mass (g) of each element is based on 1 liter aqueous fluid. To obtain total grams of each element in the WP, multiply by WP void volume of 4102 liters.

Calculation

Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposal Waste Packages: Effects of Updated Design and Rates

Document Identifier: CAL-EDC-MD-000015 REV00

Page 70 of 119

Element	Years						
	2795	3434	21294	47864	59897		
AI	1.80E-07	1.88E-08	9.37E-09	8.76E-09	1.05E-08		
В	1.00E-16	1.00E-16	1.00E-16	1.00E-16	1.00E-16		
Ва	1.00E-16	1.00E-16	1.00E-16	1.00E-16	1.00E-16		
Ca	1.03E-04	3.21E-04	2.51E-04	1.68E-04	2.70E-04		
CI	2.01E-04	2.01E-04	2.01E-04	2.01E-04	2.01E-04		
Cr	1.53E-03	1.53E-03	1.13E-03	9.71E-04	9.71E-04		
Cu	1.00E-16	1.00E-16	1.00E-16	1.00E-16	1.00E-16		
F	1.15E-04	1.15E-04	1.10E-04	9.29E-05	1.13E-04		
Fe	2.66E-12	1.75E-12	1.47E-12	1.39E-12	1.31E-12		
Gd	1.31E-09	1.14E-10	3.02E-11	1.81E-11	6.14E-11		
С	6.46E-05	1.06E-04	1.56E-04	1.86E-04	2.43E-04		
Р	4.66E-08	1.04E-07	1.85E-07	2.42E-07	6.19E-08		
К	1.29E-04	1.29E-04	1.29E-04	1.29E-04	1.29E-04		
Mg	5.14E-05	1.48E-04	8.27E-05	8.27E-05	8.27E-05		
Mn	2.85E-12	4.98E-13	1.67E-13	1.05E-13	5.61E-14		
Мо	5.68E-04	1.89E-04	4.55E-05	3.26E-05	3.26E-05		
N	1.72E-04	1.72E-04	1.63E-04	1.60E-04	1.60E-04		
Na	1.99E-03	1.99E-03	1.99E-03	1.99E-03	1.99E-03		
Ni	8.66E-04	3.72E-04	1.25E-04	7.82E-05	4.18E-05		
S	1.96E-04	1.96E-04	1.95E-04	1.94E-04	1.94E-04		
Si	5.68E-05	5.01E-05	4.82E-05	4.81E-05	4.58E-05		
Ti	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00		
U	6.15E-06	7.88E-06	1.05E-05	1.23E-05	1.55E-05		
Zn	1.00E-16	1.00E-16	1.00E-16	1.00E-16	1.00E-16		
рН	6.25	6.62	6.85	6.95	7.09		

Table 36. Case 14 (1st Stage: nm1x1033): Solution Composition in Molality

Waste Package Project	Calculation
Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codispos	al Waste Packages:
Effects of Updated Design and Rates	
Document Identifier: CAL-EDC-MD-000015 REV00	Page 71 of 119

Figure 12 and Table 37 and Table 38 show the results of the second stage of Case 14 $(nm2{xy}1303)$. The pH decreases slightly for the first 20,000 years of the run until all of the 304L stainless steel of the GPCs is completely degraded. From this point it raises rapidly to around 7.85 and continues to increase to above 8.1 over the coarse of the run. Uranium in solution increases by an order of magnitude during this first initial rise in pH, only to decrease to previous levels when the system stabilizes. After the pH reaches 8.0, CaUO₄ is the only U-bearing mineral to exist in the WP. The slightly elevated levels of U in solution during the second stage allow for the loss of another 28% of the total U.

Since the pH remains high for the rest of the case, and stable Gd minerals are able to exist within the WP, Gd loss over the entire run of the case is held to only slighly more than 4%, with most of this having been lost in the first stage during the initial period of very low pH.

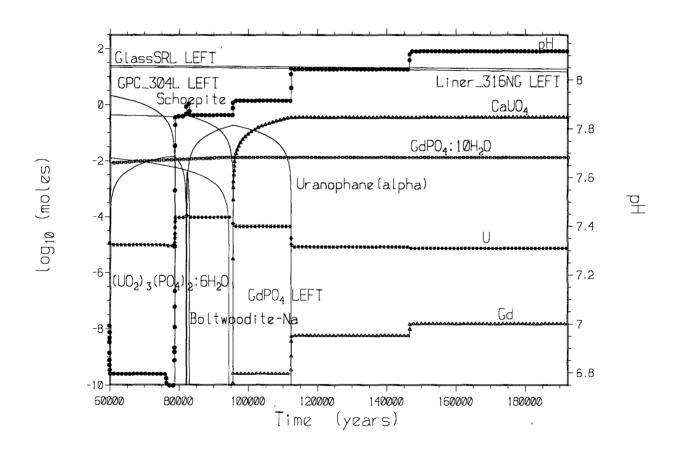


Figure 12. Case 14 (2nd Stage: nm2{xy}1303): WP Materials, Minerals, and Aqueous U

Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposal Waste Packages: Effects of Updated Design and Rates

Document Identifier: CAL-EDC-MD-000015 REV00

Page 72 of 119

Table 37. Case 14 (2 nd Stage: nm2{xy}1303): Composition of Corrosion Products (g), Total Mass, and
Density

E 1	Years					
Element	59922 78908 272040 431980 531750 633780					
0	8.95E+02	1.03E+03	1.96E+03	2.74E+03	3.00E+03	3.20E+03
Al	2.02E+01	2.11E+01	4.73E+01	6.97E+01	7.10E+01	7.10E+01
В	1.47E-19	5.56E-15	0.00E+00	2.93E-18	0.00E+00	0.00E+00
Ва	0.00E+00	7.04E-04	1.70E+00	3.14E+00	3.22E+00	3.21E+00
Са	6.10E+00	6.45E+00	4.60E+01	6.44E+01	6.18E+01	6.59E+01
CI	0.00E+00	0.00E+00	2.85E-16	0.00E+00	0.00E+00	9.61E-19
Cr	0.00E+00	0.00E+00	3.48E-13	2.82E-18	0.00E+00	0.00E+00
Cu	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
F	1.53E-01	6.81E-03	2.93E-01	3.91E-01	4.35E-01	4.64E-01
Fe	1.63E+03	1.84E+03	2.52E+03	3.09E+03	3.40E+03	3.61E+03
Gd	1.33E+00	1.77E+00	2.11E+00	2.10E+00	2.10E+00	2.09E+00
Н	4.86E+00	5.30E+00	1.10E+01	1.89E+01	1.89E+01	1.88E+01
С	0.00E+00	6.16E-05	1.48E-01	2.75E-01	2.82E-01	2.81E-01
Р	1.01E+00	1.23E+00	1.85E+00	2.33E+00	2.54E+00	2.68E+00
к	0.00E+00	0.00E+00	1.22E-15	0.00E+00	0.00E+00	1.06E-18
Mg	0.00E+00	1.33E-02	4.59E+00	1.02E+01	2.41E+00	0.00E+00
Mn	2.76E+01	3.36E+01	5.12E+01	6.59E+01	7.50E+01	8.14E+01
Мо	0.00E+00	0.00E+00	5.27E-17	1.95E-18	0.00E+00	0.00E+00
N .	1.14E-18	0.00E+00	1.81E-16	0.00E+00	0.00E+00	0.00E+00
Na	0.00E+00	0.00E+00	1.50E-14	0.00E+00	0.00E+00	0.00E+00
Ni	5.95E+01	8.42E+01	1.90E+02	2.78E+02	3.32E+02	3.70E+02
S	2.61E-18	0.00E+00	4.09E-14	0.00E+00	0.00E+00	0.00E+00
Si	7.00E+01	9.98E+01	5.48E+02	9.01E+02	1.00E+03	1.09E+03
Ti	3.15E-02	3.15E-02	3.15E-02	3.15E-02	3.15E-02	3.15E-02
U	1.03E+02	1.02E+02	9.13E+01	1.02E+02	1.00E+02	9.80E+01
Zn	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Total (Kg)	688	786	1336	1792	1967	2100
Density (g/cm³)	4.85	4.79	4.20	3.98	3.99	3.99

NOTE: Mass (g) of each element is based on 1 liter aqueous fluid. To obtain total grams of each element in the WP, multiply by WP void volume of 4102 liters.

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Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposal Waste Packages: Effects of Updated Design and Rates

Document Identifier: CAL-EDC-MD-000015 REV00

Page 73 of 119

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F 1	Years					
Element	59922	78908	272040	431980	531750	633780
AI	1.06E-15	1.18E-15	3.51E-14	1.18E-15	1.18E-15	9.89E-16
В	5.79E-05	1.00E-16	4.86E-04	4.77E-04	1.00E-16	1.00E-16
Ba	1.08E-08	1.66E-08	5.46E-09	5.76E-09	1.66E-08	5.64E-09
Са	3.30E-04	2.66E-04	2.50E-04	2.72E-04	2.66E-04	3.26E-04
CI	2.01E-04	2.01E-04	2.01E-04	2.01E-04	2.01E-04	2.01E-04
Cr	4.09E-04	4.09E-04	4.09E-04	4.09E-04	4.09E-04	1.00E-16
Cu	1.00E-16	1.00E-16	1.00E-16	1.00E-16	1.00E-16	1.00E-16
F	1.14E-04	1.14E-04	1.17E-04	1.17E-04	1.14E-04	1.15E-04
Fe	1.14E-12	1.15E-12	1.15E-12	1.15E-12	1.15E-12	1.14E-12
Gd	7.22E-09	2.68E-09	1.38E-08	1.45E-08	2.69E-09	2.40E-08
С	1.54E-03	1.24E-03	2.21E-03	2.14E-03	1.24E-03	2.10E-03
Р	2.48E-09	4.28E-09	2.74E-09	2.42E-09	4.27E-09	1.41E-09
к	1.44E-04	1.29E-04	2.54E-04	2.52E-04	1.29E-04	1.29E-04
Mg	1.72E-04	1.39E-04	1.30E-04	9.16E-05	1.39E-04	8.27E-05
Mn	1.16E-15	1.70E-15	6.89E-16	7.13E-16	1.69E-15	7.00E-16
Мо	3.28E-05	3.28E-05	3.26E-05	3.26E-05	3.26E-05	1.00E-16
N	1.49E-04	1.49E-04	1.49E-04	1.49E-04	1.49E-04	1.42E-04
Na	2.11E-03	1.99E-03	2.98E-03	2.94E-03	1.99E-03	1.99E-03
Ni	7.73E-07	1.19E-06	3.87E-07	4.09E-07	1.19E-06	4.02E-07
S	1.94E-04	1.93E-04	1.99E-04	1.99E-04	1.93E-04	1.92E-04
Si	1.92E-04	1.91E-04	1.44E-04	1.95E-04	1.91E-04	1.94E-04
Ti	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
U	2.53E-06	2.12E-06	7.69E-06	5.06E-06	2.13E-06	3.81E-06
Zn	1.00E-16	1.00E-16	1.00E-16	1.00E-16	1.00E-16	1.00E-16
pН	7.96	7.86	8.11	8.10	7.86	8.09

Table 38. Case 14 (2nd Stage: nm2{xy}1303): Solution Composition in Molality

Waste Package Project	Calculation
Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codispos	sal Waste Packages:
Effects of Updated Design and Rates	0
Document Identifier: CAL-EDC-MD-000015 REV00	Page 74 of 119

Figure 13 and Table 39 and Table 40 show the results of the first stage of Case 15 (nm1x1032). Case 15 has the same exact parameter constraints as those set for Case 14, except a lower drip rate was applied. The lower drip rate allows the acid released from steel degradation to remain in the WP longer. This has the effect of lowering the pH at the beginning of the run to below 5 for almost 30,000 years. Once again, since the pH is so low, GdPO4·10H2O is only able to form in small amounts and the level of Gd in solution remains high for this entire period. While the flush rate is slower, the lengthy amount of time at the lower pH allows for 12.9% Gd loss from the WP. This makes up the majority of the 13.01% that was lost during the entire case.

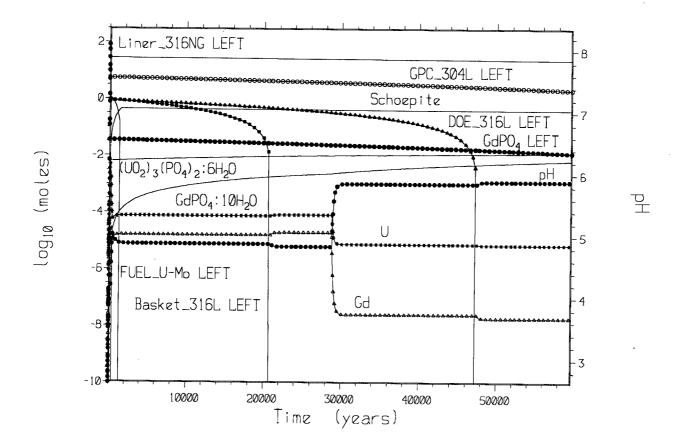


Figure 13. Case 15 (1st Stage: nm1x1032): WP Materials, Minerals, and Aqueous U

The high acidity of the system over the entire length of the first stage allows nearly all (98.11%) of the U to remain within the WP.

Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposal Waste Packages: Effects of Updated Design and Rates

Document Identifier: CAL-EDC-MD-000015 REV00

Page 75 of 119

Table 39. Case 15 (1 st Stage: nm1x1032): Composition of Corrosion Products (g), Total Mas	s, and
Density	

	Years			
Element	32128	48012	59928	
0	7.09E+02	7.69E+02	8.08E+02	
AI	2.02E+01	2.02E+01	2.02E+01	
В	0.00E+00	0.00E+00	0.00E+00	
Ва	0.00E+00	0.00E+00	0.00E+00	
Са	1.10E+00	1.21E+00	1.21E+00	
CI	9.47E-15	1.10E-15	0.00E+00	
Cr	1.40E-09	1.47E-10	0.00E+00	
Cu	0.00E+00	0.00E+00	0.00E+00	
F	8.12E-13	8.67E-14	0.00E+00	
Fe	1.42E+03	1.55E+03	1.63E+03	
Gd	4.62E-01	8.30E-01	1.11E+00	
Н	3.75E+00	3.68E+00	3.63E+00	
С	8.82E-13	0.00E+00	0.00E+00	
Р	7.56E-01	9.13E-01	1.02E+00	
К	1.20E-14	1.48E-15	0.00E+00	
Mg	8.78E-14	1.11E-14	0.00E+00	
Mn	2.14E+01	2.52E+01	2.76E+01	
Мо	2.64E+00	2.90E+00	2.90E+00	
N	1.05E-13	1.06E-14	7.59E-19	
Na	6.17E-14	7.61E-15	0.00E+00	
Ni	1.05E-12	1.10E-13	1.53E-16	
S	4.78E-13	6.53E-14	2.61E-18	
Si	1.09E+01	1.41E+01	1.64E+01	
Ti	3.15E-02	3.15E-02	3.15E-02	
U	1.07E+02	1.07E+02	1.07E+02	
Zn	0.00E+00	0.00E+00	0.00E+00	
Total (Kg)	561	609	639	
Density (g/cm³)	5.05	5.06	5.06	

NOTE: Mass (g) of each element is based on 1 liter aqueous fluid. To obtain total grams of each element in the WP, multiply by WP void volume of 4102 liters.

Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposal Waste Packages: Effects of Updated Design and Rates

Document Identifier: CAL-EDC-MD-000015 REV00

Page 76 of 119

P	Years				
Element	32128	48012	59928		
AI	1.84E-06	1.56E-06	1.52E-06		
В	1.00E-16	1.00E-16	1.00E-16		
Ba	1.00E-16	1.00E-16	1.00E-16		
Са	2.77E-04	3.18E-04	3.24E-04		
CI	2.01E-04	2.01E-04	2.01E-04		
Cr	1.13E-02	9.89E-03	9.71E-03		
Cu	1.00E-16	1.00E-16	1.00E-16		
F	1.15E-04	1.15E-04	1.15E-04		
Fe	5.26E-12	4.93E-12	4.89E-12		
Gd	2.50E-08 1.95E-0		1.88E-08		
С	4.72E-05	4.81E-05	4.82E-05		
Р	2.66E-08	2.76E-08	2.78E-08		
К	1.29E-04	1.29E-04	1.29E-04		
Mg	8.27E-05	8.27E-05	8.27E-05		
Mn	2.22E-11	1.87E-11	1.82E-11		
Мо	4.07E-04	3.34E-04	3.25E-04		
N	3.58E-04	3.27E-04	3.23E-04		
Na	1.99E-03	1.99E-03	1.99E-03		
Ni	6.19E-03	5.29E-03	5.18E-03		
S	2.22E-04	2.18E-04	2.18E-04		
Si	5.68E-05	5.68E-05	5.68E-05		
Ti	0.00E+00	0.00E+00	0.00E+00		
U	7.75E-06	7.43E-06	7.39E-06		
Zn	1.00E-16	1.00E-16	1.00E-16		
рН	5.86	5.89	5.89		

Table 40. Case 15 (1st Stage: nm1x1032): Solution Composition in Molality

Waste Package Project	Calculation
Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codispo	sal Waste Packages:
Effects of Updated Design and Rates	
Document Identifier: CAL-EDC-MD-000015 REV00	Page 77 of 119

Figure 14 and Figure 15 and Table 41 and Table 42 show the results of the second stage of Case 15 ($nm2{xy}1302$). In the second stage of Case 15, the pH remains around 6.4 for most of the run. At 600,000 years, when the 316NG liner is completely degraded, the pH increases to above 8 over a period of 15,000 years. Uranium in solution increases by an order of magnitude and over the last 33,000 years of the second stage, almost 5% more U is lost from the WP. Since the pH remained low for most of Case 15, most of the U (93.30%) was retained, however, 6.7% was lost during periods of high pH or times when there was a dramatic change in the pH of the system, allowing U to be lost while the system attempted to equilibrate itself at the new pH.

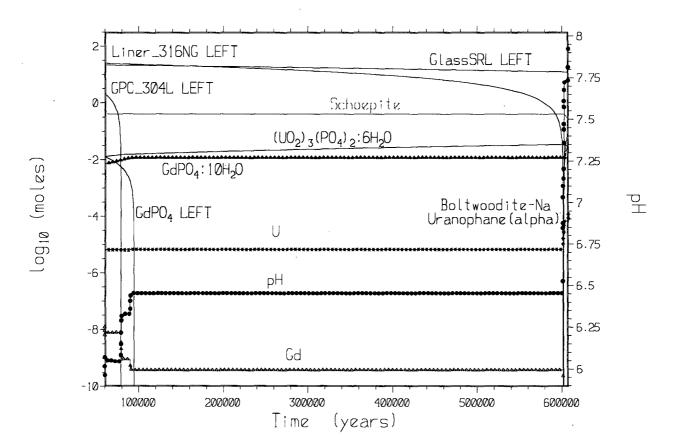


Figure 14. Case 15 (2nd Stage: nm2x1302): WP Materials, Minerals, and Aqueous U

Waste Package Project Calculation Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposal Waste Packages: Effects of Updated Design and Rates Document Identifier: CAL-EDC-MD-000015 REV00

Page 78 of 119

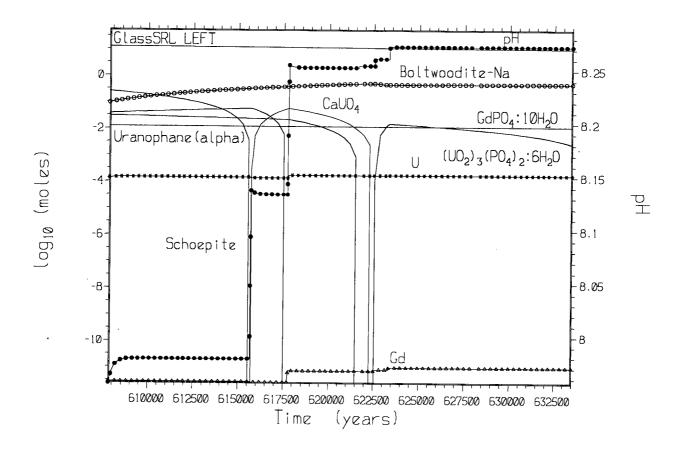


Figure 15. Case 15 (2nd Stage: nm2y1302): WP Materials, Minerals, and Aqueous U

Calculation

Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposal Waste Packages: Effects of Updated Design and Rates

Document Identifier: CAL-EDC-MD-000015 REV00

Page 79 of 119

Table 41. Case 15 (2 nd Stage: nm2{xy}1302): Composition of Corrosion Products (g), Total Mass, and
Density

Element	Years				
Element	60119	91669	607830	617790	633780
0	8.09E+02	9.49E+02	2.10E+03	2.12E+03	2.16E+03
Al	2.02E+01	2.14E+01	4.25E+01	4.38E+01	4.64E+01
В	9.65E-16	0.00E+00	5.15E-12	9.38E-17	1.88E-17
Ва	3.39E-04	6.89E-02	1.28E+00	1.37E+00	1.53E+00
Ca	1.21E+00	1.74E+00	1.07E+01	1.15E+01	1.30E+01
CI	0.00E+00	8.80E-15	0.00E+00	0.00E+00	0.00E+00
Cr	1.28E-04	2.61E-02	0.00E+00	0.00E+00	0.00E+00
Cu	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
F	0.00E+00	8.08E-14	6.07E-02	1.58E-01	3.22E-01
Fe	1.63E+03	1.88E+03	3.49E+03	3.49E+03	3.50E+03
Gd	1.11E+00	1.84E+00	1.91E+00	1.91E+00	1.91E+00
Н	3.63E+00	4.80E+00	1.02E+01	1.00E+01	1.03E+01
С	0.00E+00	2.10E-13	1.12E-01	1.19E-01	1.34E-01
Р	1.02E+00	1.34E+00	2.53E+00	2.51E+00	2.09E+00
к	0.00E+00	5.20E-14	2.67E-01	1.47E+00	3.88E+00
Mg	1.61E-04	3.41E-01	6.41E+00	6.92E+00	7.93E+00
Mn	2.77E+01	3.47E+01	8.14E+01	8.14E+01	8.14E+01
Мо	2.90E+00	2.98E-01	0.00E+00	0.00E+00	0.00E+00
N	0.00E+00	1.49E-14	0.00E+00	3.80E-19	0.00E+00
Na	0.00E+00	1.75E-13	2.13E+00	8.88E+00	1.95E+01
Ni	0.00E+00	4.05E+00	1.84E+02	1.84E+02	1.84E+02
S	0.00E+00	8.21E-13	0.00E+00	0.00E+00	0.00E+00
Si	1.65E+01	3.39E+01	3.06E+02	3.19E+02	3.45E+02
Ti	3.15E-02	3.15E-02	3.15E-02	3.15E-02	3.15E-02
U	1.07E+02	1.08E+02	1.21E+02	1.21E+02	1.21E+02
Zn	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Total (Kg)	640	741	1550	1562	1586
Density (g/cm³)	5.06	5.00	4.63	4.62	4.55

NOTE: Mass (g) of each element is based on 1 liter aqueous fluid. To obtain total grams of each element in the WP, multiply by WP void volume of 4102 liters.

Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposal Waste Packages: Effects of Updated Design and Rates

Document Identifier: CAL-EDC-MD-000015 REV00

Page 80 of 119

Floment	Years				
Element	60119	91669	607830	617790	633780
AI	5.14E-07	5.39E-08	5.81E-08	1.16E-07	1.21E-07
В	6.68E-04	1.37E-03	4.01E-03	4.99E-03	5.60E-03
Ba	5.81E-07	6.02E-07	1.06E-08	2.97E-09	2.78E-09
Са	3.87E-04	2.86E-04	1.05E-05	2.14E-05	1.77E-05
CI	2.01E-04	2.01E-04	2.01E-04	2.01E-04	2.01E-04
Cr	1.26E-02	4.09E-03	8.08E-13	1.00E-16	1.00E-16
Cu	1.00E-16	1.00E-16	1.00E-16	1.00E-16	1.00E-16
F	1.19E-04	1.23E-04	3.42E-08	2.36E-14	2.81E-14
Fe	3.68E-12	2.09E-12	1.14E-12	1.16E-12	1.16E-12
Gd	6.37E-09	3.93E-10	2.76E-12	7.20E-12	9.68E-12
С	5.56E-05	8.42E-05	1.68E-03	3.52E-03	3.68E-03
Р	3.64E-08	7.21E-08	8.64E-06	1.97E-04	2.64E-04
К	3.01E-04	4.83E-04	4.14E-04	5.52E-04	4.93E-04
Mg	1.52E-04	1.11E-04	6.11E-06	1.23E-05	1.02E-05
Mn	8.73E-12	1.22E-12	1.14E-15	5.16E-16	5.07E-16
Мо	3.51E-04	3.11E-04	1.50E-04	1.00E-16	1.00E-16
N	3.79E-04	2.13E-04	1.42E-04	1.42E-04	1.42E-04
Na	3.32E-03	4.71E-03	2.58E-03	4.77E-03	5.24E-03
Ni	6.52E-03	9.13E-04	7.56E-07	2.07E-07	1.93E-07
S	2.34E-04	2.22E-04	2.47E-04	2.60E-04	2.68E-04
Si	5.68E-05	5.28E-05	4.50E-05	4.28E-05	4.32E-05
Ti	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
U	6.46E-06	6.84E-06	1.34E-04	1.73E-04	1.77E-04
Zn	1.00E-16	1.00E-16	1.00E-16	1.00E-16	1.00E-16
рН	6.07	6.45	7.96	8.26	8.27

Table 42. Case 15 (2nd Stage: nm2{xy}1302): Solution Composition in Molality

Waste Package Project	Calculation
Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposa	1 Waste Packages:
Effects of Updated Design and Rates	
Document Identifier: CAL-EDC-MD-000015 REV00	Page 81 of 119

6.2 SOURCE TERM: EFFLUENT CONCENTRATION OF FISSILE U

Cases 20 through 23 (Table 43) are focused on maximizing the soluble concentration of fissile U (²³⁵U) from fuel flowing out of the WP, referred to as the source term. Since the U in the glass is composed primarily of ²³⁸U (Table 44), it is important to run cases where most of the U in solution is from the fuel. From the source term cases, enrichment fractions can be derived which show the fraction of fissile U to total U in the system. It is necessary to calculate ²³⁵U enrichment of effluent waters outside of EQ6 since EQ6 does not differentiate between isotopes of an element but takes the total of all isotopes as a total elemental inventory. The enrichment calculations in this section will be included in the external accumulation calculation.

Case	Case ID	Scenario	Log fCO ₂
16	nm1x3432	One-stage	-3
17	nt1x1331	One-stage - (Total surface area of liner exposed)	-3
18	nt1x1432	One-stage - (Total surface area of liner exposed)	-3
19	nm1x1031 / nm2x1402	Scenario II - Two-stage	-3
20	nc1x1031 / nc2x1402	Scenario II - Two-stage	-2

Table 43. Summary of Cases Run for Source Term Calculations

This part of the calculation focuses on the source term runs and uses input parameters designed to maximize U enrichment in solution. These cases (Sections 6.2.1 through 6.2.3) concentrate on circumstances where the fraction of 235 U in solution should be higher than the cases presented in Section 6.1 of this calculation. This includes assuming that the fuel is fully exposed to the solution in the WP, and it is degrading at the fast degradation rate. Since source term calculations are concerned with effluent (aqueous) composition, only tables for aqueous compositions are given for this section.

Table 44. Isotopic Mole Fractions of HLW Glass and Fermi	Fuel
--	------

Isotope	Mole Fraction of Total U in HLW Glass ^a	Mole Fraction of Total U in Fermi Fuel ^b	
U ²³⁴	0.002915		
U ²³⁵	0.008860	0.2593	
U ²³⁶	0.001748		
U ²³⁸	0.986477	0.7407	

Sources: ^a Ref. 16, Attachment I, p. I-7 (recalculated for mole fraction of total U in "Unenrich Fermi.xls", Attachment III)

^b Ref. 9, Section 3.1 7 (recalculated for mole fraction of total U in "Unenrich Fermi.xls", Attachment III).

Waste Package Project	Calculation
Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisp	osal Waste Packages:
Effects of Updated Design and Rates	· · ·
Document Identifier: CAL-EDC-MD-000015 REV00	Page 82 of 119

6.2.1 Influence of Degradation Rates on Source Term

Several cases (16 through 18) were run varying the degradation rates of the reactants to see the impact on U enrichment in solution. This was performed using single stage scenarios where the glass, fuel, and steels are all exposed to degradation simultaneously. All values presented in subsequent tables for Sections 6.2.1 through 6.2.3 are pulled directly from the "*.elem_aqu.txt" files (Attachment III) for each case. The times used in all cases are indicative of periods of interest due to low or high pH or significant changes in aqueous U concentration.

It is generally assumed, that during degradation of the WP, only the inside of the 316NG liner will be significantly exposed to degradation. However, there is a small gap between the 316NG liner and the Alloy 22 outer shell that may flood along with the rest of the WP. For this reason, two cases were run exposing the total surface area of the 316NG liner to degradation instead of exposing only the inner surface area. This has the general effect of increasing the degradation rate of the 316NG liner since EQ6 calculates degradation rate by multiplying the degradation rate constant (moles/cm²·sec) with the surface area of the component (cm²) to arrive at a reaction rate in moles/second. Reference 55 (Section 6.1.3) has also shown that increasing the exposed area of the liner increases U in solution and U loss.

For all source term cases, low and average drip rates are used. Not only are these more probable, but they allow better accumulation through dilution. If the drip rate is too high, the waters within the subsurface will not be able to dilute the effluent from the waste package significantly enough to cause precipitation of U minerals from the effluent until it is a great distance from the source. Therefore, it is not conservative for criticality to use a high drip rate. These results will also be input into PHREEQC (Ref. 60), and the lower rates allow PHREEQC to converge more easily.

Table 45 sums the results of the one stage source term cases. The cases are explained individually in more detail later in this section.

Case	Case ID	Peak U (moles/Kg)	Year	Enrichment Fraction	pН
16	nm1x3432	1.17E-02	144	0.2498	3.90
		5.33E-02	37,241	0.2181	8.82
17	nt1x1331	1.48E-03	136	0.2563	4.29
		4.34E-02	368,664	0.2167	8.81
18	nt1x1432	3.82E-02	44,673	0.2032	8.80

Figure 16 and Figure 17 and Table 46 show the results of Case 16 (nm1x3432). The high steel degradation rate is used to exhaust the acid producing steel components quickly. After the steels are completely depleted, at 28,000 years, glass degradation raises the pH of the system so that all of the U-bearing minerals dissolve by 38,000 years to create a high concentration of U in solution. Since the minerals were formed during the period when most of the U in the system was from the degradation of the Fermi fuel, the enrichment is expected to be high.

Waste Package Project	Calculation
Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposal	Waste Packages:
Effects of Updated Design and Rates	
Document Identifier: CAL-EDC-MD-000015 REV00	Page 83 of 119

The results from ASPRIN show that when the peak U concentration (1.17E-02 and 5.33E-02 moles/Kg) occurs, the enrichment fraction of U235/total U is 0.2498 and 0.2181 respectively. The fuel contains a mole fraction of 0.2593 U235/total U so these enrichments are close to the maximum enrichment possible.

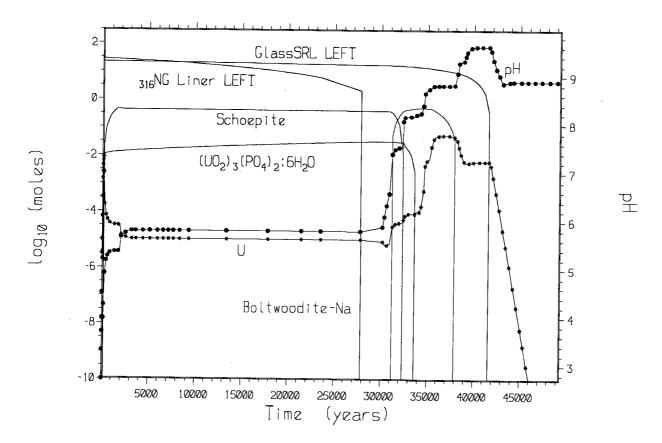


Figure 16. Case 16 (nm1x3432): WP Materials, Minerals, and Aqueous U

Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposal Waste Packages: Effects of Updated Design and Rates

Document Identifier: CAL-EDC-MD-000015 REV00

Page 84 of 119

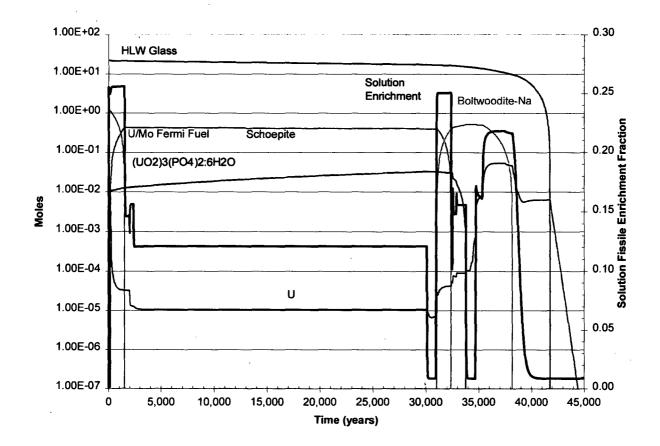


Figure 17. Case 16 (nm1x3432): Enrichment and U-bearing solids in the WP

Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposal Waste Packages: Effects of Updated Design and Rates

Document Identifier: CAL-EDC-MD-000015 REV00

Page 85 of 119

Flowert	Years			
Element	144	37246	41764	49725
AI	4.24E-04	1.56E-07	1.12E-07	1.29E-07
В	3.80E-02	1.12E-01	1.79E-01	1.06E-14
Ba	1.05E-05	9.89E-10	5.36E-11	2.12E-10
Са	2.44E-03	8.82E-06	6.70E-06	1.38E-05
CI	2.01E-04	2.01E-04	2.01E-04	2.01E-04
Cr	1.64E+00	6.65E-14	1.00E-16	1.00E-16
Cu	2.16E-04	1.00E-16	1.00E-16	1.00E-16
F	3.37E-04	7.04E-04	1.36E-03	1.15E-04
Fe	1.03E-09	1.34E-12	2.68E-12	1.33E-12
Gd	1.67E-05	4.04E-09	3.66E-07	4.50E-08
С	1.71E-05	1.78E-01	2.00E-01	1.48E-02
Р	1.67E-08	3.93E-06	1.08E-05	1.48E-07
К	3.40E-03	4.12E-03	5.42E-03	1.39E-03
Mg	6.49E-03	7.30E-05	6.53E-06	1.44E-05
Mn	3.62E-07	1.24E-15	7.93E-15	1.11E-15
Мо	1.23E-04	2.17E-07	2.55E-15	1.00E-16
N	3.21E-02	1.42E-04	1.42E-04	1.42E-04
Na	7.73E-02	2.78E-01	4.27E-01	1.49E-02
Ni	7.75E-01	4.86E-08	1.17E-09	1.28E-08
S	7.03E-04	1.73E-03	3.43E-03	1.92E-04
Si	7.82E-05	9.44E-05	5.83E-04	5.19E-05
Ti	0.00E+00	0.00E+00	0.00E+00	0.00E+00
U	1.17E-02	5.33E-02	6.32E-03	1.18E-16
Zn	1.91E-04	1.00E-16	0.00E+00	1.30E-19
рН	3.92	8.82	9.63	8.90

Table 46. Case 16 (nm1x3432): Solution Composition in Molality

Waste Package Project	Calculation
Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposal Effects of Updated Design and Rates	Waste Packages:
Document Identifier: CAL-EDC-MD-000015 REV00	Page 86 of 119

Figure 18 and Figure 19 and Table 47 show the results of Case 17. Like Case 16, A peak U concentration (1.48E-03 moles/Kg) in solution corresponds to a high enrichment fraction (0.2563). For the first 285,000 years, the pH remains around 6 until all of the steel from the 316NG liner is completely degraded. After this point, the pH slowly rises over the next 100,000 years as glass degrades and adds to the alkalinity of the system. When the pH reaches a level of 8.81 at 370,000 years, all of the U minerals remaining in the WP dissolve, creating a peak aqueous U concentration of 4.34E-02 moles/Kg having an enrichment fraction of 0.2167.

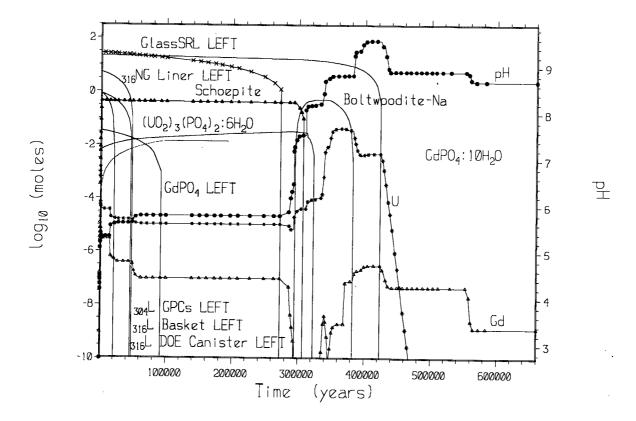


Figure 18. Case 17 (nt1x1331): WP Materials, Minerals, and Aqueous U

The results of ASPRIN (Figure 19) show that at the peak aqueous U content, the enrichment of the solution is 0.2167, very close to that for Case 16. This shows that Cases 16 and 17 produce very similar results, however, the parameters set in Case 16 allow for the enriched U concentration to peak much earlier after initial breach of the WP than in Case 17.

Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposal Waste Packages: Effects of Updated Design and Rates

Document Identifier: CAL-EDC-MD-000015 REV00

Page 87 of 119

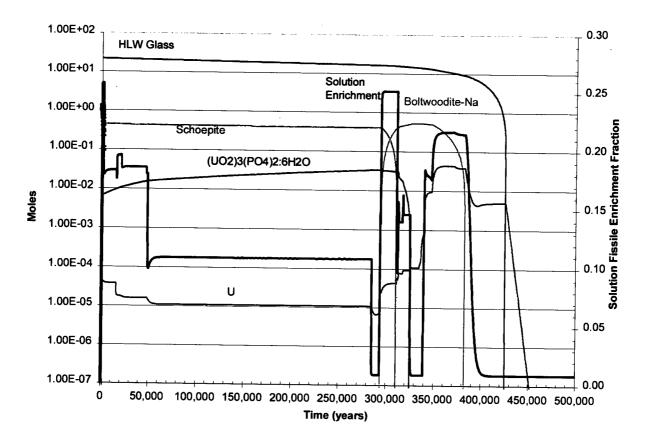


Figure 19. Case 17 (nt1x1331): Enrichment Fraction and U-bearing Solids in the WP.

Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposal Waste Packages: Effects of Updated Design and Rates

Document Identifier: CAL-EDC-MD-000015 REV00

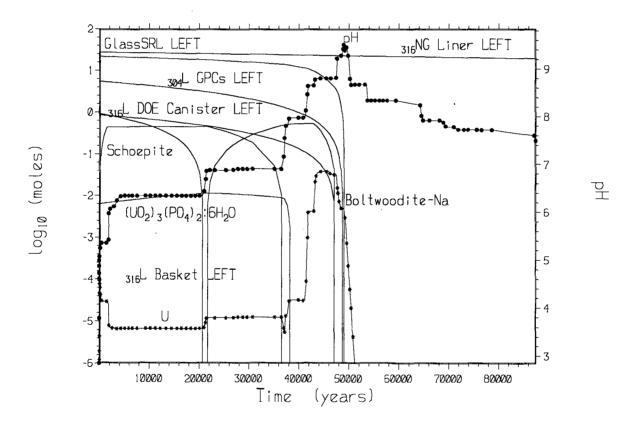
Page 88 of 119

F I	Years			
Element	136	313280	370620	660410
AI	8.26E-05	1.01E-07	1.84E-07	2.06E-07
В	3.55E-03	3.96E-02	9.16E-02	1.00E-16
Ва	6.42E-08	6.33E-09	9.36E-10	4.61E-10
Са	5.22E-04	1.91E-05	5.60E-06	3.72E-06
CI	2.01E-04	2.01E-04	2.01E-04	2.01E-04
Cr	1.26E-02	3.45E-06	3.44E-16	1.00E-16
Cu	2.56E-04	1.00E-16	1.00E-16	1.00E-16
F	1.35E-04	2.07E-14	5.99E-04	1.15E-04
Fe	2.04E-10	1.15E-12	1.34E-12	1.24E-12
Gd	1.96E-05	3.46E-11	1.96E-09	1.30E-09
С	3.39E-05	2.96E-03	1.48E-01	8.68E-03
Р	1.42E-08	9.13E-04	7.06E-06	1.10E-06
К	3.48E-06	1.94E-03	3.38E-03	8.31E-04
Mg	2.92E-03	2.00E-04	6.76E-05	2.93E-05
Mn	4.04E-08	7.76E-16	1.20E-15	6.96E-16
Мо	1.88E-04	6.34E-03	1.38E-08	1.00E-16
N	3.81E-04	1.42E-04	1.42E-04	1.42E-04
Na	9.02E-03	2.05E-02	2.28E-01	8.87E-03
Ni	6.86E-03	4.20E-07	4.75E-08	3.02E-08
S	1.00E-02	7.36E-04	1.45E-03	1.92E-04
Si	5.72E-05	4.01E-05	8.40E-05	4.45E-05
Ti	0.00E+00	0.00E+00	0.00E+00	0.00E+00
U	1.48E-03	7.92E-05	4.34E-02	1.00E-16
Zn	2.26E-04	1.00E-16	1.00E-16	1.00E-16
рН	4.29	8.17	8.81	8.69

Table 47. Case 17 (nt1x1331): Solution Composition in Molality

Waste Package Project	Calculation
Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposa	1 Waste Packages:
Effects of Updated Design and Rates	
Document Identifier: CAL-EDC-MD-000015 REV00	Page 89 of 119

Figure 20 and Figure 21 and Table 48 show the results of Case 18. In Case 18, even though the surface area of the 316NG liner was doubled, the slow steel degradation rate combined with a fast HLW glass degradation rate is not enough to keep the pH of the system as low as the previous cases. At the beginning of Case 18, the pH remains below 6.8 for the first 37,000 years. After this point, it rises to a level of 8.8 as the steel from the 316L basket and DOE canister as well as the 304L GPCs are nearing exhaustion. When the pH reaches 8.8 at around 42,000 years, all of the minerals dissolve and aqueous U rises to a high of 3.82E-02 moles/Kg. When the aqueous U reaches this high plateau, most of the glass is also degraded so the enrichment for Case 18 is not expected to be as high as that for Cases 16 and 17. This is confirmed by ASPRIN (Figure 21) which shows an enrichment fraction of 0.2032 at this point.





Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposal Waste Packages: Effects of Updated Design and Rates

Document Identifier: CAL-EDC-MD-000015 REV00

Page 90 of 119

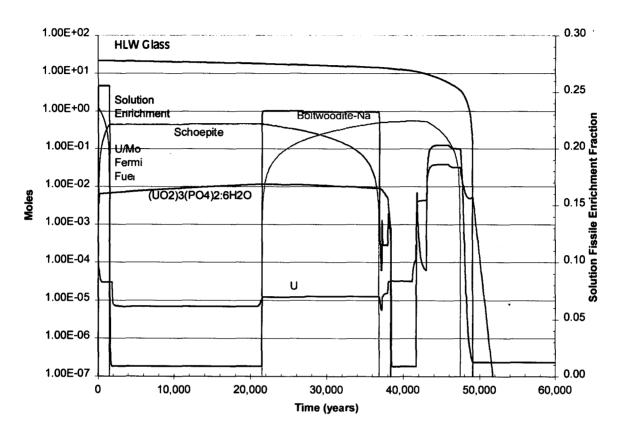


Figure 21. Case 18 (nt1x1432): Enrichment Fraction and U-bearing solids in the WP.

Calculation

Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposal Waste Packages: Effects of Updated Design and Rates

Document Identifier: CAL-EDC-MD-000015 REV00

Page 91 of 119

Florent	Years			
Element	18	29642	45890	87672
AI	4.00E-05	1.12E-08	1.64E-07	1.56E-08
В	2.62E-03	2.03E-02	1.10E-01	1.00E-16
Ва	9.07E-08	1.68E-07	1.02E-09	2.95E-07
Са	9.04E-05	7.23E-04	9.96E-06	3.17E-04
CI	2.01E-04	2.01E-04	2.01E-04	2.01E-04
Cr	1.65E-03	2.14E-02	2.15E-02	6.02E-03
Cu	3.35E-05	1.00E-16	1.00E-16	1.00E-16
F	1.30E-04	1.53E-04	6.65E-04	1.02E-04
Fe	5.03E-11	1.48E-12	1.33E-12	1.24E-12
Gd	2.62E-06	4.16E-11	2.71E-09	5.14E-11
С	3.52E-05	1.94E-04	1.32E-01	3.89E-04
Р	1.40E-08	2.84E-07	4.85E-06	1.06E-07
к	8.09E-04	4.36E-03	3.82E-03	7.07E-03
Mg	1.95E-04	7.51E-04	7.64E-05	1.88E-03
Mn	2.87E-09	2.19E-13	1.18E-15	2.81E-14
Мо	1.09E-03	4.89E-04	8.16E-04	4.81E-04
N	1.73E-04	5.47E-04	5.47È-04	2.92E-04
Na	7.18E-03	3.32E-02	2.59E-01	2.26E-03
Ni	8.99E-04	1.64E-04	5.07E-08	2.10E-05
S	3.37E-03	5.29E-04	1.76E-03	2.16E-04
Si	7.51E-05	4.49E-05	8.86E-05	3.94E-05
Ti	0.00E+00	0.00E+00	0.00E+00	0.00E+00
U	1.30E-04	1.27E-05	3.82E-02	1.00E-16
Zn	2.96E-05	1.00E-16	1.00E-16	1.00E-16
рН	4.80	6.91	8.80	7.30

Table 48. Case 18 (nt1x1432): Solution Composition in Molality

6.2.1 Influence of Degradation Order on Source Term

In an attempt to increase the enrichment fraction, the U input from HLW glass must be minimized as much as possible. For this reason, Case 19 (nm1x1031/nm2x1402) is a Scenario II two-stage run. By using this type of case, the fuel is allowed to degrade without U input from the HLW glass. The second stage then adds the glass to raise the pH and force the U into solution with minimal influence on total U in solution by the HLW glass. Figure 22 through Figure 24 and Table 49 show the effects of keeping the HLW glass from interacting with the solution in the WP until the second stage.

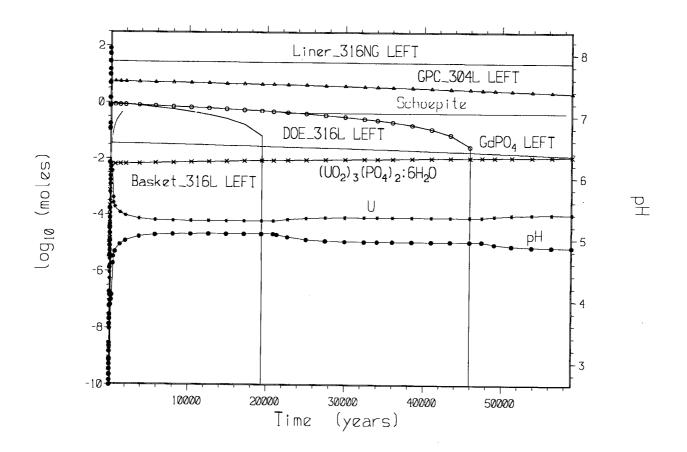


Figure 22. Case 19 (1st Stage: nm1x1031): WP Materials, Minerals, and Aqueous U

In the first stage of Case 19 (nm1x1031), the pH hovers around 5 for most of the run retaining most of the U in the package as $(UO_2)_3(PO_4)_2 \cdot 6H_2O$ and schoepite. After the second stage (nm2x1402) begins, the pH remains low until the steel from the 304L GPCs is gone just before 79,000 years. At this point, the pH begins to rise causing a like rise in aqueous U. The first U peak (1.96E-01 moles/Kg) is seen at 85,000 years when the pH is at 8.85. Four thousand years

Waste Package Project	Calculation
Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposa	al Waste Packages:
Effects of Updated Design and Rates	
Document Identifier: CAL-EDC-MD-000015 REV00	Page 93 of 119

later, the pH peaks at 10.00 at which point $Na_4UO_2(CO_3)_3$ forms causing a slight dip in aqueous U. When the pH decreases to 9.38, the U carbonate dissolves and another U peak (1.86E-01 moles/Kg) is seen at 94,000 years. Glass depletion occurs between these two U peaks. Therefore, the second peak of aqueous U should have a lower enrichment than the first, which occurs before complete degradation of the HLW glass.

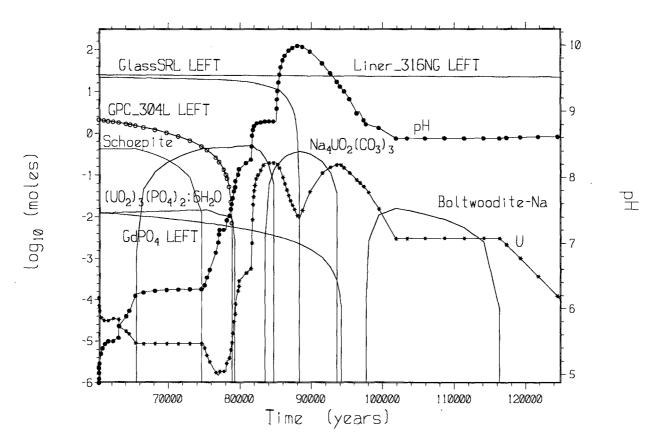


Figure 23. Case 19 (2nd Stage: nm2x1402): WP Materials, Minerals, and Aqueous U

Results from ASPRIN show that the first peak corresponds to an enrichment of 0.2200 and the second to an enrichment of 0.1802 agreeing with the above stated observations. Even though this case results in approximately the same enrichment as in Cases 16 and 17, the amount of U in solution is much higher in Case 19, over half an order of magnitude. Therefore Case 19, depending on the probability of the scenario, is a better case for source term since it is more conservative for external criticality.

Calculation

Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposal Waste Packages: Effects of Updated Design and Rates

Document Identifier: CAL-EDC-MD-000015 REV00

Page 94 of 119

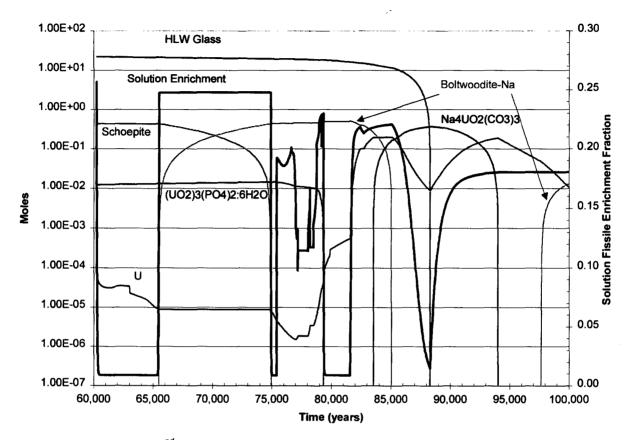


Figure 24. Case 19 (2nd Stage: nm2x1402): Enrichment Fraction and U bearing solids in the WP.

Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposal Waste Packages: Effects of Updated Design and Rates

Document Identifier: CAL-EDC-MD-000015 REV00

Page 95 of 119

	Years				
Element	60233	85077	94389	317180	
AI	3.61E-05	3.93E-08	4.64E-08	1.60E-06	
В	1.00E-16	9.74E-02	1.23E-01	1.00E-16	
Ba	1.00E-16	8.64E-10	1.32E-10	6.93E-07	
Ca	1.19E-04	6.15E-05	1.18E-05	7.25E-05	
CI	2.01E-04	2.01E-04	2.01E-04	2.01E-04	
Cr	9.72E-02	5.29E-02	4.13E-02	4.09E-02	
Cu	5.15E-14	1.04E-16	1.00E-16	1.00E-16	
F	1.15E-04	4.10E-03	1.24E-03	1.23E-04	
Fe	5.46E-11	1.32E-12	1.94E-12	5.98E-12	
Gd	3.77E-05	1.90E-07	2.61E-07	2.31E-11	
С	3.42E-05	6.20E-01	5.97E-01	4.66E-05	
Р	1.45E-08	2.24E-07	4.30E-06	2.22E-05	
к	1.29E-04	1.55E-02	1.41E-02	8.20E-04	
Mg	8.27E-05	5.12E-05	1.07E-05	2.66E-05	
Mn	3.75E-09	1.40E-15	4.36E-15	3.48E-11	
Мо	2.69E-03	7.90E-03	3.40E-03	3.52E-03	
N	1.96E-03	1.08E-03	8.63E-04	8.56E-04	
Na	1.99E-03	1.01E+00	9.72E-01	1.99E-03	
Ni	5.18E-02	4.18E-08	4.91E-09	2.61E-02	
S	4.53E-04	1.34E-02	3.47E-03	3.09E-04	
Si	5.69E-05	2.86E-04	7.24E-04	6.60E-05	
Ti	0.00E+00	0.00E+00	0.00E+00	0.00E+00	
U	1.10E-04	1.96E-01	1.62E-01	1.00E-16	
Zn	4.55E-14	0.00E+00	0.00E+00	1.00E-16	
рН	4.87	8.85	9.33	5.84	

Table 49. Case 19 (2nd Stage: nm2x1402): Solution Composition in Molality

Waste Package Project	Calculation
Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposa	Waste Packages:
Effects of Updated Design and Rates	
Document Identifier: CAL-EDC-MD-000015 REV00	Page 96 of 119

6.2.3 Influence of Higher CO₂ Partial Pressure on Source Term

There is a possibility that the partial pressure of carbon dioxide (CO_2) could increase at Yucca Mountain if there is renewed volcanic activity in the area. The higher CO_2 levels would have a profound effect on the pH of any solutions within the mountain. As shown numerous times previously in this calculation, the pH of the solution within the WP controls the solubility of U-bearing minerals. Case 20 investigates the effects of raising the partial pressure of CO_2 on the release and enrichment of U from the WP. The worst case (Case 19 – more conservative) was taken as the base case to which these results are compared.

Figure 25 and Figure 26 and Table 50 show the results of Case 20. The first stage of Cases 19 and 20 are extremely similar so the first stage of Case 20 (nc1x1031) is not presented here.

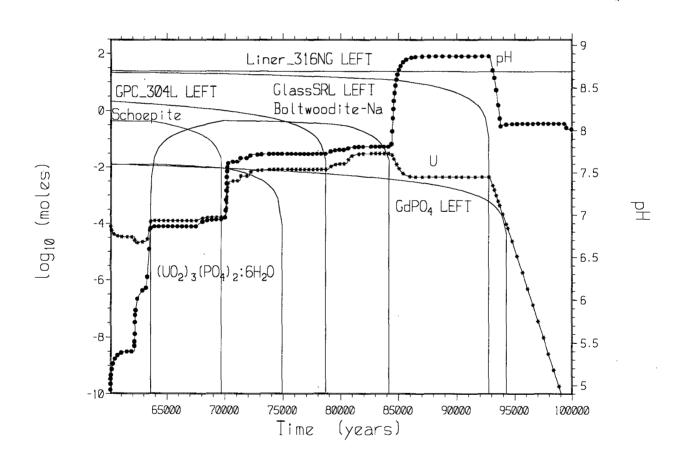


Figure 25. Case 20 (2nd Stage: nc2x1402): WP Materials, Minerals, and Aqueous U

At the start of the second stage (nc2x1402), the pH is still below 7 for the first 10,000 years as the rest of the 304L GPCs degrade. After the steel is completely exhausted, the pH rises above 7.5 and the aqueous U increases to 1.87E-3 moles/Kg. Uranium concentration in solution

Waste Package Project	Calculation
Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposa	al Waste Packages:
Effects of Updated Design and Rates	
Document Identifier: CAL-EDC-MD-000015 REV00	Page 97 of 119

continues to increase until it peaks at 3.08E-02 moles/Kg at a pH of 7.81 at 84,400 years. The pH levels at which the U-bearing minerals dissolve is much lower in Case 20 than that in Case 19. The reason for this is that U minerals are 25 times more soluble at $\log f_{CO_2} = -2$ than at $\log f_{CO_2} = -3$ (Ref. 56, Section 6.3.3). The point of highest concentration of U in solution corresponds to the dissolution of Na-boltwoodite, which contains primarily fissile U from the degradation of the fuel in the first stage. Therefore the enrichment fraction is the highest at this point, peaking at 0.2346. Although the enrichment is the highest here than seen for the other cases, due the significant increase in solubility of U-bearing minerals at higher CO₂ levels, Case 19 probably represents the more conservative source term.

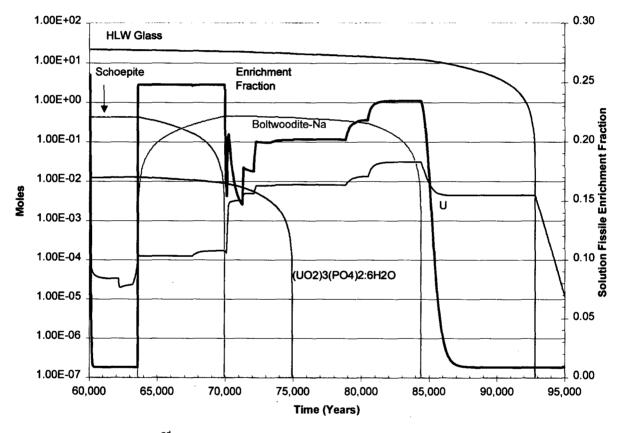


Figure 26. Case 20 (2nd Stage: nc2x1402): Enrichment Fraction and U-bearing Solids in the WP.

Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposal Waste Packages: Effects of Updated Design and Rates

Document Identifier: CAL-EDC-MD-000015 REV00

Page 98 of 119

	Years					
Element	136	1496	5436	20844	60069	
Al	2.43E-04	3.41E-05	2.60E-05	2.33E-05	3.51E-05	
В	1.00E-16	1.00E-16	1.00E-16	1.00E-16	1.00E-16	
Ва	1.00E-16	1.00E-16	1.00E-16	1.00E-16	1.00E-16	
Са	3.24E-04	9.73E-05	5.68E-05	4.96E-05	1.17E-04	
CI	2.01E-04	2.01E-04	2.01E-04	2.01E-04	2.01E-04	
Cr	7.70E-03	7.04E-02	1.66E-01	2.16E-01	1.38E-01	
Cu	2.58E-04	6.56E-04	2.25E-04	3.24E-06	6.27E-11	
F	1.15E-04	1.15E-04	1.15E-04	1.15E-04	1.15E-04	
Fe	6.23E-10	4.65E-11	3.49E-11	3.24E-11	5.33E-11	
Gd	1.98E-05	5.01E-05	1.45E-05	1.01E-05	3.68E-05	
С	3.38E-04	3.35E-04	3.36E-04	3.36E-04	3.37E-04	
Р	1.58E-08	1.43E-08	1.54E-08	1.59E-08	1.47E-08	
к	3.10E-07	1.43E-04	1.34E-04	1.29E-04	1.29E-04	
Mg	2.53E-03	6.32E-03	2.22E-03	1.13E-04	8.27E-05	
Mn	2.22E-07	2.99E-09	1.72E-09	1.49E-09	3.68E-09	
Мо	4.90E-05	3.17E-03	8.25E-03	1.09E-02	3.39E-03	
N	2.90E-04	1.53E-03	3.43E-03	4.42E-03	2.72E-03	
Na	1.99E-03	1.99E-03	1.99E-03	1.99E-03	1.99E-03	
Ni	4.24E-03	3.96E-02	9.41E-02	1.22E-01	7.38E-02	
S	1.19E-02	8.87E-03	3.56E-03	8.27E-04	5.63E-04	
Si	5.83E-05	5.53E-05	5.63E-05	5.68E-05	5.69E-05	
Ti	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	
U	7.54E-03	1.20E-04	7.01E-05	6.13E-05	1.12E-04	
Zn	2.28E-04	5.79E-04	1.99E-04	2.86E-06	5.54E-11	
рН	3.91	4.92	5.08	5.12	4.90	

Table 50. Case 20 (2nd Stage: nc2x1402): Solution Composition in Molality

6.3 SENSITIVITY ANALYSES

6.3.1 GdPO₄ Degradation Rate and Mass

Due to the uncertainty in the degradation rate of the GdPO₄ shot within the basket of the DOE canister and the results of the Enrico-Fermi criticality analysis (Ref. 7, Section 8.5), additional calculations have been made to determine the effects of faster degradation rates and greater masses of GdPO₄ on the retention of Gd in the WP. Because an increase of Gd loss was indicated using faster rates (Section 6.3.1.1), these higher degradation rates are also combined with larger masses of GdPO₄ to examine the effect of higher Gd concentrations on the losses from the WP (Section 6.3.1.2).

6.3.1.1 Effects of Increasing GdPO₄ Degradation Rate on Gd Loss

This section examines the effect of faster GdPO₄ degradation rates. Since there is no reference for the degradation rate of GdPO₄ in an aqueous environment, the cases presented earlier in the calculation used a rate equal to the dissolution of quartz (See Assumption 3-22). The cases presented in Section 6.3.1 use degradation rates equal to those of 304L stainless steel and A516 carbon steel. Although these rates may also not be representative of how GdPO₄ truly degrades in a fully saturated environment, it explores the effects of increased degradation rates on the retention of the Gd in the WP. The runs chosen as the base cases to which to compare these results are those one-stage runs which lost the most Gd, Cases 7 and 8. Table 51 presents the results of the sensitivity runs.

Case ^a	File Name ^a	Length of Run (Years) ^a	Gd Retention ^a	U Retention ^a
21	nA1{xyz}3323	633,780	95.53%	70.01%
22	nL1{xyz}3323	633,780	95.53%	70.01%
23	nA1x3333	245,930	38.16%	60.74%
24	nL1x3333	228,640	63.13%	61.89%
Case ^b	File Name ^b	Length of Run (Years) ^b	Gd Retention ^b	U Retention ^b
7	nm1{xyz}3323	633,780	95.53%	70.01%
8	nm1{xyz}3333	622,460	94.64%	46.97%

Table 51	Gd and U Retention: S	Sensitivity of Easter	GdPO ₄ Degradation Rates
	ou una o ricicinaon. o	choling of radici	Our Of Degraduation reacts

Source: ^a Calculated in "fermi-losses.xls" (Attachment III) ^b From Section 6.1.1

NOTE: Percent retention values presented for Gd and U represent percent of total initial moles of those elements.

The losses of Gd and U between Cases 21, 22, and 7 are exactly the same indicating that at the lower fuel degradation rate, the effect of differing the GdPO₄ degradation rate is inconsequential to the overall losses from the WP. This may be due to the virtual absence of U in the system because of the slowly degrading fuel. Without the U taking up the P in the system, even at low pH values GdPO₄·10H₂O can successfully form.

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Waste Package Project	Calculation
Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposal	Waste Packages:
Effects of Updated Design and Rates	
Document Identifier: CAL-EDC-MD-000015 REV00	Page 100 of 119

Cases 23 and 24, however, differ greatly from the base case, Case 8. For Cases 8, 23, and 24 it can be seen that as the GdPO₄ degradation rate increases, Gd retention decreases. Looking at Cases 23 and 24, most of the Gd loss occurs before the first 1000 years. Figure 27 shows that for Cases 8, 23, and 24 (all of which have a 3333 extension), the pH dips below 4 for a period of over 200 years. During this extreme period of low pH, Gd in solution for the two sensitivity cases is very high. It is during this period that most of the Gd is lost from the WP. For Case 23, all of the GdPO₄ is degraded during the pH low. Case 24 only has about half of the GdPO₄ degraded during this period. Case 8 on the other hand has almost all of the GdPO₄ intact during this period. Therefore, with cases that have a period of very low pH at the beginning of the run, Gd retention will decrease with increasing degradation rate. Since Case 23 gives the most conservative losses of Gd, only tables for Case 23 are presented in this section.

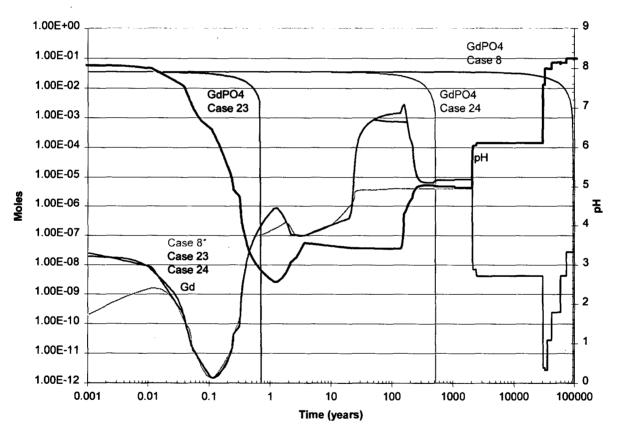


Figure 27. Cases 8, 23, and 24: GdPO₄ Degradation, Aqueous Gd, and pH

Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposal Waste Packages:
Effects of Updated Design and RatesDocument Identifier: CAL-EDC-MD-000015 REV00Page 101 of 119

Flowert	Years					
Element	1043 2114 33132 245930					
0	7.92E+02	8.45E+02	1.70E+03	2.49E+03		
AI	1.97E+01	1.97E+01	2.10E+01	5.41E+01		
В	0.00E+00	3.81E-18	0.00E+00	2.34E-18		
Ba	1.24E-03	0.00E+00	1.54E-02	2.16E+00		
Ca	3.77E-01	8.35E-01	7.93E+00	7.09E+01		
CI	0.00E+00	0.00E+00	0.00E+00	9.61E-19		
Cr	0.00E+00	0.00E+00	0.00E+00	0.00E+00		
Cu	0.00E+00	0.00E+00	0.00E+00	0.00E+00		
F	0.00E+00	0.00E+00	2.15E-01	4.90E-01		
Fe	1.63E+03	1.72E+03	3.40E+03	3.54E+03		
Gd	9.11E-01	8.64E-01	8.63E-01	8.36E-01		
н	3.15E+00	3.59E+00	5.25E+00	1.21E+01		
С	1.03E-12	8.35E-13	1.34E-03	9.63E+00		
Р	1.16E+00	1.23E+00	2.38E+00	2.56E+00		
к	0.00E+00	0.00E+00	0.00E+00	4.24E-18		
Mg	0.00E+00	0.00E+00	7.67E-01	1.14E+01		
Mn	2.73E+01	3.00E+01	8.14E+01	8.14E+01		
Мо	3.95E+00	2.00E+00	0.00E+00	0.00E+00		
N	0.00E+00	0.00E+00	0.00E+00	1.14E-18		
Na	0.00E+00	0.00E+00	1.38E-01	5.52E-01		
Ni	0.00E+00	3.46E-04	1.06E+01	1.05E+01		
S	2.89E-04	0.00E+00	7.82E-18	0.00E+00		
Si	1.24E+01	1.57E+01	8.42E+01	6.07E+02		
Ti	3.15E-02	3.15E-02	3.15E-02	3.15E-02		
U	7.55E+01	1.08E+02	1.07E+02	7.88E+01		
Zn	0.00E+00	0.00E+00	0.00E+00	3.38E-11		
Total (Kg)	625	670	1321	1699		
Density (g/cm³)	5.07	5.07	5.00	4.28		

Table 52. Case 23 (nA1x3333): Composition of Corrosion Products (g), Total Mass, and Density

NOTE: Mass (g) of each element is based on 1 liter aqueous fluid. To obtain total grams of each element in the WP, multiply by WP void volume of 4102 liters.

Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposal Waste Packages: Effects of Updated Design and Rates

Document Identifier: CAL-EDC-MD-000015 REV00

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Page 102 of 119

Flower		Yea	ars	
Element	1043	2114	33132	245930
AI	3.12E-05	5.42E-07	6.30E-08	6.82E-08
В	2.71E-04	1.49E-04	4.35E-04	5.44E-04
Ва	2.05E-06	5.63E-07	8.70E-09	2.96E-09
Ca	4.07E-05	1.46E-04	8.53E-06	1.78E-04
CI	2.01E-04	2.01E-04	2.01E-04	2.01E-04
Cr	1.93E-02	1.14E-02	1.00E-16	1.00E-16
Cu	6.15E-15	1.00E-16	1.00E-16	1.00E-16
F	1.16E-04	1.16E-04	3.72E-08	1.18E-04
Fe	3.33E-11	3.79E-12	1.14E-12	1.15E-12
Gd	7.86E-06	7.14E-09	2.80E-12	2.68E-08
C	3.57E-05	5.46E-05	1.84E-03	2.99E-03
Р	1.48E-08	3.52E-08	9.98E-06	2.86E-09
к	1.99E-04	1.67E-04	2.41E-04	2.69E-04
Mg	1.14E-04	9.97E-05	4.97E-06	1.02E-04
Mn	1.29E-09	9.51E-12	9.63E-16	5.07E-16
Мо	3.34E-03	8.99E-04	5.06E-10	1.00E-16
N	5.28E-04	3.55E-04	1.42E-04	1.42E-04
Na	2.53E-03	2.29E-03	2.35E-03	3.09E-03
Ni	1.21E-02	7.13E-03	6.21E-07	2.09E-07
S	2.52E-04	2.26E-04	1.98E-04	1.99E-04
Si	5.69E-05	5.68E-05	4.51E-05	4.02E-05
Ti	0.00E+00	0.00E+00	0.00E+00	0.00E+00
U	5.46E-05	6.50E-06	1.52E-04	1.33E-05
Zn	5.44E-15	1.00E-16	1.00E-16	1.78E-17
рН	5.01	6.05	7.99	8.24

Table 53. Case 23 (nA1x3333): Solution Composition in Molality

Waste Package Project	Calculation
Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposal W	Vaste Packages:
Effects of Updated Design and Rates	
Document Identifier: CAL-EDC-MD-000015 REV00	Page 103 of 119

6.3.1.2 Effects of Increased GdPO₄ Mass on Gd Loss

Due to the highly reactive nature of the Enrico Fermi-Fuel and losses seen in Section 6.3.1.1, the mass of $GdPO_4$ in the WP was doubled in an attempt to keep more (mass) of Gd in the WP. Table 54 presents the results of the cases where the mass of $GdPO_4$ was doubled.

Table 54. Gd and U Retention¹: Cases with an Increase in GdPO₄ Mass

Case	File Name	Gd Retention ^a	U Retention ^a	Length of Run (Years)	Mass Retained (Kg) ^{b,c}	Case	File Name	Mass Retained (Kg) ^{d,e}
25	nA1d3333	68.85%	61.53%	245,970	12.37	23	nA1x3333	3.43
26	nL1d3333	69.51%	62.15%	228,780	12.49	24	nL1x3333	5.66

NOTES: ^a Calculated in "moresense.xls" (Attachment III)

^b Calculated in "S+A sensitivity.xls" (Attachment III)

^cOut of a maximum of 17.9708 Kg

^dCalculated in "S+A.xls" (Attachment III)

⁹ Out of a maximum of 8.9854 Kg

^f Gd and U Retention presented as percentage of total initial moles within the WP.

Figure 28 shows a comparison between Cases 23, 24, 25, and 26. The number in parentheses indicates the case number.

Comparing Cases 24 and 26, which both simulate GdPO₄ degradation at the 304L stainless steel degradation rate, the results between the case with 3% Gd (Case 24) and the case with 6% Gd (Case 26) are very similar. The GdPO₄ is fully degraded around 500 and 600 years. GdPO₄·10H₂O quickly forms in the first few hours of degradation. When the pH reaches a plateau at 3.4, the Gd in solution rises significantly. For Case 24, all of the GdPO₄·10H₂O dissolves at this pH. For Case 26, this also occurs but not until slightly over a hundred years later as the extra Gd released by the larger amount of GdPO₄ succumbs to the lower pH. At 155 years into the run GdPO₄·10H₂O is able to form again when the pH increases.

Comparing Cases 23 and 25, which both simulate GdPO₄ degradation at the A516 steel degradation rate, there is a significant increase in the retention of Gd in Case 25. Similar to Cases 24 and 26, GdPO₄·10H₂O forms for Cases 23 and 25, with more of it forming for Case 25 due to the doubled mass of Gd. As the pH low is approached, the GdPO₄·10H₂O content in the WP for Case 23 is cut in half while that for Case 25 remains stable. This is possibly due to the significant reserve of Gd in the system from the doubled mass and fast degradation rate. Since the Gd reservoir is so high, even at very low pH levels, GdPO₄·10H₂O levels are affected very little. Because of this, a larger percentage of Gd is lost from the WP for Case 23.

Since only Case 25 is significantly different from the previous section, only tables for this case are presented here.

Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposal Waste Packages: Effects of Updated Design and RatesDocument Identifier: CAL-EDC-MD-000015 REV00Page 104 of 119

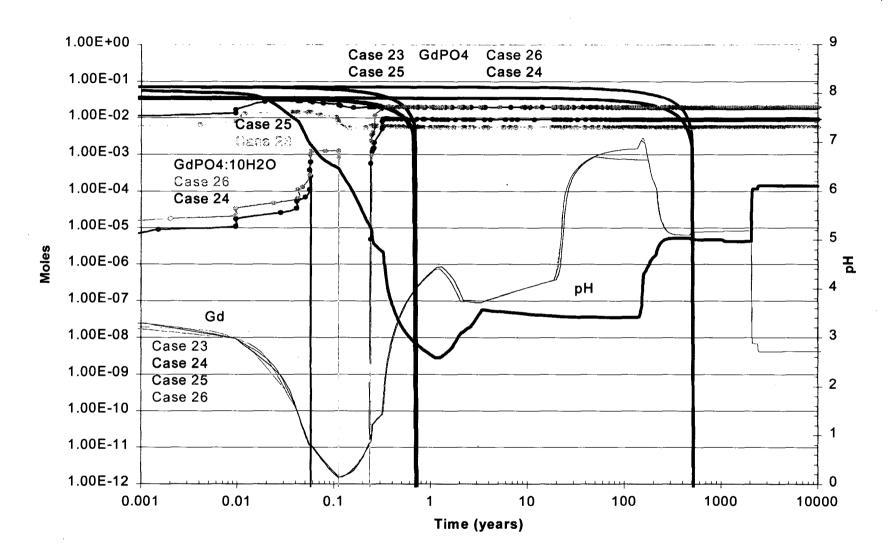


Figure 28. Cases 23-26: Gd Solids, Aqueous Gd, and pH

Calculation

Waste Package Project

Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposal Waste Packages: Effects of Updated Design and Rates

Document Identifier: CAL-EDC-MD-000015 REV00

Page 105 of 119

Flowert	Years						
Element	15064	40096	65071	100280	245970		
0	5.06E+03	7.05E+03	7.33E+03	7.88E+03	1.02E+04		
AI	8.29E+01	8.99E+01	1.05E+02	1.27E+02	2.22E+02		
В	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00		
Ва	0.00E+00	2.96E-01	1.25E+00	2.70E+00	8.86E+00		
Ca	1.43E+01	4.67E+01	9.44E+01	1.36E+02	2.91E+02		
CI	0.00E+00	0.00E+00	1.58E-17	3.94E-18	3.94E-18		
Cr	2.96E-15	0.00E+00	0.00E+00	0.00E+00	0.00E+00		
Cu	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00		
F	2.11E-18	1.83E+00	1.84E+00	1.88E+00	2.01E+00		
Fe	1.02E+04	1.39E+04	1.40E+04	1.41E+04	1.45E+04		
Gd	1.25E+01	1.25E+01	1.25E+01	1.25E+01	1.24E+01		
Н	1.67E+01	2.36E+01	1.91E+01	2.44E+01	5.09E+01		
С	0.00E+00	2.59E-02	1.09E-01	6.19E+00	3.95E+01		
Р	9.00E+00	1.14E+01	1.15E+01	1.16E+01	1.23E+01		
к	0.00E+00	0.00E+00	1.74E-17	0.00E+00	1.74E-17		
Mg	9.04E-01	6.37E+00	1.72E+01	2.39E+01	4.66E+01		
Mn	2.21E+02	3.33E+02	3.33E+02	3.33E+02	3.33E+02		
Мо	2.13E+01	0.00E+00	0.00E+00	0.00E+00	0.00E+00		
N	9.34E-18	1.56E-18	1.56E-18	3.11E-18	4.67E-18		
Na	0.00E+00	1.18E+01	6.22E+00	1.35E+01	2.27E+00		
Ni	2.20E+01	4.33E+01	4.33E+01	4.32E+01	4.29E+01		
S	0.00E+00	7.13E-18	0.00E+00	0.00E+00	0.00E+00		
Si	1.84E+02	4.08E+02	6.48E+02	1.00E+03	2.49E+03		
Ti	1.29E-01	1.29E-01	1.29E-01	1.29E-01	1.29E-01		
U	4.43E+02	4.03E+02	3.17E+02	3.17E+02	3.23E+02		
Zn	0.00E+00	0.00E+00	0.00E+00	2.98E-11	1.94E-10		
Total (Kg)	1.63E+04	2.24E+04	2.29E+04	2.40E+04	2.86E+04		
Density (g/cm ³)	5.05	4.97	4.90	4.73	4.28		

Table 55. Case 25 (nA1d3333): Composition of Corrosion Products (Kg), Total Mass, and Density

Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposal Waste Packages: Effects of Updated Design and Rates

Document Identifier: CAL-EDC-MD-000015 REV00

Page 106 of 119

Element.	Years					
Element	15064	40096	65071	100280	245970	
AI	3.69E-07	6.17E-08	8.60E-08	6.82E-08	6.82E-08	
В	1.29E-04	4.31E-04	4.93E-04	5.44E-04	5.44E-04	
Ba	4.88E-07	9.10E-09	4.74E-09	2.96E-09	2.96E-09	
Са	1.89E-04	8.89E-06	9.56E-05	1.78E-04	1.78E-04	
CI	2.01E-04	2.01E-04	2.01E-04	2.01E-04	2.01E-04	
Cr	8.17E-03	1.00E-16	1.00E-16	1.00E-16	1.00E-16	
Cu	1.00E-16	1.00E-16	1.00E-16	1.00E-16	1.00E-16	
F	1.16E-04	1.17E-04	1.17E-04	1.18E-04	1.18E-04	
Fe	3.37E-12	1.14E-12	1.15E-12	1.15E-12	1.15E-12	
Gd	4.23E-09	2.83E-11	4.17E-09	2.68E-08	2.68E-08	
С	5.76E-05	1.80E-03	2.32E-03	2.99E-03	2.99E-03	
Р	3.86E-08	6.50E-07	9.17E-09	2.86E-09	2.86E-09	
К	1.62E-04	2.40E-04	2.56E-04	2.69E-04	2.69E-04	
Mg	7.45E-05	5.19E-06	5.54E-05	1.02E-04	1.02E-04	
Mn	6.59E-12	1.00E-15	6.28E-16	5.07E-16	5.07E-16	
Мо	5.92E-04	1.00E-16	1.00E-16	1.00E-16	1.00E-16	
N	2.84E-04	1.42E-04	1.42E-04	1.42E-04	1.42E-04	
Na	2.25E-03	2.40E-03	2.66E-03	3.09E-03	3.09E-03	
Ni	4.93E-03	6.51E-07	3.37E-07	2.09E-07	2.09E-07	
S	2.17E-04	1.97E-04	1.98E-04	1.99E-04	1.99E-04	
Si	5.80E-05	4.51E-05	3.99E-05	4.02E-05	4.02E-05	
Ti	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	
υ	6.30E-06	1.47E-04	1.73E-05	1.33E-05	1.33E-05	
Zn	1.00E-16	1.00E-16	1.00E-16	1.78E-17	1.78E-17	
рН	6.11	7.98	8.13	8.24	8.24	

Table 56. Case 25 (nA1d3333): Solution Composition in Molality

Waste Package Project	Calculation
Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposal	Waste Packages:
Effects of Updated Design and Rates	
Document Identifier: CAL-EDC-MD-000015 REV00	Page 107 of 119

6.3.2 New Glass Degradation Rate

Section 6.2.3.3 of Reference 46 presents an updated model for the degradation of HLW glass. Specific changes to the model involve changes to the K_{eff} of the low pH leg. K_{eff} is a term which combines the intrinsic dissolution rate (k_0 , dependent only on glass composition) and the reaction affinity (Q/K) into a single term. The K_{eff} for the low pH leg of the model was changed from 9.2 to 14.0 due to uncertainties at lower pH values and unavailability of test results. This has the net effect of increasing the glass dissolution rate at pH values below 7. The cases presented previously in this calculation were run at the old glass rate from Reference 28. This section investigates the consequences of using the new glass rate proposed in Reference 46. The new glass rates can be found in Table 4 of this calculation.

6.3.2.1 Effects on Internal Accumulation

To study the effects of the new glass dissolution rate on the retention of U in the WP, via formation of U-bearing minerals, one case was rerun with the new glass rate. Case 27 is Case 2 run with the new glass rate. Case 2 was chosen because it is the only case that has a fast fuel degradation rate and retains half of the glass by the end of 634,000 years. The results are presented below in Table 57 through Table 59 and Figure 29 as well as in "moresense.xls" (Attachment III).

Case	File Name	Gd Retention	U Retention	Length of Run (Years)
27	nm1n1331	100%	99.75%	634,730
2	nm1x1331	99.77%	99.60%	634,370

Table 57 Gd and U Retention for Different HLW Glass Degradation Rates

NOTE: Gd and U retention expressed in percentage of total initial moles in the WP

The end results of Cases 27 and 2 are similar but the cases themselves are very different. Where Case 2 retains a pH of around 6 for most of the run, the pH in Case 27 rises above 7 around 80,000 years when the basket, DOE canister, and GPCs are fully degraded. The pH then decreases to around 6 after the glass is completely degraded at about 380,000 years. The pH remains near 6 until the 316NG liner is completely exhausted at around 580,000 years. At 634,000 years it has only risen to 6.60. This differs from Case 2 where half the glass still remains intact within the WP at 634,000 years. The slightly higher U loss in Case 2 is due to the pH rise at the very end of the run. In other cases, it is expected that more U would be lost from the WP using the new HLW glass rate, which might cause a higher pH earlier in the case, allowing more U loss from the package. Therefore, the older glass rate is more conservative for internal criticality.

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Calculation

Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposal Waste Packages: Effects of Updated Design and Rates

Document Identifier: CAL-EDC-MD-000015 REV00

Page 108 of 119

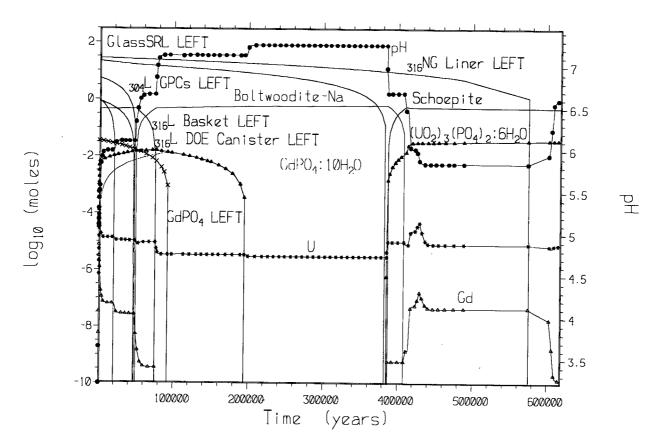


Figure 29. Case 27 (nm1n1331): WP Materials, Minerals, and Aqueous U

Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposal Waste Packages: Effects of Updated Design and Rates

Document Identifier: CAL-EDC-MD-000015 REV00

Page 109 of 119

Flomont	Years						
Element	76156	143380	307030	407530	427840	553340	634730
0	4.92E+03	5.83E+03	8.03E+03	9.22E+03	9.30E+03	9.99E+03	1.03E+04
Al	1.53E+02	1.84E+02	2.57E+02	2.92E+02	2.91E+02	2.91E+02	2.91E+02
В	0.00E+00	0.00E+00	5.83E-13	2.84E-15	0.00E+00	0.00E+00	0.00E+00
Ba	4.54E+00	6.51E+00	1.13E+01	1.35E+01	1.35E+01	1.35E+01	1.34E+01
Ca	1.80E+01	2.68E+01	4.68E+01	5.42E+01	5.28E+01	5.49E+01	5.63E+01
CI	3.00E-15	2.28E-14	0.00E+00	0.00E+00	2.61E-12	0.00E+00	0.00E+00
Cr	1.72E+00	2.47E+00	4.26E+00	5.11E+00	5.11E+00	5.11E+00	4.56E+00
Cu	0.00E+00						
F	1.51E-14	6.21E-01	1.37E+00	1.03E+00	3.73E-08	0.00E+00	0.00E+00
Fe	7.78E+03	8.73E+03	1.10E+04	1.24E+04	1.27E+04	1.42E+04	1.48E+04
Gd	7.25E+00	8.98E+00	8.98E+00	8.98E+00	8.98E+00	8.98E+00	8.98E+00
H	3.32E+01	4.01E+01	5.64E+01	6.48E+01	5.91E+01	5.95E+01	6.12E+01
С	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.89E-11	8.22E-13	5.09E-02
Р	5.50E+00	6.60E+00	8.45E+00	9.53E+00	9.70E+00	1.08E+01	1.12E+01
ĸ	3.19E+01	4.31E+01	6.94E+01	7.50E+01	7.16E+01	6.78E+01	6.54E+01
Mg	5.30E+00	1.12E+01	2.52E+01	3.10E+01	3.08E+01	3.11E+01	3.13E+01
Mn	1.37E+02	1.62E+02	2.23E+02	2.61E+02	2.69E+02	3.16E+02	3.34E+02
Мо	4.30E+01	4.84E+01	7.74E+01	1.05E+02	1.13E+02	6.77E+01	3.58E+01
Ν	1.18E-15	1.59E-15	0.00E+00	0.00E+00	4.47E-11	0.00E+00	0.00E+00
Na	6.40E+01	7.29E+01	9.11E+01	5.82E+01	3.78E+01	1.75E+01	5.03E+00
Ni	4.14E+02	5.65E+02	9.32E+02	1.16E+03	1.19E+03	1.18E+03	1.18E+03
S _.	5.32E-13	3.36E-12	0.00E+00	0.00E+00	9.20E-11	0.00E+00	1.89E-01
Si	7.12E+02	1.01E+03	1.73E+03	2.08E+03	2.09E+03	2.12E+03	2.13E+03
Ti	1.29E-01						
U	5.07E+02	5.31E+02	5.90E+02	6.17E+02	6.17E+02	6.17E+02	6.16E+02
Zn	0.00E+00						
Total (Kg)	1.48E+04	1.73E+04	2.32E+04	2.65E+04	2.68E+04	2.90E+04	2.99E+04
Density (g/cm ³)	4.55	4.46	4.32	4.28	4.30	4.36	4.38

Table 58. Case 27 (nm1n1331): Composition of Corrosion Products (Kg), Total Mass, and Density

Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposal Waste Packages: Effects of Updated Design and Rates

Document Identifier: CAL-EDC-MD-000015 REV00

Page 110 of 119

Flowert	Years						
Element	76156	110680	307030	407530	427840	553340	634730
AI	1.93E-07	1.24E-08	1.65E-08	1.70E-06	1.17E-03	1.25E-06	2.02E-08
В	4.72E-02	3.76E-02	3.71E-02	3.63E-06	9.09E-10	1.00E-16	1.00E-16
Ва	1.62E-07	1.27E-07	1.21E-07	1.57E-07	5.49E-07	7.11E-07	6.35E-06
Са	5.72E-04	2.55E-04	4.18E-04	1.60E-03	2.55E-04	4.54E-05	1.96E-05
CI	2.01E-04						
Cr	4.07E-02	4.08E-02	4.08E-02	4.09E-02	4.09E-02	4.09E-02	3.00E-04
Cu	1.52E-16	1.00E-16	1.00E-16	1.00E-16	1.00E-16	1.00E-16	1.00E-16
F	3.90E-04	1.45E-05	2.50E-04	8.69E-04	5.22E-03	1.15E-04	1.15E-04
Fe	1.81E-12	1.34E-12	1.28E-12	1.78E-12	5.11E-12	5.97E-12	1.80E-12
Gd	3.51E-10	3.22E-12	2.49E-11	5.91E-10	1.76E-07	4.51E-08	1.39E-10
С	1.30E-04	3.19E-04	4.11E-04	1.34E-04	5.02E-05	4.74E-05	1.05E-04
Р	1.51E-07	3.65E-06	4.50E-07	1.59E-07	3.06E-08	2.77E-08	1.00E-07
К	5.69E-03	7.03E-03	7.01E-03	5.44E-03	1.49E-03	6.50E-04	5.48E-04
Mg	1.30E-03	1.99E-03	2.00E-03	1.18E-03	8.84E-05	1.67E-05	1.08E-05
Mn	7.83E-13	9.71E-14	5.55E-14	7.11E-13	2.32E-11	3.48E-11	6.07E-13
Мо	8.80E-04	2.70E-03	1.70E-03	3.14E-04	9.93E-04	5.81E-03	3.12E-03
N	8.56E-04	8.56E-04	8.56E-04	8.56E-04	8.56E-04	8.56E-04	1.42E-04
Na	5.91E-02	7.27E-02	7.25E-02	5.65E-02	1.55E-02	6.73E-03	5.79E-03
Ni	5.84E-04	7.26E-05	4.15E-05	5.34E-04	1.75E-02	2.62E-02	4.57E-04
S	9.57E-04	8.25E-04	8.18E-04	3.09E-04	3.09E-04	3.09E-04	4.05E-05
Si	4.63E-05	4.18E-05	4.10E-05	4.64E-05	6.12E-05	6.76E-05	5.68E-05
Ti	0.00E+00						
U	9.32E-06	3.45E-06	3.00E-06	1.01E-05	6.55E-05	8.18E-06	7.81E-06
Zn	1.46E-16	1.00E-16	1.00E-16	1.00E-16	1.00E-16	1.00E-16	1.00E-16
рН	6.66	7.13	7.25	6.68	5.92	5.84	6.60

Table 59. Case 27 (nm1n1331): Solution Composition in Molality

 $\sim G_{1,2n\mu} A$

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Waste Package Project	Calculation
Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codispos	al Waste Packages:
Effects of Updated Design and Rates	
Document Identifier: CAL-EDC-MD-000015 REV00	Page 111 of 119

6.3.2.2 Effects on Source Term

Case 28 (nm2n1402) demonstrates the effects that using the new glass degradation rate has on the effluent concentration of fissile U. The results of Case 28 are presented in Figure 30 and Figure 31 and Table 60. Case 19 and Case 28 are very similar and show similar results. The major difference between the two cases is the timing in which everything occurs. In Case 28, the first U peak of 1.57E-01 moles/Kg occurs 67,600 years when the pH is 8.83. The second peak occurs nearly 12,000 years later with an intensity of 1.71E-01 moles/Kg at a pH of 8.84. The peak U in Case 19 (Figure 23) is slightly higher and occurs later in the case than do the peaks for Case 28 (Figure 30).

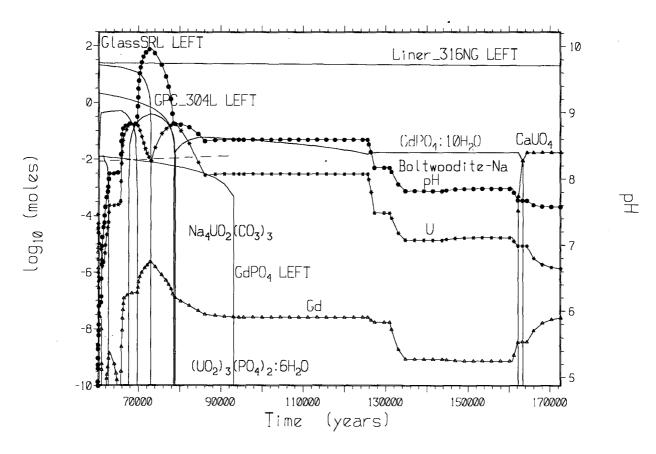


Figure 30. Case 28 (nm2n1402): WP Materials, Minerals, and Aqueous U

The enrichment fraction of the U peaks in Case 28 are very close to those seen in Case 19. The first peak corresponds to an enrichment of 0.2168 and the second to 0.1820. This is comparable to the 0.2200 and 0.1802 in Case 19. Since Case 19 (Figure 24) has the larger peaks in U, more fissile U is able to leave the WP for this case than for Case 28 (Figure 31). Therefore, the older glass rate from Reference 28 is more conservative for source term.

Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposal Waste Packages: Effects of Updated Design and Rates

Document Identifier: CAL-EDC-MD-000015 REV00

Page 112 of 119

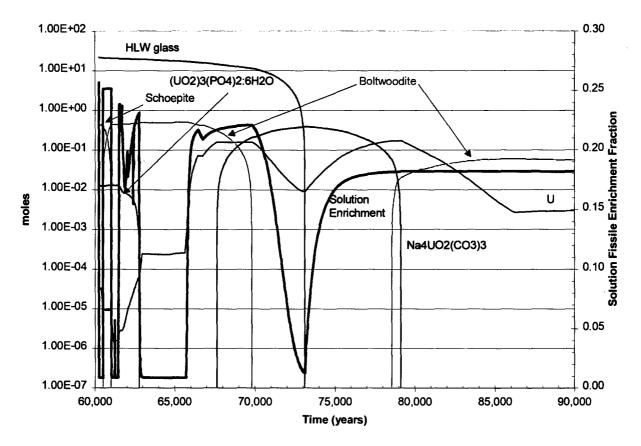


Figure 31. Case 28 (nm2n1402): Enrichment and U-bearing Solids in the WP

Calculation

Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposal Waste Packages: Effects of Updated Design and Rates

Document Identifier: CAL-EDC-MD-000015 REV00

Page 113 of 119

Element	Years						
Element	60487	62033	64606	67634	73116	78608	94389
AI	9.28E-06	3.34E-08	1.02E-07	3.79E-08	3.67E-09	3.91E-08	5.52E-08
В	1.63E-01	3.63E-01	2.04E-01	9.67E-02	2.03E-01	9.90E-02	2.17E-01
Ba	6.00E-07	1.19E-07	2.55E-08	9.37E-10	2.43E-11	9.42E-10	2.27E-09
Ca	6.82E-06	3.33E-05	5.80E-05	1.06E-04	4.67E-06	1.06E-04	2.76E-04
CI	2.01E-04						
Cr	1.02E-01	1.23E-01	1.43E-01	1.50E-01	1.53E-01	1.53E-01	4.12E-02
Cu	4.69E-14	2.66E-14	1.03E-14	3.45E-15	5.43E-16	1.56E-16	1.00E-16
F	5.05E-04	4.21E-08	1.58E-11	3.19E-03	1.21E-02	1.43E-03	5.72E-05
Fe	4.38E-12	1.18E-12	1.14E-12	1.31E-12	4.23E-12	1.34E-12	1.24E-12
Gd	3.76E-08	4.01E-11	2.74E-10	1.73E-07	2.49E-06	1.35E-07	2.62E-08
С	6.18E-05	1.07E-03	4.05E-03	5.00E-01	1.43E+00	5.34E-01	1.84E-02
Р	4.81E-08	1.28E-03	1.90E-03	2.19E-07	6.68E-05	3.02E-07	8.68E-08
к	2.69E-02	1.42E-02	6.23E-03	1.62E-02	8.36E-02	1.63E-02	6.68E-03
Mg	1.86E-02	1.38E-02	1.63E-03	5.47E-05	3.10E-06	5.41E-05	2.03E-04
Mn	1.95E-11	2.00E-14	2.13E-15	1.36E-15	2.14E-14	1.40E-15	7.86E-16
Мо	1.15E-01	6.49E-02	4.38E-02	1.70E-02	5.07E-03	3.49E-03	3.26E-03
N	2.05E-03	2.49E-03	2.83E-03	2.98E-03	3.04E-03	3.05E-03	8.62E-04
Na	2.67E-01	3.63E-01	4.12E-01	1.06E+00	2.89E+00	1.07E+00	1.60E-01
Ni	1.46E-02	1.48E-05	1.41E-06	4.56E-08	2.76E-10	4.56E-08	1.06E-07
S	2.71E-03	5.51E-03	7.58E-03	1.19E-02	3.27E-02	4.62E-03	3.18E-04
[•] Si	4.59E-05	3.80E-05	4.61E-05	2.85E-04	8.22E-03	2.92E-04	6.26E-05
Ti	0.00E+00						
U	1.02E-05	9.24E-06	2.33E-04	1.57E-01	8.75E-03	1.68E-01	3.03E-03
Zn	4.15E-14	2.35E-14	9.12E-15	3.15E-19	0.00E+00	0.00E+00	2.47E-19
рН	6.07	7.57	8.08	8.83	9.97	8.84	8.59

Table 60. Case 28 (nm2n1402): Solution Composition in Molality

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Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposal Waste Packages: Effects of Updated Design and Rates

Document Identifier: CAL-EDC-MD-000015 REV00

Page 114 of 119

7. REFERENCES

- CRWMS M&O 1999. Electronic Media (CD); the Calculation Files for EQ6 Calculation for Chemical Degradation of Enrico Fermi Spent Nuclear Fuel Waste Packages. BBA000000-01717-0210-00029 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: <u>MOL.19990507.0237</u>.
- 2. Stockman, H.W. 1994. *PP: A Graphics Post-Processor for the EQ6 Reaction Path Code.*. SAND94-1955. Albuquerque, New Mexico: Sandia National Laboratories. TIC: <u>241246</u>.
- 3. <u>MO0009THRMODYN.001</u>. Input Transmittal for Thermodynamic Data Input Files for Geochemical Calculations. Submittal date: 09/20/2000.
- 4. CRWMS M&O 1998. EQ6 Calculations for Chemical Degradation of Fast Flux Test Facility (FFTF) Waste Packages. BBA000000-01717-0210-00028 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19981229.0081.
- DOE (U.S. Department of Energy) 1998. Total System Performance Assessment. Volume 3 of Viability Assessment of a Repository at Yucca Mountain. DOE/RW-0508. Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: <u>MOL.19981007.0030</u>.
- 6. Hillner, E.; Franklin, D.G.; and Smee, J.D. 1998. *The Corrosion of Zircaloy-Clad Fuel* Assemblies in a Geologic Repository Environment. WAPD-T-3173. West Mifflin, Pennsylvania: Bettis Atomic Power Laboratory. TIC: <u>237127</u>.
- CRWMS M&O 2000. Evaluation of Codisposal Viability for U-Zr/U-Mo Alloy (Enrico Fermi) DOE-Owned Fuel. TDR-EDC-NU-000002 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: <u>MOL.20000815.0317</u>.
- CRWMS M&O 1996. Second Waste Package Probabilistic Criticality Analysis: Generation and Evaluation of Internal Criticality Configurations. BBA000000-01717-2200-00005 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19960924.0193.
- 9. DOE (U.S. Department of Energy) 1999. Fermi (U-Mo) Fuel Characteristics for Disposal Criticality Analysis. DOE/SNF/REP-035, Rev. 0. Washington, D.C.: U.S. Department of Energy. TIC: 242461.
- CRWMS M&O 2000. Total System Performance Assessment for the Site Recommendation. TDR-WIS-PA-000001 REV 00 ICN 01. Las Vegas, Nevada: CRWMS M&O. ACC: <u>MOL.20001220.0045</u>.
- 11. Audi, G. and Wapstra, A.H. 1995. Atomic Mass Adjustment, Mass List for Analysis. [Upton, New York: Brookhaven National Laboratory, National Nuclear Data Center]. TIC: 242718.
- Parrington, J.R.; Knox, H.D.; Breneman, S.L.; Baum, E.M.; and Feiner, F. 1996. Nuclides and Isotopes, Chart of the Nuclides. 15th Edition. San Jose, California: General Electric Company and KAPL, Inc.. TIC: 233705.
- 13. Estill, J.C. 1998. "Long-Term Corrosion Studies." 2.2 of Engineered Materials Characterization Report. McCright, R.D., ed., UCRL-ID-119564 Volume 3 Rev.1.1.

Waste Package Project	Calculation
Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposal W	aste Packages:
Effects of Updated Design and Rates	

Document Identifier: CAL-EDC-MD-000015 REV00

Page 115 of 119

Livermore, California: Lawrence Livermore National Laboratory. ACC: MOL.19981222.0137.

- CRWMS M&O 1998. Evaluation of Codisposal Viability for Aluminum-Clad DOE-Owned Spent Fuel: Phase II Degraded Codisposal Waste Package Internal Criticality. BBA000000-01717-5705-00017 REV 01. Las Vegas, Nevada: CRWMS M&O. ACC: <u>MOL.19981014.0038</u>.
- 15. <u>MO0006J13WTRCM.000</u>. Recommended Mean Values of Major Constituents in J-13 Well Water. Submittal date: 06/07/2000.
- 16. CRWMS M&O 1999. DOE SRS HLW Glass Chemical Composition. BBA000000-01717-0210-00038 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19990215.0397.
- 17. CRWMS M&O 2000. Technical Work Plan for: Department of Energy Spent Nuclear Fuel Work Packages. TWP-MGR-MD-000010 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.20001107.0305.
- 18. ASM International 1987. *Corrosion*. Volume 13 of *ASM Handbook*. Formerly 9th Edition, Metals Handbook. [Materials Park, Ohio]: ASM International. TIC: <u>240704</u>.
- 19. CRWMS M&O 2000. Waste Package Degradation Process Model Report. TDR-WIS-MD-000002 REV 00 ICN 02. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.20001228.0229.
- 20. CRWMS M&O 2001. EQ6 Calculations for Chemical Degradation of N Reactor (U-metal) Spent Nuclear Fuel Waste Packages. CAL-EDC-MD-000010 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.20010227.0017.
- 21. CRWMS M&O 1999. Software Code: EQ6, Version 7.2bLV. V7.2bLV. 10075-7.2bLV-00.
- 22. YMP (Yucca Mountain Site Characterization Project) 2000. Disposal Criticality Analysis Methodology Topical Report. YMP/TR-004Q, Rev. 01. Las Vegas, Nevada: Yucca Mountain Site Characterization Office. ACC: MOL.20001214.0001.
- 23. ASTM G 1-90 (Reapproved 1999). 1990. Standard Practice for Preparing, Cleaning, and Evaluating Corrosion Test Specimens. West Conshohocken, Pennsylvania: American Society for Testing and Materials, TIC: 238771.
- 24. CRWMS M&O 2000. In-Drift Accumulation of Fissile Material from Waste Packages Containing Plutonium Disposition Waste Forms. CAL-EDC-GS-000001 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.20001016.0008.
- 25. AP-SI.1Q, Rev. 3, ICN 2, ECN 1. *Software Management*. Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: <u>MOL.20011030.0598</u>.
- 26. CRWMS M&O 1997. Criticality Evaluation of Degraded Internal Configurations for the *PWR AUCF WP Designs*. BBA000000-01717-0200-00056 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: <u>MOL.19971231.0251</u>.
- 27. McCright, R.D. 1998. Corrosion Data and Modeling, Update for Viability Assessment. Volume 3 of Engineered Materials Characterization Report. UCRL-ID-119564, Rev. 1.1.

Waste Package Project	Calculation
Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposal	Waste Packages:
Effects of Updated Design and Rates	
Document Identifier: CAL-EDC-MD-000015 REV00	Page 116 of 119

Livermore, California: Lawrence Livermore National Laboratory. ACC: MOL.19980806.0177.

- 28. CRWMS M&O 2000. Defense High Level Waste Glass Degradation. ANL-EBS-MD-000016 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.20000329.1183.
- 29. AP-3.12Q, Rev. 0, ICN 4. *Calculations*. Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: <u>MOL.20010404.0008</u>.
- DOE (U.S. Department of Energy) 2000. Quality Assurance Requirements and Description. DOE/RW-0333P, Rev. 10. Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: MOL.20000427.0422.
- 31. National Research Council 1995. *Technical Bases for Yucca Mountain Standards*. Washington, D.C.: National Academy Press. TIC: <u>217588</u>.
- 32. CRWMS M&O 1999. EQ6 Calculations for Chemical Degradation of Enrico Fermi Spent Nuclear Fuel Waste Packages. BBA000000-01717-0210-00029 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: <u>MOL.19990702.0030</u>.
- 33. ASTM A 20/A20M-99a. 1999. Standard Specification for General Requirements for Steel Plates for Pressure Vessels. West Conshohocken, Pennsylvania: American Society for Testing and Materials. TIC: 247403.
- 34. ASTM A 240/A 240M-99b. 2000. Standard Specification for Heat-Resisting Chromium and Chromium-Nickel Stainless Steel Plate, Sheet, and Strip for Pressure Vessels. West Conshohocken, Pennsylvania: American Society for Testing and Materials. TIC: <u>248529</u>.
- 35. Wolery, T.J. and Daveler, S.A. 1992. EQ6, A Computer Program for Reaction Path Modeling of Aqueous Geochemical Systems: Theoretical Manual, User's Guide, and Related Documentation (Version 7.0). UCRL-MA-110662 PT IV. Livermore, California: Lawrence Livermore National Laboratory. ACC: MOL.19980701.0459.
- 36. CRWMS M&O 1999. User's Manual for EQ6 V7.2bLV. SDN: 10075-ITP-7.2bLV-00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.20000126.0158.
- 37. CRWMS M&O 1998. Software Qualification Report (SQR) Addendum to Existing LLNL Document UCRL-MA-110662 PT IV: Implementation of a Solid-Centered Flow-Through Mode for EQ6 Version 7.2B. CSCI: UCRL-MA-110662 V 7.2b. SCR: LSCR198. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19990920.0169.
- 38. AP-SV.1Q, Rev. 0, ICN 2. Control of the Electronic Management of Information. Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: <u>MOL.20000831.0065</u>.
- 39. Yang, I.C.; Rattray, G.W.; and Yu, P. 1996. Interpretation of Chemical and Isotopic Data from Boreholes in the Unsaturated Zone at Yucca Mountain, Nevada. Water-Resources Investigations Report 96-4058. Denver, Colorado: U.S. Geological Survey. ACC: <u>MOL.19980528.0216</u>.

Waste Package Project	Calculation
Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Co	disposal Waste Packages:
Effects of Updated Design and Rates	
Document Identifier: CAL-EDC-MD-000015 REV00	Page 117 of 119

- 40. Weast, R.C., ed. 1977. CRC Handbook of Chemistry and Physics. 58th Edition. Cleveland, Ohio: CRC Press. TIC: 242376.
- 41. ASTM A 276-00. 2000. *Standard Specification for Stainless Steel Bars and Shapes*. West Conshohocken, Pennsylvania: American Society for Testing and Materials. TIC: <u>248098</u>.
- 42. CRWMS M&O 1999. Software Code: EQ3/6. V7.2b. UCRL-MA-110662 (LSCR198).
- 43. Stout, R.B. and Leider, H.R., eds. 1991. Preliminary Waste Form Characteristics Report. Version 1.0. Livermore, California: Lawrence Livermore National Laboratory. ACC: <u>MOL.19940726.0118</u>.
- 44. ASTM A 516/A 516M-90. 1991. Standard Specification for Pressure Vessel Plates, Carbon Steel, for Moderate- and Lower-Temperature Service. Philadelphia, Pennsylvania: American Society for Testing and Materials. TIC: <u>240032</u>.
- 45. BSC 2001. Software Code: ASPRIN. V1.0. 10487-1.0-00.
- 46. BSC (Bechtel SAIC Company) 2001. Defense High Level Waste Glass Degradation. ANL-EBS-MD-000016 REV 00 ICN 02. Las Vegas, Nevada: Bechtel SAIC Company. ACC: MOL.20011015.0502.
- 47. CRWMS M&O 1999. EQ6 Calculations for Chemical Degradation of TRIGA Codisposal Waste Packages. CAL-EDC-MD-000001 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19991118.0050.
- 48. DOE (U.S. Department of Energy) 2000. Review of Oxidation Rates of DOE Spent Nuclear Fuel, Part 1: Metallic Fuel. DOE/SNF/REP-054, Rev. 0. Washington, D.C.: U.S. Department of Energy. TIC: 248978.
- 49. CRWMS M&O 1998. "Waste Form Degradation, Radionuclide Mobilization, and Transport Through the Engineered Barrier System." Chapter 6 of Total System Performance Assessment-Viability Assessment (TSPA-VA) Analyses Technical Basis Document. B0000000-01717-4301-00006 REV 01. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19981008.0006.
- 50. BSC (Bechtel SAIC Company) 2001. EQ6 Calculation for Chemical Degradation of Fort St. Vrain (Th/U Carbide) Waste Packages. CAL-EDC-MD-000011 REV 00. Las Vegas, Nevada: Bechtel SAIC Company. ACC: MOL.20010831.0300.
- 51. ASME (American Society of Mechanical Engineers) 1998. "Section II: Materials, Part A Ferrous Materials Specifications." 1998 ASME Boiler and Pressure Vessel Code. New York, New York: American Society of Mechanical Engineers. TIC: <u>247429</u>.
- 52. ASM International 1987. Corrosion. Volume 13 of Metals Handbook. 9th Edition. Metals Park, Ohio: ASM International. TIC: 209807.
- 53. BSC (Bechtel SAIC Company) 2001. *EQ6 Calculations for Chemical Degradation of Melt and Dilute Waste Packages.* CAL-EDC-MD-000012 REV 00. Las Vegas, Nevada: Bechtel SAIC Company. ACC: MOL.20010719.0064.

Waste Package Project	Calculation
Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codis	sposal Waste Packages:
Effects of Updated Design and Rates	
Document Identifier: CAL-EDC-MD-000015 REV00	Page 118 of 119

- 54. BSC (Bechtel SAIC Company) 2001. EQ6 Calculation for Chemical Degradation of Pu-Ceramic Waste Packages: Effects Updated Waste Package Design and Rates. CAL-EDC-MD-000009 REV 00. Las Vegas, Nevada: Bechtel SAIC Company. ACC: MOL.20010606.0284.
- 55. BSC (Bechtel SAIC Company) 2001. EQ6 Calculation for Chemical Degradation of Shippingport PWR Codisposal Waste Packages: Effects of Updated Design and Rates. CAL-EDC-MD-000016 REV 00. Las Vegas, Nevada: Bechtel SAIC Conpany. ACC: MOL.20011112.0069.
- 56. CRWMS M&O 2000. Summary of Dissolved Concentration Limits. ANL-WIS-MD-000010 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.20000525.0372.
- 57. Roberts, W.L.; Campbell, T.J.; and Rapp, G.R., Jr. 1990. *Encyclopedia of Minerals*. 2nd Edition. New York, New York: Van Nostrand Reinhold. TIC: <u>242976</u>.
- 58. Brady, P.V. and Walther, J.V. 1989. "Controls on Silicate Dissolution Rates in Neutral and Basic pH Solutions at 25°C." *Geochimica et Cosmochimica Acta*, 53, 2823-2830. New York, New York: Pergamon Press. TIC: <u>235216</u>.
- Brady, P.V. and Walther, J.V. 1990. "Kinetics of Quartz Dissolution at Low Temperatures." *Chemical Geology*, 82, 253-264. Amsterdam, The Netherlands: Elsevier Science Publishers B.V.. TIC: <u>235349</u>.
- 60. BSC 2001. Software Code: PHREEQC. V2.3. PC. 10068-2.3-00.
- 61. DOE (U.S. Department of Energy) 1998. Design Specification. Volume 1 of Preliminary Design Specification for Department of Energy Standardized Spent Nuclear Fuel Canisters. DOE/SNF/REP-011, Rev. 1. Washington, D.C.: U.S. Department of Energy, Office of Spent Fuel Management and Special Projects. TIC: <u>241528</u>.
- 62. DOE (U.S. Department of Energy) 1999. Waste Acceptance System Requirements Document. DOE/RW-0351, Rev. 03. Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: <u>HQO.19990226.0001</u>.

Title: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposal Waste Packages:
Effects of Updated Design and Rates
Document Identifier: CAL-EDC-MD-000015 REV00Page 119 of 119

8. ATTACHMENTS

Attachment I. Listing of Files on Compact Disks (11 pages)

Attachment II. Sketch SK-0200 REV 04 (2 pages)

Attachment III. Two Compact Discs

ATTACHMENT I. LISTING OF FILES ON COMPACT DISKS

This attachment contains the MS-DOS directory for files placed on the electronic media (Attachment I). The files are of various types:

- 1. Excel files (extensions = xls).
- 2. EQ3/6 input files (extension = 3i or 6i).

ASCII text file: provides input parameters for EQ3/6.

3. EQ3/6 output files (extension = 30 or 60).

ASCII text file: provides detailed information about the system at each print point, which is specified by the user in the input file.

4. EQ3/6 pickup files (extension = 3p or 6p).

ASCII text file: provides a description of the system at the end of that run to be used as an input file for a continuation run.

5. EQ6 Tab-delimited text files (extension = txt).

*.elem_aqu: total aqueous moles of elements.

*.elem min: total moles of elements in minerals.

- *.elem_tot: total moles of elements (aqueous + mineral).
- *.min_info: moles of each mineral.
- 6. EQ6 binary output file (extension = bin).

Binary file: provides detailed information about the system at the full numerical precision for *every* time step.

- 7. EQ3/6 text data files used for the calculations, "data0.ymd".
- 8. Batch files (extension = bat) used to start EQ6 runs.
- 9. Winzip files (extension = zip).

Below are listed the contents of the DOS directories within the electronic attachment:

The first column is the DOS file name.

The second column lists <DIR> if it is a directory or gives the files size (bytes) if it is a file.

The third and fourth columns are the date and time of the last update.

The fifth column is the filename.

Directory of Fermi-IA1

DATA0	NUC	2,302,224	09-15-99	11:40a	DATA0.NUC
DATA0	YMD	2,657,459	03-16-01	1:22p	data0.ymd
DATAO	YMP	2,649,470	09-11-00	5:23p	data0.ymp
ENRIC~34	XLS	1,075,200	11-14-01	3:24p	enrich-fermi1.xls
ENRIC~38	XLS	1,047,552	11-14-01	3:49p	enrich-fermi2.xls
ENRIC~44	XLS	535,040	11-15-01	10:15a	enrich-sens-Fermi.xls
FERMI~48	XLS	39,424	09-20-01	8:28a	Fermi-IA-2001.xls
FERMI~50	XLS	256,512	09-13-01	10:24a	fermi-losses.xls
HLWGL~52	XLS	57,856	08-01-01	10:17a	HLWglass-2001.xls
J13NOM20	31	13,734	10-23-00	12:44p	j13nom20.3i
J13NOM20	30	114,582	10-23-00	12:45p	j13nom20.30
J13NOM20	3P	11,786	10-23-00	12:45p	j13nom20.3p
J13NOM30	3I	13,660	10-10-00	1:31p	j13nom30.3i
J13NOM30	30	115,224	10-10-00	1:32p	j13nom30.30
J13NOM30	3P	11,712	10-10-00	1:32p	j13nom30.3p
LOSSE~66	XLS	18,944	08-20-01	3:59p	losses-oldtime.xls
MORES~68	XLS	18,944	09-17-01	7:22a	moresense.xls
OLDFE~72	XLS	16,896	09-13-01	8:19a	oldfermi-recalc.xls
ONE-ST~5		<dir></dir>	11-15-01	8:50a	One-Stage
S_ASE~76	XLS	108,544	08-23-01	7:32a	S+A sensitivity.xls
S_A~78	XLS	790,016	09-19-01	9:02a	S+A.xls
SENSI~82	XLS	9,253,888	11-15-01	9:27a	Sensitivity.xls
SOURCE~7		<dir></dir>	11-15-01	10:37a	Source Term
UENR~112			11-13-01	-	Uenrich Fermi.xls
	22 fil	e(s) 21,12	28,635 by	tes	

Directory of D:\One-Stage

•	<dir></dir>	11-13-01	3:01p .
	<dir></dir>	11-13-01	3:01p
NG1X3323 61	45,736	07-16-01	5:11p ng1x3323.6i
NG1X3323 60	31,486,614	07-16-01	9:01p ng1x3323.60
NG1X3323 6F	43,166	07-16-01	9:01p ng1x3323.6p
NG1X~104 TX	XT 232,706	07-16-01	9:00p ng1x3323.elem_aqu.txt
NG1X~106 TX	KT 218,217	07-16-01	9:00p ng1x3323.elem_min.txt
NG1X~108 TX	XT 218,230	07-16-01	9:00p ng1x3323.elem_tot.txt
NG1X~112 TX	KT 465,870	07-16-01	9:00p ng1x3323.min_info.txt
NM1X1321 61	46,466	07-11-01	1:16p nmlx1321.6i
NM1X1321 60	2,802,843	07-11-01	1:25p nmlx1321.60
NM1X1321 6E	2 43,554	07-11-01	1:25p nmlx1321.6p
NM1X~128 TX	XT 28,656	07-11-01	1:25p nm1x1321.elem_aqu.txt
NM1X~130 TX	(T 26,887	07-11-01	1:25p nmlx1321.elem_min.txt
NM1X~132 TX	KT 26,900	07-11-01	1:25p nmlx1321.elem_tot.txt
NM1X~134 TX	KT 58,272	07-11-01	1:25p nmlx1321.min_info.txt
NM1X1331 61	46,466	07-11-01	1:16p nmlx1331.6i
NM1X1331 60	2,784,787	07-11-01	1:31p nmlx1331.60
NM1X1331 61	2 43,226	07-11-01	1:31p nm1x1331.6p
NM1X~150 TX	(T 27,886	07-11-01	1:31p nm1x1331.elem_aqu.txt
NM1X~152 TX	(T 26,165	07-11-01	1:31p nm1x1331.elem_min.txt
NM1X~154 TX	KT 26,178	07-11-01	1:31p nm1x1331.elem_tot.txt
NM1X~156 TX	KT 53,551	07-11-01	1:31p nm1x1331.min_info.txt
NM1X1333 61	I 46,466	07-25-01	1:34p nmlx1333.6i
NM1X1333 60	17,695,889	07-25-01	2:05p nmlx1333.60
NM1X1333 6F	42,816	07-25-01	2:05p nmlx1333.6p

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NM1X~216		183,811	07-25-01		nm1x1333.elem_aqu.txt
NM1X~218		172,370	07-25-01		nm1x1333.elem_min.txt
NM1X~222		172,383	07-25-01		nmlx1333.elem_tot.txt
NM1X~224	TXT	364,691	07-25-01	-	nm1x1333.min_info.txt
NM1X2331		46,466	07-11-01	-	nm1x2331.6i
NM1X2331	60	3,499,254	07-11-01	-	nm1x2331.60
NM1X2331		43,636	07-11-01	_	nm1x2331.6p
NM1X~244	TXT	35,201	07-11-01		nm1x2331.elem_aqu.txt
NM1X~246	TXT	33,024	07-11-01	_	nm1x2331.elem_min.txt
NM1X~248	TXT	33,037	07-11-01	-	nm1x2331.elem_tot.txt
NM1X~250	TXT	77,821	07-11-01	_	nm1x2331.min_info.txt
NM1X2422	61	45,652	07-12-01		nm1x2422.6i
NM1X2422	60	12,646,847	07-12-01	2:28p	nm1x2422.60
NM1X2422	6P	42,668	07-12-01	2:28p	nm1x2422.6p
NM1X~296	TXT	102,961	07-12-01		nm1x2422.elem_aqu.txt
NM1X~298	TXT	96,560	07-12-01	2:28p	nm1x2422.elem_min.txt
NM1X~300	TXT	96,573	07-12-01	2:28p	nm1x2422.elem_tot.txt
NM1X~302	TXT	254,139	07-12-01	2:28p	nm1x2422.min_info.txt
NM1X2432	6I	45,651	07-12-01	1:53p	nm1x2432.6i
NM1X2432	60	12,914,822	07-12-01	3:00p	nm1x2432.60
NM1X2432	6P	42,586	07-12-01		nm1x2432.6p
NM1X~348	TXT	107,581	07-12-01		nm1x2432.elem aqu.txt
NM1X~350	TXT	100,892	07-12-01	-	nm1x2432.elem_min.txt
NM1X~352	TXT	100,905	07-12-01	_	nm1x2432.elem_tot.txt
NM1X~354		274,469	07-12-01	-	nm1x2432.min info.txt
NM1X3323		45,655	07-12-01	-	nm1x3323.6i
NM1X3323		31,856,704	07-12-01	-	nm1x3323.60
NM1X3323		43,078	07-12-01	_	nm1x3323.6p
NM1X~456		235,786	07-12-01	-	nm1x3323.elem aqu.txt
NM1X~458		221,105	07-12-01		nm1x3323.elem min.txt
NM1X~462		221,103	07-12-01	-	nm1x3323.elem tot.txt
NM1X~464		504,572	07-12-01		nm1x3323.min info.txt
NM1X3333		45,655	07-12-01	-	nm1x3333.6i
NM1X3333		30,373,686			nm1x3333.60
NM1X3333		43,078			nm1x3333.6p
NM1X~562		219,231			nm1x3333.elem aqu.txt
NM1X~566		205,582			nm1x3333.elem min.txt
NM1X~568		205,582			nm1x3333.elem tot.txt
NM1X~588 NM1X~570		444,410			nm1x3333.min info.txt
	_	•			—
NM1X3433		45,655 30,750,097			nm1x3433.6i
NM1X3433			07-12-01	-	nm1x3433.60
NM1X3433		42,996	07-12-01		nmlx3433.6p
NM1X~670		229,626	07-12-01	-	nmlx3433.elem_aqu.txt
NM1X~674		215,329	07-12-01		nm1x3433.elem_min.txt
NM1X~676		215,342	07-12-01		nm1x3433.elem_tot.txt
NM1X~678		572,539	07-12-01	_	nm1x3433.min_info.txt
SECOND~5		<dir></dir>	11-15-01		second part
THIRDP~7		<dir></dir>			third part
	70 file	(S) 184,8	08,385 byt	ces	

Directory of D:\One-Stage\second part

•		<dir></dir>	11-15-01	10:46a	•
		<dir></dir>	11-15-01	10:46a	••
NG1Y3323	61	30,372	07-17-01	6:53a	ng1y3323.6i
NG1Y3323	60	27,899,955	07-17-01	8:41a	ng1y3323.60
NG1Y3323	6P	30,367	07-17-01	8:41a	ng1y3323.6p

1701172 04	m 3/ m	010 616	07 17 01	0 40-	
NG1Y3~94		219,616	07-17-01		ng1y3323.elem_aqu.txt
NG1Y3~96		205,943	07-17-01		ng1y3323.elem_min.txt
NG1Y~100		205,956	07-17-01		ng1y3323.elem_tot.txt
NG1Y~102		343,174	07-17-01		ng1y3323.min_info.txt
NM1Y1333		30,577	07-25-01	-	nm1y1333.6i
NM1Y1333		20,670,995	07-25-01	-	nm1y1333.60
NM1Y1333	6P	30,585	07-25-01	-	nmly1333.6p
NM1Y~172	$\mathbf{T}\mathbf{X}\mathbf{T}$	228,471	07-25-01	_	nmly1333.elem_aqu.txt
NM1Y~174	TXT	214,246	07-25-01	-	nm1y1333.elem_min.txt
NM1Y~176	TXT	214,259	07-25-01	-	nmly1333.elem_tot.txt
NM1Y~180	TXT	315,064	07-25-01	3:54p	nmly1333.min_info.txt
NM1Y3323	6I	30,289	07-12-01	5:36p	nm1y3323.6i
NM1Y3323	60	28,171,181	07-12-01	10:25p	nm1y3323.60
NM1Y3323	6P	30,289	07-12-01	10:25p	nm1y3323.6p
NM1Y~270	TXT	219,616	07-12-01	10:25p	nm1y3323.elem aqu.txt
NM1Y~274	TXT	205,943	07-12-01	10:25p	nm1y3323.elem min.txt
NM1Y~276	TXT	205,956	07-12-01	10:25p	nm1y3323.elem_tot.txt
NM1Y~278	TXT	340,774	07-12-01		nm1y3323.min info.txt
NM1Y3333	61	29,310	07-12-01	2:02p	nmly3333.6i
NM1Y3333	60	28,916,112	07-12-01	11:58p	nm1y3333.60
NM1Y3333	6P	29,310	07-12-01	11:58p	nm1y3333.6p
NM1Y~372	TXT	222,696	07-12-01	11:57p	nm1y3333.elem aqu.txt
NM1Y~374	TXT	208,831		_	nm1y3333.elem min.txt
NM1Y~378	TXT	208,844		-	nm1y3333.elem_tot.txt
NM1Y~380	TXT	324,558	07-12-01	11:57p	nm1y3333.min info.txt
NM1Y3433	61	28,027	07-12-01		nmly3433.6i
NM1Y3433	60	26,458,687	07-13-01		nm1y3433.60
NM1Y3433	6P	27,618			nm1y3433.6p
NM1Y~466	TXT	221,156			nm1y3433.elem aqu.txt
NM1Y~470	TXT	207,387			nm1y3433.elem min.txt
NM1Y~472	TXT	207,400			nm1y3433.elem_tot.txt
NM1Y~474	TXT	304,930			nmly3433.min info.txt
	35 file		38,494 byt		• · · · · · · · · · · · · · · · · · · ·
		•			

Directory of D:\One-Stage\third part

•	<dir></dir>	07-13-01	12:58a	
••	<dir></dir>	07-13-01	12:58a	••
NG1Z3323 6I	29,164	07-17-01	12:12p	ng1z3323.6i
NG1Z3323 60	20,531,160	07-17-01	1:39p	ng1z3323.60
NG1Z3323 6P	29,163	07-17-01	1:39p	ng1z3323.6p
NG1Z3~72 TXT	170,336	07-17-01	1:39p	ng1z3323.elem_aqu.txt
NG1Z3~74 TXT	159,735	07-17-01	1:39p	ng1z3323.elem_min.txt
NG1Z3~76 TXT	159,748	07-17-01	1:39p	ng1z3323.elem_tot.txt
NG1Z3~80 TXT	242,384	07-17-01	1:39p	ng1z3323.min_info.txt
NM1Z3323 6I	29,086	07-13-01	6:58a	nm1z3323.6i
NM1Z3323 60	20,814,521	07-13-01	9:32a	nm1z3323.60
NM1Z3323 6P	29,003	07-13-01	9:32a	nm1z3323.6p
NM1Z3323 6T	683,102	07-13-01	9:32a	nm1z3323.6t
NM1Z3323 6TX	690,396	07-13-01	9:32a	nm1z3323.6tx
NM1Z~156 TXT	171,491	07-13-01	9:31a	nm1z3323.elem_aqu.txt
NM1Z~160 TXT	160,818	07-13-01	9:31a	nm1z3323.elem_min.txt
NM1Z~162 TXT	160,831	07-13-01	9:31a	nm1z3323.elem_tot.txt
NM1Z~164 TXT	244,016	07-13-01	9:32a	nmlz3323.min_info.txt
NM1Z3333 6I	28,107	07-13-01	6:57a	nm1z3333.6i
NM1Z3333 60	28,944,873	07-13-01	11:17a	nm1z3333.60
NM1Z3333 6P	28,106	07-13-01	11:17a	nm1z3333.6p

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NM1Z3333 6T 929,403 07-13-01 11:17a nmlz3333.6t 1,022,828 07-13-01 11:17a nmlz3333.6tx NM1Z3333 6TX 258,116 07-13-01 11:16a nmlz3333.elem_aqu.txt 242,043 07-13-01 11:16a nmlz3333.elem_min.txt NM1Z~268 TXT NM1Z~270 TXT 242,056 07-13-01 11:16a nmlz3333.elem_tot.txt 366,416 07-13-01 11:17a nmlz3333.min_info.txt 27,617 07-13-01 6:56a nmlz3433.6i NM1Z~274 TXT NM1Z~276 TXT 27,617 07-13-01 6:56a nmlz3433.6i 27,644,398 07-13-01 12:18p nmlz3433.6o NM1Z3433 6I NM1Z3433 60

 NM123433 60
 27,644,398
 07-13-01
 12:18p
 nm123433.60

 NM1Z3433 6P
 27,616
 07-13-01
 12:18p
 nm1z3433.6p

 NM1Z3433 6T
 842,656
 07-13-01
 12:18p
 nm1z3433.6t

 NM1Z3433 6T
 842,656
 07-13-01
 12:18p
 nm1z3433.6t

 NM1Z3433 6TX
 851,516
 07-13-01
 12:18p
 nm1z3433.6tx

 NM1Z~376
 TXT
 257,731
 07-13-01
 12:18p
 nm1z3433.elem_aqu.txt

 NM1Z~378
 TXT
 241,682
 07-13-01
 12:18p
 nm1z3433.elem_tot.txt

 NM1Z~380
 TXT
 241,695
 07-13-01
 12:18p
 nm1z3433.elem_tot.txt

 NM1Z~384
 TXT
 293,503
 07-13-01
 12:18p
 nm1z3433.min_info.txt

 34 file(s) 106,795,316 bytes

Directory of D:\Source Term

•	<dir></dir>		11-15-01	10:00a	
	<dir></dir>		11-15-01	10:00a	
ASPRIN	EXE 299	,130	07-03-01	9:07a	asprin.exe
DEFLTS~8	TXT	187	07-26-01	9:25a	defltsolids.txt
DEFLT~10	TXT	858	07-10-01	2:35p	defltsolids_longlist.txt
ONESTA~5	<dir></dir>		11-15-01	10:37a	one stage
TWOSTA~7	<dir></dir>		11-15-01	10:46a	two stage
	3 file(s)	3	00,175 by	tes	-

Directory of D:\Source Term\one stage

•	<dir></dir>	07-13-01 12:18	p.	
• •	<dir></dir>	07-13-01 12:18	p	
NM1X3432 6I	46,471	07-26-01 8:58	a nm1x3432.6i	
NM1X3432 60	3,236,897	07-26-01 9:03	a nm1x3432.60	
NM1X3432 6P		07-26-01 9:03		
NM1X3432 BIN	6,049,296	07-26-01 9:03	a nmlx3432.bin	
NM1X3~42 TXT	32,121	07-26-01 9:03	a nm1x3432.elem_aqu.txt	
NM1X3~44 TXT	30,136	07-26-01 9:03	a nm1x3432,elem_min.txt	
NM1X3~46 TXT	30,149	07-26-01 9:03	a nm1x3432.elem_tot.txt	
NM1X3~48 TXT	65,619	07-26-01 9:03	a nmlx3432.min_info.txt	
NM1X3432 TXT	1,455,396	11-14-01 9:44	a nm1x3432.txt	
NT1X1331 6I	46,478	07-18-01 10:21	a nt1x1331.6i	
NT1X1331 60	3,464,822	07-18-01 10:26	a nt1x1331.60	
NT1X1331 6P	43,324	07-18-01 10:26	a nt1x1331.6p	
NT1X1331 BIN	7,102,184	07-18-01 10:26	a ntlx1331.bin	
NT1X1~96 TXT	34,816	07-18-01 10:26	a nt1x1331.elem_aqu.txt	
NT1X1~98 TXT	32,663	07-18-01 10:26	a nt1x1331.elem_min.txt	
NT1X~100 TXT	•		a nt1x1331.elem_tot.txt	
NT1X~102 TXT	76,137	07-18-01 10:26	a nt1x1331.min_info.txt	e de la composición d
NT1X1331 TXT	1,703,332	11-14-01 9:46	a ntlx1331.txt	
NT1X1432 6I	46,467	07-25-01 7:10	p nt1x1432.6i	
NT1X1432 60	3,765,523	07-25-01 7:16	p nt1x1432.60	
NT1X1432 6P	42,898	07-25-01 7:16	p nt1x1432.6p	
NT1X1432 BIN	7,965,424	07-25-01 7:16	p ntlx1432.bin	
NT1X~154 TXT	37,511	07-25-01 7:16	<pre>p nt1x1432.elem_aqu.txt</pre>	
NT1X~156 TXT	35,190	07-25-01 7:16	<pre>p nt1x1432.elem_min.txt</pre>	
NT1X~158 TXT	35,203	07-25-01 7:16	<pre>p nt1x1432.elem_tot.txt</pre>	

NT1X~160 TXT88,57307-25-017:16p ntlx1432.min_info.txtNT1X1432 TXT1,908,65411-14-019:48a ntlx1432.txt 27 file(s) 37,451,596 bytes

Directory of D:\Source Term\two stage

	<dir></dir>	11-14-01	9:48a	
	<dir></dir>	11-14-01	9:48a	•••
NC1X1031 6I	44,775	07-18-01	1:18p	nc1x1031.6i
NC1X1031 60	1,326,343	07-18-01	1:21p	nc1x1031.60
NC1X1031 6P	41,236	07-18-01	1:21p	nc1x1031.6p
NC1X1031 BIN	6,003,824	07-25-01	8:21a	nc1x1031.bin
NC1X1~36 TXT	14,026	07-18-01	1:21p	nclx1031.elem aqu.txt
NC1X1~38 TXT	13,169	07-18-01	1:21p	nc1x1031.elem min.txt
NC1X1~40 TXT	13,182	07-18-01	1:21p	nc1x1031.elem_tot.txt
NC1X1~42 TXT	20,145	07-18-01	1:21p	nc1x1031.min info.txt
NC1X1031 TXT	1,043,308	11-14-01	10:00a	nclx1031.txt
NC2X1402 6I	32,777	07-18-01	1:58p	nc2x1402.6i
NC2X1402 60	5,117,352	07-18-01	2:17p	nc2x1402.60
NC2X1402 6P	32,855	07-18-01	2:17p	nc2x1402.6p
NC2X1402 BIN	51,507,080	07-25-01	8:34a	nc2x1402.bin
NC2X~222 TXT	44,441	07-18-01	2:17p	nc2x1402.elem_aqu.txt
NC2X~224 TXT	41,688	07-18-01	2:17p	nc2x1402.elem_min.txt
NC2X~226 TXT	41,701	07-18-01	2:17p	nc2x1402.elem_tot.txt
NC2X~228 TXT	92,412	07-18-01	2:17p	nc2x1402.min_info.txt
NC2X1402 TXT	10,667,092	11-14-01	9:51a	nc2x1402.txt
NM1X1031 6I	44,527	07-18-01	8:53a	nm1x1031.6i
NM1X1031 60	1,726,189	07-18-01	1:24p	nm1x1031.60
NM1X1031 6P	41,384	07-18-01	1:24p	nm1x1031.6p
NM1X1031 BIN	7,452,600	07-25-01	8:37a	nm1x1031.bin
NM1X~300 TXT	18,646	07-18-01	1:24p	nm1x1031.elem_aqu.txt
NM1X~302 TXT	17,501	07-18-01	1:24p	nm1x1031.elem_min.txt
NM1X~304 TXT	17,514	07-18-01	1:24p	nm1x1031.elem_tot.txt
NM1X~306 TXT	29,947	07-18-01	1:24p	nm1x1031.min_info.txt
NM1X1031 TXT	1,813,835	11-14-01	9:57a	nm1x1031.txt
NM2X1402 6I	32,923	07-19-01	9:07a	nm2x1402.6i
NM2X1402 60	2,886,235	07-19-01	9:17a	nm2x1402.60
NM2X1402 6P	33,167	07-19-01	9:17a	nm2x1402.6p
NM2X1402 BIN	15,910,448	07-25-01	8:44a	nm2x1402.bin
NM2X~378 TXT	27,501	07-19-01	9:17a	nm2x1402.elem_aqu.txt
NM2X~380 TXT	25,804	07-19-01	9:17a	nm2x1402.elem_min.txt
NM2X~382 TXT	25,817	07-19-01		nm2x1402.elem_tot.txt
NM2X~384 TXT	63,787	07-19-01	9:17a	nm2x1402.min_info.txt
NM2X1402 TXT	3,836,115		-	nm2x1402.txt
36 fil	le(s) 110,1	01,346 by	tes	

Total files listed: 227 file(s) 597,823,948 bytes - . ·

Directory of Fermi-IA2

SENSIT~5	<dir></dir>	11-15-01	11:23a	Sensitivity
TWO-ST~7	<dir></dir>	11-15-01	12:31p	Two-Stage
	0 file(s)	0 byt	ces	

Directory of D:\Sensitivity

Attachment I Page I-7 of I-11

•	<dir></dir>	11-15-01 12:31p	•
••	<dir></dir>	11-15-01 12:31p	••
GDPO4M~5	<dir></dir>	11-15-01 11:23a	GdPO4 mass
GDPO4R~7	<dir></dir>	11-15-01 11:37a	GdPO4 rate
GLASSR~9	<dir></dir>	11-15-01 12:29p	glass rate
	0 file(s)	0 bytes	

Directory of D:\Sensitivity\GdPO4 mass

	<dir></dir>	11-15-01	12:35p	
••	<dir></dir>	11-15-01	12:35p	
NA1D3333 6I	45,731	08-20-01	1:39p	nA1d3333.6i
NA1D3333 60	33,509,003	08-20-01	4:08p	na1d3333.60
NA1D3333 6P	43,226	08-20-01	4:08p	na1d3333.6p
NA1D~110 TXT	255,806	08-20-01	4:08p	nA1d3333.elem_aqu.txt
NA1D~112 TXT	239,877	08-20-01	4:08p	nA1d3333.elem_min.txt
NA1D~114 TXT	239,890	08-20-01	4:08p	nA1d3333.elem_tot.txt
NA1D~118 TXT	530,449	08-20-01	4:08p	nAld3333.min_info.txt
NL1D3333 6I	45,733	08-20-01	1:41p	nL1d3333.6i
NL1D3333 60	32,192,728	08-20-01	5:46p	nl1d3333.60
NL1D3333 6P	43,230	08-20-01	5:46p	nl1d3333.6p
NL1D~222 TXT	240,406	08-20-01	5:45p	nL1d3333.elem_aqu.txt
NL1D~224 TXT	225,437	08-20-01	5:45p	nL1d3333.elem_min.txt
NL1D~226 TXT	225,450	08-20-01	5:45p	nL1d3333.elem_tot.txt
NL1D~230 TXT	495,897	08-20-01	5:45p	nL1d3333.min_info.txt
14 fil	.e(s) 68,3	32,863 by	tes	

Directory of D:\Sensitivity\GdPO4 rate

		<dir></dir>	08-20-01	5:45p	
••		<dir></dir>	08-20-01	5:45p	
NA1X3323	6I	45,731	07-16-01	7:10p	nA1x3323.6i
NA1X3323	60	33,581,652	07-16-01	10:41p	na1x3323.60
NA1X3323	6P	43,226	07-16-01	10:41p	na1x3323.6p
NA1X~112	TXT	255,806	07-16-01	10:40p	nA1x3323.elem_aqu.txt
NA1X~114	TXT	239,877	07-16-01	10:40p	nA1x3323.elem_min.txt
NA1X~116	TXT	239,890	07-16-01	10:40p	nA1x3323.elem_tot.txt
NA1X~120	TXT	550,810	07-16-01	10:40p	nA1x3323.min_info.txt
NA1X3333	61	45,731	07-24-01	9:13a	nA1x3333.6i
NA1X3333	60	33,507,357	07-24-01	12:34p	na1x3333.60
NA1X3333	6P	43,226	07-24-01	12:34p	na1x3333.6p
NA1X~228	TXT	255,806	07-24-01	12:34p	nA1x3333.elem_aqu.txt
NA1X~230	TXT	239,877	07-24-01	12:34p	nA1x3333.elem_min.txt
NA1X~232	TXT	239,890	07-24-01	12:34p	nA1x3333.elem_tot.txt
NA1X~236	TXT	530,456	07-24-01	12:34p	nA1x3333.min_info.txt
NA1Y3323	6I	30,437	07-17-01	6:52a	nAly3323.6i
NA1Y3323	60	29,606,682	07-17-01	10:26a	naly3323.60
NA1Y3323	6P	30,437	07-17-01	10:26a	naly3323.6p 💦 🗤
NA1Y~332	TXT	241,176	07-17-01	10:25a	nA1y3323.elem_aqu.txt
NA1Y~334	$\mathbf{T}\mathbf{X}\mathbf{T}$	226,159	07-17-01	10:25a	nA1y3323.elem_min.txt
NA1Y~338	TXT	226,172	07-17-01	10:25a	nA1y3323.elem_tot.txt
NA1Y~340	TXT	379,240	07-17-01	10:25a	nA1y3323.min_info.txt
NA1Z3323	61	29,235	07-17-01	12:12p	nalz3323.6i
NA1Z3323	60	15,049,863	07-17-01	-	na1z3323.60
NA1Z3323	6P	29,153	07-17-01	2:39p	nalz3323.6p
NA1Z~394	TXT	129,141	07-17-01	2:39p	nA1z3323.elem_aqu.txt

NA1Z~396	TXT	121,108	07-17-01	2:39p	nA1z3323.elem_min.txt
NA1Z~398	TXT	121,121	07-17-01	2:39p	nA1z3323.elem_tot.txt
NA1Z~400	TXT	184,258	07-17-01	2:39p	nA1z3323.min_info.txt
NL1X3323	61	45,732	07-17-01	6:54a	nL1x3323.6i
NL1X3323	60	32,225,921	07-17-01	12:09p	nl1x3323.60
NL1X3323	6P	43,228	07-17-01	12:09p	nl1x3323.6p
NL1X~504	TXT	240,021	07-17-01	12:09p	nL1x3323.elem_aqu.txt
NL1X~506	TXT	225,076	07-17-01	12:09p	nL1x3323.elem_min.txt
NL1X~508	TXT	225,089	07-17-01	12:09p	nL1x3323.elem_tot.txt
NL1X~512	TXT	514,946	07-17-01	12:09p	nL1x3323.min_info.txt
NL1X3333	6I	45,732	07-24-01	9:13a	nL1x3333.6i
NL1X3333	60	32,263,697	07-25-01	9:32p	nl1x3333.60
NL1X3333	6P	43,228	07-25-01		nl1x3333.6p
NL1X~616	TXT	241,176	07-25-01	9:31p	nL1x3333.elem_aqu.txt
NL1X~618	TXT	226,159	07-25-01	9:31p	nL1x3333.elem_min.txt
NL1X~620	TXT	226,172	07-25-01	9:31p	nL1x3333.elem_tot.txt
NL1X~624	TXT	497,364	07-25-01	9:31p	nL1x3333.min_info.txt
NL1Y3323	61	30,439	07-17-01	12:14p	nl1y3323.6i
NL1Y3323	60	28,503,399	07-17-01	4:25p	nl1y3323.60
NL1Y3323	6P	30,439	07-17-01	4:25p	nl1y3323.6p
NL1Y~716	TXT	224,621	07-17-01	-	nL1y3323.elem_aqu.txt
NL1Y~720	TXT	210,636	07-17-01	4:25p	nL1y3323.elem_min.txt
NL1Y~722	TXT	210,649	07-17-01	_	nL1y3323.elem_tot.txt
NL1Y~724	TXT	349,800	07-17-01	4:25p	nLly3323.min_info.txt
NL1Z3323	61	29,236	07-18-01	6:48a	nl1z3323.6i
NL1Z3323	60	19,410,445	07-18-01	8:06a	nl1z3323.60
NL1Z3323	6P	29,153	07-18-01		nl1z3323.6p
NL1Z~790	TXT	161,481			nL1z3323.elem_aqu.txt
NL1Z~794	TXT	151,432	07-18-01	8:05a	nL1z3323.elem_min.txt
NI.17~796	TYT	151 445	07-18-01	8·05a	nL173323 elem tot tyt

151,445 07-18-01 8:05a nL1z3323.elem tot.txt

229,954 07-18-01 8:05a nL1z3323.min_info.txt

Directory of D:\Sensitivity\glass rate

56 file(s) 233,010,187 bytes

NL1Z~796 TXT

NL1Z~798 TXT

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	<di< th=""><th>ર></th><th>07-18-01</th><th>8:05a</th><th></th></di<>	ર >	07-18-01	8:05a	
••	<dii< td=""><td>२></td><td>07-18-01</td><td>8:05a</td><td>••</td></dii<>	२>	07-18-01	8:05a	••
NM1N1331	61	46,392	08-20-01	1:30p	nm1n1331.6i
NM1N1331	60 3	,124,338	08-20-01	5:51p	nm1n1331.60
NM1N1331	6P	43,160	08-20-01	5:51p	nm1n1331.6p
NM1N1~22	TXT	29,811	08-20-01	5:51p	nm1n1331.elem_aqu.txt
NM1N1~24	TXT	27,970	08-20-01	5:51p	nm1n1331.elem_min.txt
NM1N1~26	TXT	27,983	08-20-01	5:51p	nm1n1331.elem_tot.txt
NM1N1~28	TXT	58,660	08-20-01	5:51p	nm1n1331.min_info.txt
NM2N1402	61	32,923	08-21-01	3:58p	nm2n1402.6i
NM2N1402	60 2	,544,605	08-21-01	4:04p	nm2n1402.60
NM2N1402	6P	33,659	08-21-01	4:04p	nm2n1402.6p
NM2N1~44	TXT	24,036	08-21-01	4:04p	nm2n1402.elem_aqu.txt
NM2N1~46	TXT	22,555	08-21-01	4:04p	nm2n1492.elem_min.txt
NM2N1~48	TXT	22,568	08-21-01	4:04p	nm2n1402.elem_tot.txt
NM2N1~50	TXT	52,712	08-21-01	4:04p	nm2n1402.min_info.txt
NM2N1402	TXT 3	,332,738	11-15-01	8:31a	nm2n1402.txt
1	5 file(s)	9,42	4,110 byte	es	

Directory of D:\Two-Stage

<DIR> 11-15-01 12:29p .

••	<dir></dir>	11-15-01 12:29p
SCENAR~5	<dir></dir>	11-15-01 12:31p Scenario I
SCENAR~7	<dir></dir>	11-15-01 12:35p Scenario II
	0 file(s)	0 bytes

Directory of D:\Two-Stage\Scenario I

	<dir></dir>	11-15-01	8:31a			
••	<dir></dir>	11-15-01	8:31a			
NM1X1303 6I	38,545	07-16-01	7:35a	nm1x1303.6i		
NM1X1303 60	3,664,654	07-16-01	7:41a	nm1x1303.60		
NM1X1303 6P	34,824	07-16-01	7:41a	nm1x1303.6p		
NM1X1~24 TXT	43,671	07-16-01	7:41a	nm1x1303.elem_aqu.txt		
NM1X1~26 TXT	40,966	07-16-01	7:41a	nm1x1303.elem_min.txt		
NM1X1~28 TXT	40,979	07-16-01	7:41a	nmlx1303.elem_tot.txt		
NM1X1~30 TXT	67,345	07-16-01	7:41a	nm1x1303.min_info.txt		
NM1X1403 6I	38,544	07-16-01	7:30a	nmlx1403.6i		
NM1X1403 60	4,224,287	07-16-01	7:48a	nmlx1403.60		
NM1X1403 6P	34,988	07-16-01	7:48a	nm1x1403.6p		
NM1X1~50 TXT	46,751	07-16-01	7:48a	nm1x1403.elem_aqu.txt		
NM1X1~52 TXT	43,854	07-16-01	7:48a	nm1x1403.elem_min.txt		
NM1X1~54 TXT	43,867	07-16-01	7:48a	nm1x1403.elem_tot.txt		
NM1X1~56 TXT	88,503	07-16-01	7:48a	nm1x1403.min_info.txt		
SECOND~5	<dir></dir>	11-15-01	12:33p	second stage		
14 file(s) 8,451,778 bytes						

Directory of D:\Two-Stage\Scenario I\second stage

. <d< th=""><th>IR></th><th>11-15-01</th><th>12:40p</th><th>•</th></d<>	IR>	11-15-01	12:40p	•
<d< td=""><td>IR></td><td>11-15-01</td><td>12:40p</td><td></td></d<>	IR>	11-15-01	12:40p	
NM2X1031 6I	40,418	07-16-01	12:38p	nm2x1031.6i
NM2X1031 60	1,183,740	07-16-01	12:39p	nm2x1031.60
NM2X1031 6P	40,405	07-16-01	12:39p	nm2x1031.6p
NM2X1~14 TXT	12,871	07-16-01	12:39p	nm2x1031.elem_aqu.txt
NM2X1~16 TXT	12,086	07-16-01	12:39p	nm2x1031.elem_min.txt
NM2X1~18 TXT	12,099	07-16-01	12:39p	nm2x1031.elem_tot.txt
NM2X1~20 TXT	22,629	07-16-01	12:39p	nm2x1031.min_info.txt
NM2X1332 6I	41,457	07-16-01	4:51p	nm2x1332.6i
NM2X1332 60	7,506,988	07-16-01	5:07p	nm2x1332.60
NM2X1332 6P	41,771	07-16-01	5:07p	nm2x1332.6p
NM2X1~52 TXT	75,626	07-16-01	5:07p	nm2x1332.elem_aqu.txt
NM2X1~54 TXT	70,929	07-16-01	5:07p	nm2x1332.elem_min.txt
NM2X1~56 TXT	70,942	07-16-01	5:07p	nm2x1332.elem_tot.txt
NM2X1~58 TXT	144,331	07-16-01	5:07p	nm2x1332.min_info.txt
NM2Y1031 6I	29,531	07-16-01	12:41p	nm2y1031.6i
NM2Y1031 60	357,876	07-16-01	12:41p	nm2y1031.60
NM2Y1031 6P	29,695	07-16-01	12:41p	nm2y1031.6p
NM2Y1~68 TXT	4,401	07-16-01	12:41p	nm2y1031.elem_aqu.txt
NM2Y1~70 TXT	4,144	07-16-01	12:41p	nm2y1031.elem_min.txt
NM2Y1~72 TXT	4,157	07-16-01	12:41p	nm2y1031.elem_tot.txt
NM2Y1~74 TXT	7,627	07-16-01	12:41p	nm2y1031.min_info.txt
21 file(s) 9,7	13,723 byt	ces	

Directory of D:\Two-Stage\Scenario II

	<dir></dir>	11-15-01	12:33p	•
• •	<dir></dir>	11-15-01	12:33p	••

and shows

.

NM1X1023	61	44,52	7 07-12-01	5:32p	nmlx1023.6i
NM1X1023	60	10,068,66		-	nm1x1023.60
NM1X1023	6P	41,22	0 07-12-01	5:55p	nm1x1023.6p
NM1X1~42	TXT	85,63	6 07-12-01	-	nm1x1023.elem aqu.txt
NM1X1~44	TXT	80,31	.5 07-12-01	_	nm1x1023.elem min.txt
NM1X1~46	TXT	80,32	8 07-12-01	5:55p	nm1x1023.elem_tot.txt
NM1X1~48	TXT	149,60	9 07-12-01	5:55p	nmlx1023.min info.txt
NM1X1032	6I	44,52	27 07-16-01	11:40a	nm1x1032.6i
NM1X1032	60	2,591,20	0 07-16-01	11:48a	nm1x1032.60
NM1X1032	6P	41,30	07-16-01	11:48a	nm1x1032.6p
NM1X1032	6T	116,73	86 07-16-01	11:48a	nm1x1032.6t
NM1X1032	6TX	118,33	81 07-16-01	11:48a	nm1x1032.6tx
NM1X1~68	TXT	25,19	07-16-01	11:48a	nm1x1032.elem_aqu.txt
NM1X1~70	TXT	23,63	88 07-16-01	11:48a	nm1x1032.elem_min.txt
NM1X1~72	TXT	23,65	51 07-16-01	11:48a	nm1x1032.elem_tot.txt
NM1X1~74	TXT	42,25	5 07-16-01	11:48a	nm1x1032.min_info.txt
NM1X1033	6I	44,52	27 07-12-01	5:32p	nmlx1033.6i
NM1X1033	60	10,139,04	4 07-12-01	6:17p	nm1x1033.60
NM1X1033	6P	41,30	07-12-01	6:17p	nm1x1033.6p
NM1X~112	TXT	84,86	6 07-12-01	6:16p	nm1x1033.elem_aqu.txt
NM1X~114	TXT	79,59	93 07-12-01	6:16p	nm1x1033.elem_min.txt
NM1X~116	TXT	79,60	06 07-12-01	6:16p	nm1x1033.elem_tot.txt
NM1X~118	TXT	154,49	99 07-12-01	6:16p	nmlx1033.min_info.txt
SECOND~5		<dir></dir>	11-15-01	12:40p	second stage
:	23 file	(s) 24	1,200,571 by	tes	

Directory of D:\Two-Stage\Scenario II\second stage

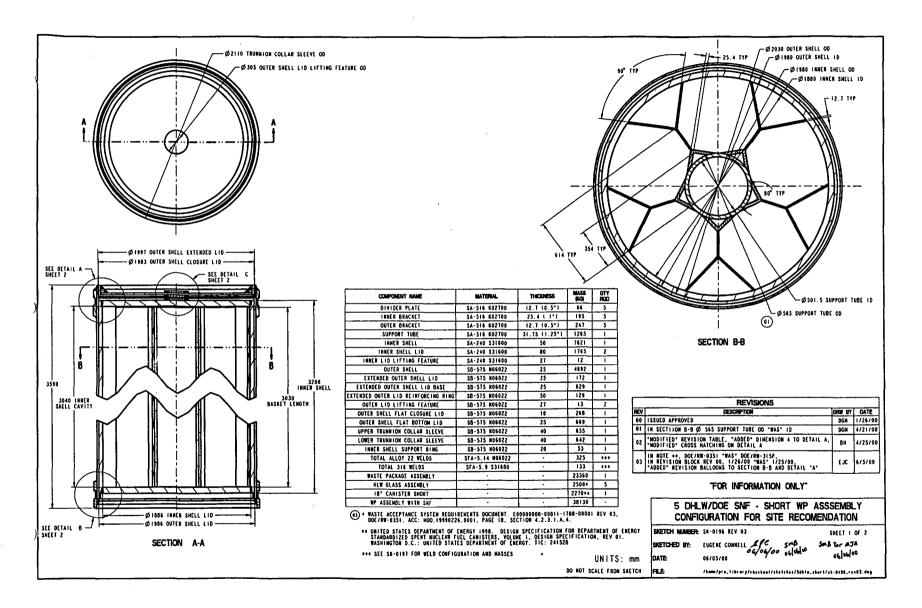
•	<dir></dir>	07-16-01		
••	<dir></dir>	07-16-01	-	
NM2X1302 6I	32,920	07-16-01	_	nm2x1302.6i
NM2X1302 60	8,420,000	07-16-01	_	nm2x1302.60
NM2X1302 6P	33,413	07-16-01	÷	nm2x1302.6p
NM2X1~38 TXT	66,386	07-16-01	3:05p	nm2x1302.elem_aqu.txt
NM2X1~40 TXT	62,265	07-16-01	3:05p	nm2x1302.elem_min.txt
NM2X1~42 TXT	62,278	07-16-01	3:05p	nm2x1302.elem_tot.txt
NM2X1~44 TXT	90,003	07-16-01	3:05p	nm2x1302.min_info.txt
NM2X1303 6I	32,920	07-12-01	6:29p	nm2x1303.6i
NM2X1303 60	27,393,171	07-13-01	2:58a	nm2x1303.60
NM2X1303 6P	33,085	07-13-01	2:58a	nm2x1303.6p
NM2X~132 TXT	194,206	07-13-01	2:58a	nm2x1303.elem_aqu.txt
NM2X~136 TXT	182,117	07-13-01	2:58a	nm2x1303.elem_min.txt
NM2X~138 TXT	182,130	07-13-01	2:58a	nm2x1303.elem_tot.txt
NM2X~140 TXT	288,249	07-13-01	2:58a	nm2x1303.min_info.txt
NM2X1323 6I	33,817	07-12-01	6:24p	nm2x1323.6i
NM2X1323 60	27,310,618	07-13-01	1:58a	nm2x1323.60
NM2X1323 6P	34,064	07-13-01	1:58a	nm2x1323.6p
NM2X~230 TXT	191,896	07-13-01	1:57a	nm2x1323.elem_aqu.txt
NM2X~232 TXT		07-13-01	1:57a	nm2x1323.elem_min.txt
NM2X~234 TXT	179,964	07-13-01	1:57a	nm2x1323.elem_tot.txt
NM2X~236 TXT	267,941	07-13-01	1:57a	nm2x1323.min_info.txt
NM2Y1302 6I	29,228	07-16-01	3:24p	nm2y1302.6i
NM2Y1302 60	826,333	07-16-01	3:26p	nm2y1302.60
NM2Y1302 6P	29,228	07-16-01	3:26p	nm2y1302.6p
NM2Y~248 TXT	7,866	07-16-01	3:26p	nm2y1302.elem_aqu.txt
NM2Y~250 TXT	7,393	07-16-01		nm2y1302.elem_min.txt
NM2Y~252 TXT	7,406	07-16-01	-	nm2y1302.elem_tot.txt
			_	

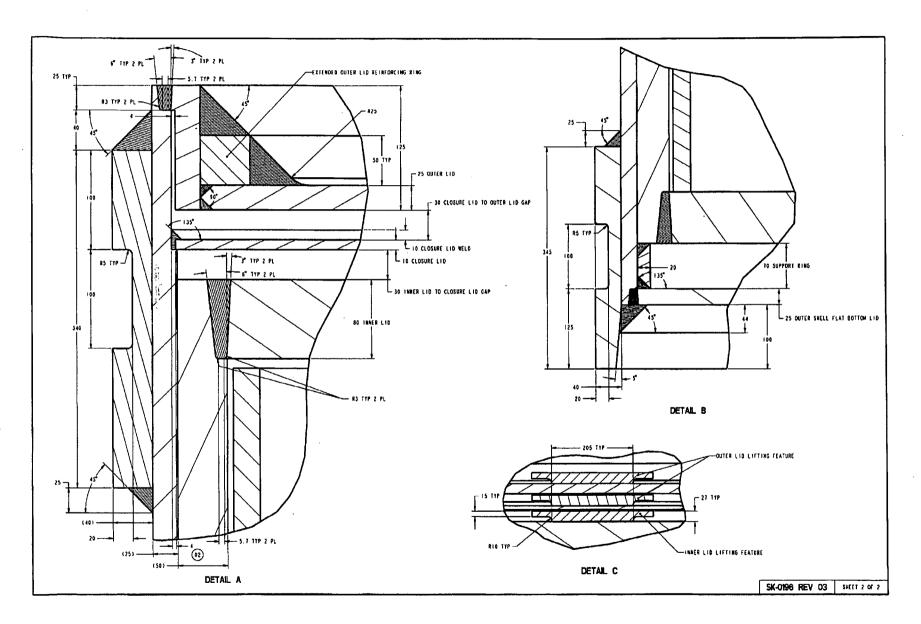
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NM2Y~254	TXT	14,349	07-16-01	3:26p	nm2y1302.min_info.txt
NM2Y1303	61	30,503	07-13-01	6:55a	nm2y1303.6i
NM2Y1303	60	30,205,779	07-13-01	2:23p	nm2y1303.60
NM2Y1303	6P	30,503	07-13-01	2:23p	nm2y1303.6p
NM2Y~350	TXT	243,871	07-13-01	2:23p	nm2y1303.elem_aqu.txt
NM2Y~354	TXT	228,686	07-13-01	2:23p	nm2y1303.elem_min.txt
NM2Y~356	TXT	228,699	07-13-01	2:23p	nm2y1303.elem_tot.txt
NM2Y~360	TXT	347,794	07-13-01	2:23p	nm2y1303.min_info.txt
NM2Y1323	6I	31,482	07-13-01	6:54a	nm2y1323.6i
NM2Y1323	60	30,293,869	07-13-01	1:20p	nm2y1323.60
NM2Y1323	6P	31,482	07-13-01	1:20p	nm2y1323.6p
NM2Y~456	TXT	243,101	07-13-01	1:20p	nm2y1323.elem_aqu.txt
NM2Y~460	TXT	227,964	07-13-01	1:20p	nm2y1323.elem_min.txt
NM2Y~462	TXT	227,977	07-13-01	1:20p	nm2y1323.elem_tot.txt
NM2Y~464	TXT	319,735	07-13-01	1:20p	nm2y1323.min_info.txt
NM2Z1303	6I	30,503	07-16-01	6:47a	nm2z1303.6i
NM2Z1303	60	22,538,351	07-16-01	10:43a	nm2z1303.60
NM2Z1303	6P	30,421	07-16-01	10:43a	nm2z1303.6p
NM2Z~540	TXT	192,666	07-16-01	10:43a	nm2z1303.elem_aqu.txt
NM2Z~542	TXT	180,673	07-16-01	10:43a	nm2z1303.elem_min.txt
NM2Z~546	TXT	180,686	07-16-01	10:43a	nm2z1303.elem_tot.txt
NM2Z~548	TXT	243,295	07-16-01	10:43a	nm2z1303.min_info.txt
NM2Z1323	61	31,480	07-16-01	12:46p	nm2z1323.6i
NM2Z1323	60	23,506,589	07-16-01	1:57p	nm2z1323.60
NM2Z1323	6P	31,400	07-16-01	1:57p	nm2z1323.6p
NM2Z~626	TXT	194,206	07-16-01	1:57p	nm2z1323.elem_aqu.txt
NM2Z~628	TXT	182,117	07-16-01	1:57p	nm2z1323.elem_min.txt
NM2Z~630	TXT	182,130	07-16-01	1:57p	nm2z1323.elem_tot.txt
NM2Z~634	TXT	245,423	07-16-01	1:57p	nm2z1323.min_info.txt
	56 file	(s) 176,65	54,582 byt	ces	

Total files listed: 199 file(s) 529,787,814 bytes

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EQ6 CALCULATION FOR CHEMICAL DEGRADATION OF ENRICO CODISPOSAL WASTE PACKAGE: EFFECTS OF UPDATED DESIGN AND RATES 7. Document Number(s) CAL-EDC-MD-000015 8. Version Designate REV. 00	
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QA: N/A

1. DOCUMENT TITLE:	<u> </u>			
EQ6 Calculation for Chemical Degradation 2. IDENTIFIER (e.g., DI OR PI):	of Enrico Fermi Codi	sposal Waste Package 3. REVISION DESIGNA		ed Design and Rates
CAL-EDC-MD-000015		Rev. 00		
ATTACHED SOFTWARE FILE INFORM	ATION	4. PDF FILE SUBMITTE	D: YES	✓ NO
5. FILE NAMES(S) WITH FILE EXTENSION(S) PI	ROVIDED BY THE SOFT	WARE:		
See Attacked				
See Attached 6. DATE LAST MODIFIED:	7. NATIVE APPLICATIO	N:	8. FILE SIZE IN KIL	OBYTES:
	(i.e., EXCEL, WORD, CORE	ELDRAW)		
See Attached 9. FILE LINKAGE INSTRUCTIONS/INFORMATIO	Word		See Attached	
9. FILE LINKAGE INSTRUCTIONS/INFORMATIO	IN:			
Standard				
10. PRINTER SPECIFICATION (I.E., HP4SI) INCLU	JDING POSTSCRIPT INF	ORMATION (i.e., PRINTER	R DRIVER) AND PRIN	TING PAGE SETUP: (i.e.,
LANDSCAPE, 11 X 17 PAPER)				
·				
T1024AHP5Si 8 1/2 x 11 Color- 8 1/2 X 11. COMPUTING PLATFORM USED: (i.e., PC, SU		12. OPERATING SYST	EM AND VERSION.	(i.e., WINDOWS UNIX, SOLARIS)
PC#117728		Windows 95		
13. ADDITIONAL HARDWARE/SOFTWARE REC	QUIREMENT USED TO CI	REATE FILE(S):	14. ACCESS REST LICENSE ISSUES)	RICTIONS: (COPYRIGHT OR
None			None	
COMMENTS/SPECIAL INSTRUCTION		<u> </u>		
15. IS SOFTWARE AVAILABLE FROM SOFTWA	·	ANAGEMENT?	ES NO	
SOFTWARE MEDIA TRACKING NUMBER				
Note: The software product(s) to develop th				
Software Media Number (SMN). The COT	is software products a	re under Sonware Con	inguration Manag	ement (SCM).
Originator: Patricia Bernot & Emma Parke	er			
CERTIFICATION				
16. DOCUMENT OWNER (Print and Sign):	6	······································	17. D	
	1/2 1		12	114/2001
Dan Thomas DUA 18. ORGANIZATION: 19. DEPAR	RTMENT:	20. LOCATION/MAIL S		/ HONE:
1				
BSC Waste Pa 22. SUBMITTED BY (Print and Sign):	ckage Criticality	MS423/1006	295 23. D	
			23. 0.	∖≀⊑ .
Daynett D. Vosicky Down With,	D. Vosich	/	1	2-14-2001
DC USE ONLY		0		
24. DATE RECEIVED:	25. DATE FILES TRAN	SFERRED:	26. DC NO.:	<u></u>
12-14-01	\sim	A	1 na 71-	<u>`</u> م
27. NAME (Print and Sign):	L	<u></u>	28. DATE:	<u> </u>
	ALA		NA	
	1 / 1/			
AP-6.1Q.8				Rev. 06/01/200

Waste Package ProjectCalculationTitle: EQ6 Calculation for Chemical Degradation of Enrico Fermi Codisposal Waste Packages:
Effects of Updated Design and RatesPage 119 of 119Document Identifier: CAL-EDC-MD-000015 REV00Page 119 of 119

8. ATTACHMENTS

Attachment I. Listing of Files on Compact Disks (11 pages)

Attachment II. Sketch SK-0200 REV 04 (2 pages)

Attachment III. Two Compact Discs

ATTACHMENT I. LISTING OF FILES ON COMPACT DISKS

This attachment contains the MS-DOS directory for files placed on the electronic media (Attachment I). The files are of various types:

- 1. Excel files (extensions = xls).
- 2. EQ3/6 input files (extension = 3i or 6i).

ASCII text file: provides input parameters for EQ3/6.

3. EQ3/6 output files (extension = 30 or 60).

ASCII text file: provides detailed information about the system at each print point, which is specified by the user in the input file.

4. EQ3/6 pickup files (extension = 3p or 6p).

ASCII text file: provides a description of the system at the end of that run to be used as an input file for a continuation run.

5. EQ6 Tab-delimited text files (extension = txt).

*.elem_aqu: total aqueous moles of elements.

*.elem_min: total moles of elements in minerals.

*.elem_tot: total moles of elements (aqueous + mineral).

*.min_info: moles of each mineral.

6. EQ6 binary output file (extension = bin).

Binary file: provides detailed information about the system at the full numerical precision for *every* time step.

- 7. EQ3/6 text data files used for the calculations, "data0.ymd".
- 8. Batch files (extension = bat) used to start EQ6 runs.
- 9. Winzip files (extension = zip).

Below are listed the contents of the DOS directories within the electronic attachment:

The first column is the DOS file name.

The second column lists <DIR> if it is a directory or gives the files size (bytes) if it is a file.

The third and fourth columns are the date and time of the last update.

The fifth column is the filename.

Directory of Fermi-IA1

DATA0	NUC	2,302,224	09-15-99	11:40a	DATAO.NUC
DATAO	YMD	2,657,459	03-16-01	1:22p	data0.ymd
DATA0	YMP	2,649,470	09-11-00	5:23p	data0.ymp
ENRIC~34	XLS	1,075,200	11-14-01	3:24p	enrich-fermi1.xls
ENRIC~38	XLS	1,047,552	11-14-01	3:49p	enrich-fermi2.xls
ENRIC~44	XLS	535,040	11-15-01	10:15a	enrich-sens-Fermi.xls
FERMI~48	XLS	39,424	09-20-01	8:28a	Fermi-IA-2001.xls
FERMI~50	XLS	256,512	09-13-01	10:24a	fermi-losses.xls
HLWGL~52	XLS	57,856	08-01-01	10:17a	HLWglass-2001.xls
J13NOM20	31	13,734	10-23-00	12:44p	j13nom20.3i
J13NOM20	30	114,582	10-23-00	12:45p	j13nom20.30
J13NOM20	3P	11,786	10-23-00	12:45p	j13nom20.3p
J13NOM30	31	13,660	10-10-00	1:31p	j13nom30.3i
J13NOM30	30	115,224	10-10-00	1:32p	j13nom30.30
J13NOM30	3P	11,712	10-10-00	1:32p	j13nom30.3p
LOSSE~66	XLS	18,944	08-20-01	3:59p	losses-oldtime.xls
MORES~68	XLS	18,944	09-17-01	7:22a	moresense.xls
OLDFE~72	XLS	16,896	09-13-01	8:19a	oldfermi-recalc.xls
ONE-ST~5		<dir></dir>	11-15-01	8:50a	One-Stage
S_ASE~76	XLS	108,544	08-23-01	7:32a	S+A sensitivity.xls
S_A~78	XLS	790,016	09-19-01	9:02a	S+A.xls
SENSI~82	XLS	9,253,888	11-15-01	9:27a	Sensitivity.xls
SOURCE~7		<dir></dir>	11-15-01	10:37a	Source Term
UENR~112	XLS	19,968	11-13-01	3:01p	Uenrich Fermi.xls
:	22 file	e(s) 21,12	28,635 by	tes	

Directory of D:\One-Stage

		<dir></dir>	11-13-01	3:01p .
		<dir></dir>	11-13-01	3:01p
NG1X3323	61	45,736	07-16-01	5:11p ng1x3323.6i
NG1X3323	60	31,486,614	07-16-01	9:01p ng1x3323.60
NG1X3323	6P	43,166	07-16-01	9:01p ng1x3323.6p
NG1X~104	TXT	232,706	07-16-01	9:00p ng1x3323.elem aqu.txt
NG1X~106	TXT	218,217	07-16-01	9:00p ng1x3323.elem min.txt
NG1X~108	TXT	218,230	07-16-01	9:00p ng1x3323.elem tot.txt
NG1X~112	TXT	465,870	07-16-01	9:00p ng1x3323.min info.txt
NM1X1321	6I	46,466	07-11-01	1:16p nmlx1321.6i
NM1X1321	60	2,802,843	07-11-01	1:25p nmlx1321.60
NM1X1321	6P	43,554	07-11-01	1:25p nmlx1321.6p
NM1X~128	TXT	28,656	07-11-01	1:25p nm1x1321.elem aqu.txt
NM1X~130	TXT	26,887	07-11-01	1:25p nmlx1321.elem min.txt
NM1X~132	TXT	26,900	07-11-01	1:25p nmlx1321.elem tot.txt
NM1X~134	TXT	58,272	07-11-01	1:25p nmlx1321.min_info.txt
NM1X1331	6I	46,466	07-11-01	1:16p nm1x1331.6i
NM1X1331	60	2,784,787	07-11-01	1:31p nm1x1331.60
NM1X1331	6P	43,226	07-11-01	1:31p nm1x1331.6p
NM1X~150	TXT	27,886	07-11-01	1:31p nm1x1331.elem_aqu.txt
NM1X~152	TXT	26,165	07-11-01	1:31p nm1x1331.elem_min.txt
NM1X~154	TXT	26,178	07-11-01	1:31p nm1x1331.elem_tot.txt
NM1X~156	TXT	53,551	07-11-01	1:31p nm1x1331.min_info.txt
NM1X1333	61	46,466	07-25-01	1:34p nmlx1333.6i
NM1X1333	60	17,695,889	07-25-01	2:05p nmlx1333.60
NM1X1333	6 P	42,816	07-25-01	2:05p nmlx1333.6p

NM1X~216 TX1	183,811	07-25-01	2:05p	nm1x1333.elem aqu.txt					
NM1X~218 TXT		07-25-01		nmlx1333.elem min.txt					
NM1X~222 TX1		07-25-01	2:05p	nmlx1333.elem_tot.txt					
NM1X~224 TX1		07-25-01	-	nmlx1333.min info.txt					
NM1X2331 6I	46,466	07-11-01		nm1x2331.6i					
NM1X2331 60	3,499,254	07-11-01	-	nm1x2331.60					
NM1X2331 6P	43,636	07-11-01	-	nm1x2331.6p					
NM1X~244 TXT		07-11-01	_	nm1x2331.elem aqu.txt					
NM1X~246 TX1		07-11-01		nm1x2331.elem_min.txt					
NM1X~248 TXT	•	07-11-01		nm1x2331.elem_tot.txt					
NM1X~250 TX1	•	07-11-01	-	nmlx2331.min info.txt					
NM1X2422 6I	45,652	07-12-01	-	nm1x2422.6i					
NM1X2422 60	12,646,847	07-12-01	-	nm1x2422.60					
NM1X2422 6P	42,668	07-12-01	-	nm1x2422.6p					
NM1X~296 TX7		07-12-01	-	nmlx2422.elem aqu.txt					
NM1X~298 TX1	•	07-12-01	-	nm1x2422.elem min.txt					
NM1X~300 TX7	•	07-12-01		nm1x2422.elem_tot.txt					
NM1X~302 TX7	•	07-12-01		nmlx2422.min_info.txt					
NM1X2432 6I	45,651	07-12-01		nmlx2432.6i					
NM1X2432 60	12,914,822	07-12-01	-	nm1x2432.60					
NM1X2432 6P	42,586	07-12-01		nm1x2432.6p					
NM1X~348 TX1			_	nm1x2432.elem aqu.txt					
NM1X~348 1X1 NM1X~350 TX1		07-12-01		nm1x2432.elem_aqu.txt					
		07-12-01	-						
NM1X~352 TX1	•	07-12-01	-	nmlx2432.elem_tot.txt					
NM1X~354 TX1	•	07-12-01	_	nmlx2432.min_info.txt					
NM1X3323 6I	45,655	07-12-01		nm1x3323.6i					
NM1X3323 60	31,856,704	07-12-01		nm1x3323.60					
NM1X3323 6P	43,078	07-12-01	-	nm1x3323.6p					
NM1X~456 TXT	•	07-12-01	-	nm1x3323.elem_aqu.txt					
NM1X~458 TX1	•	07-12-01		nm1x3323.elem_min.txt					
NM1X~462 TXT	•	07-12-01	-	nm1x3323.elem_tot.txt					
NM1X~464 TX1	•	07-12-01	-	nmlx3323.min_info.txt					
NM1X3333 6I	45,655	07-12-01		nm1x3333.6i					
NM1X3333 60	30,373,686	07-12-01		nm1x3333.60					
NM1X3333 6P	43,078	07-12-01		nmlx3333.6p					
NM1X~562 TX1	, •			nm1x3333.elem_aqu.txt					
NM1X~566 TX1 NM1X~568 TX1				nm1x3333.elem_min.txt					
				nm1x3333.elem_tot.txt					
NM1X~570 TX1	•			nm1x3333.min_info.txt					
NM1X3433 6I	45,655			nm1x3433.6i					
NM1X3433 60	30,750,097	07-12-01	-	nm1x3433.60					
NM1X3433 6P	42,996	07-12-01		nm1x3433.6p					
NM1X~670 TX		07-12-01	-	nmlx3433.elem_aqu.txt					
NM1X~674 TX	•	07-12-01	-	nmlx3433.elem_min.txt					
NM1X~676 TX	-	07-12-01		nm1x3433.elem_tot.txt					
NM1X~678 TX	•	07-12-01		nm1x3433.min_info.txt					
SECOND~5	<dir></dir>	11-15-01		second part					
THIRDP~7	<dir></dir>			third part					
70 1	70 file(s) 184,808,385 bytes								

Directory of D:\One-Stage\second part

		<dir></dir>	11-15-01	10:46a	•
••		<dir></dir>	11-15-01	10:46a	
NG1Y3323	61	30,372	07-17-01	6:53a	ng1y3323.6i
NG1Y3323	60	27,899,955	07-17-01	8:41a	ng1y3323.60
NG1Y3323	6 P	30,367	07-17-01	8:41a	ng1y3323.6p
					•

NG1Y3~94	TXT	219,616	07-17-01	8:40a	ng1y3323.elem_aqu.txt
NG1Y3~96	TXT	205,943	07-17-01	8:40a	ng1y3323.elem_min.txt
NG1Y~100	TXT	205,956	07-17-01	8:40a	ng1y3323.elem_tot.txt
NG1Y~102	TXT	343,174	07-17-01	8:40a	ng1y3323.min_info.txt
NM1Y1333	61	30,577	07-25-01	3:02p	nm1y1333.6i
NM1Y1333	60	20,670,995	07-25-01	3:54p	nm1y1333.60
NM1Y1333	6 P	30,585	07-25-01	3:54p	nmly1333.6p
NM1Y~172	TXT	228,471	07-25-01	3:54p	nm1y1333.elem_aqu.txt
NM1Y~174	TXT	214,246	07-25-01	3:54p	nm1y1333.elem_min.txt
NM1Y~176	TXT	214,259	07-25-01	3:54p	nm1y1333.elem_tot.txt
NM1Y~180	TXT	315,064	07-25-01	3:54p	nmly1333.min_info.txt
NM1Y3323	6I	30,289	07-12-01	5:36p	nm1y3323.6i
NM1Y3323	60	28,171,181	07-12-01	10:25p	nm1y3323.60
NM1Y3323	6P	30,289	07-12-01	10:25p	nm1y3323.6p
NM1Y~270	TXT	219,616	07-12-01	10:25p	nm1y3323.elem_aqu.txt
NM1Y~274	TXT	205,943	07-12-01	10:25p	nm1y3323.elem_min.txt
NM1Y~276	TXT	205,956	07-12-01	10:25p	nm1y3323.elem_tot.txt
NM1Y~278	TXT	340,774	07-12-01	10:25p	nm1y3323.min_info.txt
NM1Y3333	61	29,310	07-12-01	2:02p	nm1y3333.6i
NM1Y3333	60	28,916,112	07-12-01	11:58p	nm1y3333.60
NM1Y3333	6P	29,310	07-12-01	11:58p	nm1y3333.6p
NM1Y~372	TXT	222,696	07-12-01	11:57p	nm1y3333.elem_aqu.txt
NM1Y~374	$\mathbf{T}\mathbf{X}\mathbf{T}$	208,831	07-12-01	11:57p	nm1y3333.elem_min.txt
NM1Y~378	TXT	208,844	07-12-01	11:57p	nmly3333.elem_tot.txt
NM1Y~380	TXT	324,558	07-12-01	11:57p	nm1y3333.min_info.txt
NM1Y3433	6I	28,027	07-12-01	2:04p	nm1y3433.6i
NM1Y3433	60	26,458,687			nmly3433.60
NM1Y3433	6P	27,618	07-13-01	12:58a	nm1y3433.6p
NM1Y~466	TXT	221,156	07-13-01	12:58a	nm1y3433.elem_aqu.txt
NM1Y~470	TXT	207,387	07-13-01	12:58a	nm1y3433.elem_min.txt
NM1Y~472	$\mathbf{T}\mathbf{X}\mathbf{T}$	207,400	07-13-01	12:58a	nm1y3433.elem_tot.txt
NM1Y~474		304,930			nmly3433.min_info.txt
	35 file	(s) 137,23	38,494 by	tes	

Directory of D:\One-Stage\third part

		<dir></dir>	07-13-01	12·58a	
		<dir></dir>	07-13-01	12:58a	
NG1Z3323	61	29,164			ng1z3323.6i
NG1Z3323	60	20,531,160	07-17-01	-	ng1z3323.60
NG1Z3323		29,163	07-17-01	-	ng1z3323.6p
NG1Z3~72	TXT	170,336	07-17-01	*	ng1z3323.elem agu.txt
NG1Z3~74	TXT	159,735	07-17-01	-	ng1z3323.elem min.txt
NG1Z3~76	TXT	159,748	07-17-01	-	ng1z3323.elem_tot.txt
NG1Z3~80	TXT	242,384	07-17-01	1:39p	ng1z3323.min info.txt
NM1Z3323	61	29,086	07-13-01	-	nm1z3323.6i
NM1Z3323	60	20,814,521	07-13-01	9:32a	nm1z3323.60
NM1Z3323	6 P	29,003	07-13-01	9:32a	nm1z3323.6p
NM1Z3323	6T	683,102	07-13-01	9:32a	nm1z3323.6t
NM1Z3323	6TX	690,396	07-13-01	9:32a	nm1z3323.6tx
NM1Z~156	TXT	171,491	07-13-01	9:31a	nm1z3323.elem aqu.txt
NM1Z~160	TXT	160,818	07-13-01	9:31a	nm1z3323.elem min.txt
NM1Z~162	TXT	160,831	07-13-01	9:31a	nm1z3323.elem_tot.txt
NM1Z~164	TXT	244,016	07-13-01	9:32a	nm1z3323.min_info.txt
NM1Z3333	61	28,107	07-13-01	6:57a	nm1z3333.6i
NM1Z3333	60	28,944,873	07-13-01	11:17a	nm1z3333.60
NM1Z3333	6 P	28,106	07-13-01	11:17a	nm1z3333.6p

929,403 07-13-01 11:17a nmlz3333.6t NM1Z3333 6T 1,022,828 07-13-01 11:17a nmlz3333.6tx NM1Z3333 6TX 258,116 07-13-01 11:16a nm1z3333.elem aqu.txt NM1Z~268 TXT 242,043 07-13-01 11:16a nm1z3333.elem min.txt NM1Z~270 TXT NM1Z~274 TXT 242,056 07-13-01 11:16a nmlz3333.elem tot.txt NM1Z~276 TXT 366,416 07-13-01 11:17a nmlz3333.min info.txt 27,617 07-13-01 6:56a nmlz3433.6i NM1Z3433 6I 27,644,398 07-13-01 12:18p nm1z3433.60 NM1Z3433 60 NM1Z3433 6P 27,616 07-13-01 12:18p nmlz3433.6p NM1Z3433 6T 842,656 07-13-01 12:18p nm1z3433.6t 851,516 07-13-01 12:18p nm1z3433.6tx NM1Z3433 6TX NM1Z~376 TXT 257,731 07-13-01 12:18p nm1z3433.elem aqu.txt NM1Z~378 TXT 241,682 07-13-01 12:18p nm1z3433.elem min.txt 241,695 07-13-01 12:18p nmlz3433.elem_tot.txt NM1Z~380 TXT 293,503 07-13-01 12:18p nmlz3433.min_info.txt NM1Z~384 TXT 34 file(s) 106,795,316 bytes

Directory of D:\Source Term

•	<	DIR>		11-15-01	10:00a	
••	<	DIR>		11-15-01	10:00a	
ASPRIN	EXE	299,1	130	07-03-01	9:07a	asprin.exe
DEFLTS~8	TXT	1	187	07-26-01	9:25a	defltsolids.txt
DEFLT~10	TXT	8	858	07-10-01	2:35p	defltsolids_longlist.txt
ONESTA~5	<	DIR>		11-15-01	10:37a	one stage
TWOSTA~7	<	DIR>		11-15-01	10:46a	two stage
	3 file(s)	30	0,175 byt	ces	

Directory of D:\Source Term\one stage

	<dir></dir>	07-13-01	12:18p	
• •	<dir></dir>	07-13-01	12:18p	
NM1X3432 6I	46,471	07-26-01	8:58a	nm1x3432.6i
NM1X3432 60	3,236,897	07-26-01	9:03a	nm1x3432.60
NM1X3432 6P	43,636	07-26-01	9:03a	nm1x3432.6p
NM1X3432 BIN	6,049,296	07-26-01	9:03a	nmlx3432.bin
NM1X3~42 TXT	32,121	07-26-01	9:03a	nm1x3432.elem_aqu.txt
NM1X3~44 TXT	30,136	07-26-01	9:03a	nm1x3432.elem_min.txt
NM1X3~46 TXT	30,149	07-26-01	9:03a	nm1x3432.elem_tot.txt
NM1X3~48 TXT	65,619	07-26-01	9:03a	nm1x3432.min_info.txt
NM1X3432 TXT	1,455,396	11-14-01	9:44a	nm1x3432.txt
NT1X1331 6I	46,478	07-18-01	10:21a	nt1x1331.6i
NT1X1331 60	3,464,822	07-18-01	10:26a	nt1x1331.60
NT1X1331 6P	43,324	07-18-01	10:26a	nt1x1331.6p
NT1X1331 BIN	7,102,184	07-18-01	10:26a	nt1x1331.bin
NT1X1~96 TXT	34,816	07-18-01	10:26a	nt1x1331.elem_aqu.txt
NT1X1~98 TXT	32,663	07-18-01	10:26a	nt1x1331.elem_min.txt
NT1X~100 TXT	32,676	07-18-01	10:26a	nt1x1331.elem_tot.txt
NT1X~102 TXT	76,137	07-18-01	10:26a	nt1x1331.min_info.txt
NT1X1331 TXT	1,703,332	11-14-01	9:46a	ntlx1331.txt
NT1X1432 6I	46,467	07-25-01	7:10p	nt1x1432.6i
NT1X1432 60	3,765,523	07-25-01	7:16p	nt1x1432.60
NT1X1432 6P	42,898	07-25-01	7:16p	nt1x1432.6p
NT1X1432 BIN	7,965,424	07-25-01	7:16p	ntlx1432.bin
NT1X~154 TXT	37,511	07-25-01	7:16p	nt1x1432.elem_aqu.txt
NT1X~156 TXT	35,190	07-25-01	-	ntlx1432.elem_min.txt
NT1X~158 TXT	35,203	07-25-01	7:16p	ntlx1432.elem_tot.txt

Attachment I Page I-6 of I-11

NT1X~160 TXT 88,573 07-25-01 7:16p nt1x1432.min_info.txt NT1X1432 TXT 1,908,654 11-14-01 9:48a nt1x1432.txt 27 file(s) 37,451,596 bytes

Directory of D:\Source Term\two stage

	<dir></dir>	11-14-01	9:48a				
••	<dir></dir>	11-14-01	9:48a				
NC1X1031 6I	44,775	07-18-01	1:18p	nc1x1031.6i			
NC1X1031 60	1,326,343	07-18-01	1:21p	nc1x1031.60			
NC1X1031 6P	41,236	07-18-01		nclx1031.6p			
NC1X1031 BIN	6,003,824	07-25-01	8:21a	nclx1031.bin			
NC1X1~36 TXT	14,026	07-18-01		nc1x1031.elem_aqu.txt			
NC1X1~38 TXT	13,169	07-18-01		nc1x1031.elem_min.txt			
NC1X1~40 TXT	13,182	07-18-01		nc1x1031.elem_tot.txt			
NC1X1~42 TXT	20,145	07-18-01	_	nclx1031.min info.txt			
NC1X1031 TXT	1,043,308	11-14-01	-	nclx1031.txt			
NC2X1402 6I	32,777	07-18-01	1:58p	nc2x1402.6i			
NC2X1402 60	5,117,352	07-18-01	-	nc2x1402.60			
NC2X1402 6P	32,855	07-18-01		nc2x1402.6p			
NC2X1402 BIN	51,507,080	07-25-01		nc2x1402.bin			
NC2X~222 TXT	44,441	07-18-01		nc2x1402.elem_aqu.txt			
NC2X~224 TXT	41,688	07-18-01		nc2x1402.elem_min.txt			
NC2X~226 TXT	41,701	07-18-01		nc2x1402.elem_tot.txt			
NC2X~228 TXT	92,412	07-18-01	2:17p	nc2x1402.min info.txt			
NC2X1402 TXT	10,667,092	11-14-01	9:51a	nc2x1402.txt			
NM1X1031 6I	44,527	07-18-01	8:53a	nm1x1031.6i			
NM1X1031 60	1,726,189	07-18-01	1:24p	nm1x1031.60			
NM1X1031 6P	41,384	07-18-01	1:24p	nm1x1031.6p			
NM1X1031 BIN	7,452,600	07-25-01	8:37a	nm1x1031.bin			
NM1X~300 TXT	18,646	07-18-01	1:24p	nm1x1031.elem_aqu.txt			
NM1X~302 TXT	17,501	07-18-01		nm1x1031.elem_min.txt			
NM1X~304 TXT	17,514	07-18-01	1:24p	nm1x1031.elem_tot.txt			
NM1X~306 TXT	29,947	07-18-01	1:24p	nmlx1031.min_info.txt			
NM1X1031 TXT	1,813,835	11-14-01	9:57a	nmlx1031.txt			
NM2X1402 6I	32,923	07-19-01	9:07a	nm2x1402.6i			
NM2X1402 60	2,886,235	07-19-01	9:17a	nm2x1402.60			
NM2X1402 6P	33,167	07-19-01	9:17a	nm2x1402.6p			
NM2X1402 BIN	15,910,448	07-25-01	8:44a	nm2x1402.bin			
NM2X~378 TXT	27,501	07-19-01	9:17a	nm2x1402.elem_aqu.txt			
NM2X~380 TXT	25,804	07-19-01	9:17a	nm2x1402.elem_min.txt			
NM2X~382 TXT	25,817	07-19-01	9:17a	nm2x1402.elem tot.txt			
NM2X~384 TXT	63,787	07-19-01		nm2x1402.min_info.txt			
NM2X1402 TXT	3,836,115	11-14-01	12:48p	nm2x1402.txt			
36 file(s) 110,101,346 bytes							

Total files listed: 227 file(s) 597,823,948 bytes

Directory of Fermi-IA2

SENSIT~5	<dir></dir>	11-15-01 11:23a Sensitivity
TWO-ST~7	<dir></dir>	11-15-01 12:31p Two-Stage
	0 file(s)	0 bytes

Directory of D:\Sensitivity

Attachment I

•	<dir></dir>	11-15-01	12:31p	•	
••	<dir></dir>	11-15-01	12:31p	••	
GDPO4M~5	<dir></dir>	11-15-01	11:23a	GdPO4	mass
GDPO4R~7	<dir></dir>	11-15-01	11:37a	GdPO4	rate
GLASSR~9	<dir></dir>	11-15-01	12:29p	glass	rate
	0 file(s)	0 by	tes		

Directory of D:\Sensitivity\GdPO4 mass

•	<dir></dir>	11-15-01	12:35p	
••	<dir></dir>	11-15-01	12:35p	
NA1D3333 6I	45,731	08-20-01	1:39p	nAld3333.6i
NA1D3333 60	33,509,003	08-20-01	4:08p	na1d3333.60
NA1D3333 6P	43,226	08-20-01	4:08p	na1d3333.6p
NA1D~110 TXT	255,806	08-20-01	4:08p	nA1d3333.elem_aqu.txt
NA1D~112 TXT	239,877	08-20-01	4:08p	nA1d3333.elem_min.txt
NA1D~114 TXT	239,890	08-20-01	4:08p	nA1d3333.elem_tot.txt
NA1D~118 TXT	530,449	08-20-01	4:08p	nAld3333.min_info.txt
NL1D3333 6I	45,733	08-20-01	1:41p	nL1d3333.6i
NL1D3333 60	32,192,728	08-20-01	5:46p	nl1d3333.60
NL1D3333 6P	43,230	08-20-01	5:46p	nl1d3333.6p
NL1D~222 TXT	240,406	08-20-01	5:45p	nL1d3333.elem_aqu.txt
NL1D~224 TXT	225,437	08-20-01	5:45p	nL1d3333.elem_min.txt
NL1D~226 TXT	225,450	08-20-01	5:45p	nL1d3333.elem_tot.txt
NL1D~230 TXT	495,897	08-20-01	5:45p	nL1d3333.min_info.txt
14 fil	e(s) 68,3	32,863 by	tes	

Directory of D:\Sensitivity\GdPO4 rate

	<dir></dir>	08-20-01	5:45p	
••	<dir></dir>	08-20-01	5:45p	
NA1X3323 6I	45,731	07-16-01	7:10p	nA1x3323.6i
NA1X3323 60	33,581,652			na1x3323.60
NA1X3323 6P	43,226	07-16-01 1	10:41p	na1x3323.6p
NA1X~112 TXT	255,806	07-16-01 1	10:40p	nA1x3323.elem_aqu.txt
NA1X~114 TXT	239,877	07-16-01 1	L0:40p	nA1x3323.elem_min.txt
NA1X~116 TXT	239,890	07-16-01 1	10:40p	nA1x3323.elem_tot.txt
NA1X~120 TXT	550,810	07-16-01 1	10:40p	nA1x3323.min_info.txt
NA1X3333 6I	45,731	07-24-01	9:13a	nA1x3333.6i
NA1X3333 60	33,507,357	07-24-01 1	12:34p	na1x3333.60
NA1X3333 6P	43,226	07-24-01 1	12:34p	na1x3333.6p
NA1X~228 TXT	255,806	07-24-01 1	12:34p	nA1x3333.elem_aqu.txt
NA1X~230 TXT	239,877	07-24-01 1	12:34p	nA1x3333.elem_min.txt
NA1X~232 TXT	239,890	07-24-01 1	12:34p	nA1x3333.elem_tot.txt
NA1X~236 TXT	530,456	07-24-01 1	12:34p	nA1x3333.min_info.txt
NA1Y3323 6I	30,437	07-17-01	6:52a	nAly3323.6i
NA1Y3323 60	29,606,682	07-17-01 1	10:26a	naly3323.60
MA1Y3323 6P	30,437	07-17-01 1	10:26a	naly3323.6p
NA1Y~332 TXT	241,176	07-17-01 1	10:25a	nA1y3323.elem_aqu.txt
NA1Y~334 TXT	226,159	07-17-01 1	10:25a	nA1y3323.elem_min.txt
NA1Y~338 TXT	226,172	07-17-01 1	10:25a	nA1y3323.elem_tot.txt
NA1Y~340 TXT	379,240	07-17-01 1	10:25a	nA1y3323.min_info.txt
NA1Z3323 6I	29,235	07-17-01 1	12:12p	nalz3323.6i
NA1Z3323 60	15,049,863	07-17-01	2:39p	na1z3323.60
NA1Z3323 6P	29,153	07-17-01	2:39p	nalz3323.6p
NA1Z~394 TXT	129,141	07-17-01	2:39p	nAlz3323.elem_aqu.txt

9813 Page I-7 of I-11

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NA1Z~396	ΨVΨ	121,108	07 17 01	2.200	nalazzzz olom min tyt
NA12~398		•			nAlz3323.elem_min.txt nAlz3323.elem_tot.txt
		121,121		-	—
NA1Z~400		184,258	07-17-01	-	nAlz3323.min_info.txt
NL1X3323		45,732	07-17-01		nL1x3323.6i
NL1X3323		32,225,921		-	nl1x3323.60
NL1X3323		43,228		-	nl1x3323.6p
NL1X~504		240,021		-	nL1x3323.elem_aqu.txt
NL1X~506	TXT	225,076	07-17-01	12:09p	nL1x3323.elem_min.txt
NL1X~508	TXT	225,089	07-17-01	12:09p	nL1x3323.elem_tot.txt
NL1X~512	TXT	514,946	07-17-01	12:09p	nL1x3323.min_info.txt
NL1X3333	6I	45,732	07-24-01	9:13a	nL1x3333.6i
NL1X3333	60	32,263,697	07-25-01	9:32p	nl1x3333.60
NL1X3333	6P	43,228	07-25-01	9:32p	nl1x3333.6p
NL1X~616	TXT	241,176	07-25-01	9:31p	nL1x3333.elem aqu.txt
NL1X~618	TXT	226,159	07-25-01	9:31p	nL1x3333.elem_min.txt
NL1X~620	TXT	226,172	07-25-01	9:31p	nL1x3333.elem_tot.txt
NL1X~624	TXT	497,364	07-25-01	9:31p	nL1x3333.min_info.txt
NL1Y3323	6I	30,439	07-17-01	12:14p	nl1y3323.6i
NL1Y3323	60	28,503,399	07-17-01	4:25p	nl1y3323.60
NL1Y3323	6P	30,439	07-17-01	4:25p	nl1y3323.6p
NL1Y~716	TXT	224,621	07-17-01	4:25p	nL1y3323.elem aqu.txt
NL1Y~720	TXT	210,636	07-17-01	4:25p	nL1y3323.elem min.txt
NL1Y~722	TXT	210,649	07-17-01	4:25p	nL1y3323.elem_tot.txt
NL1Y~724	TXT	349,800	07-17-01	4:25p	nL1y3323.min info.txt
NL1Z3323	61	29,236	07-18-01	6:48a	nl1z3323.6i
NL1Z3323	60	19,410,445	07-18-01	8:06a	nl1z3323.60
NL1Z3323	6P	29,153	07-18-01	8:06a	nl1z3323.6p
NL1Z~790	TXT	161,481	07-18-01		nL1z3323.elem aqu.txt
NL1Z~794	TXT	151,432	07-18-01	8:05a	nL1z3323.elem_min.txt
NL1Z~796	TXT	151,445	07-18-01	8:05a	nL1z3323.elem_tot.txt
NL1Z~798	TXT	229,954	07-18-01	8:05a	nL1z3323.min info.txt
	56 file		10,187 by		=
		•	. 1		

Directory of D:\Sensitivity\glass rate

	<dir></dir>	07-18-01	8:05a	•
• •	<dir></dir>	07-18-01	8:05a	
NM1N1331 6I	46,392	08-20-01	1:30p	nm1n1331.6i
NM1N1331 60	3,124,338	08-20-01	5:51p	nm1n1331.60
NM1N1331 6P	43,160	08-20-01	5:51p	nm1n1331.6p
NM1N1~22 TXT	29,811	08-20-01	5:51p	nm1n1331.elem_aqu.txt
NM1N1~24 TXT	27,970	08-20-01	5:51p	nmln1331.elem_min.txt
NM1N1~26 TXT	27,983	08-20-01	5:51p	nm1n1331.elem_tot.txt
NM1N1~28 TXT	58,660	08-20-01	5:51p	nmln1331.min_info.txt
NM2N1402 6I	32,923	08-21-01	3:58p	nm2n1402.6i
NM2N1402 60	2,544,605	08-21-01	4:04p	nm2n1402.60
NM2N1402 6P	33,659	08-21-01	4:04p	nm2n1402.6p
NM2N1~44 TXT	24,036	08-21-01	4:04p	nm2n1402.elem_aqu.txt
NM2N1~46 TXT	22,555	08-21-01	4:04p	nm2n1402.elem_min.txt
NM2N1~48 TXT	22,568	08-21-01	4:04p	nm2n1402.elem_tot.txt
NM2N1~50 TXT	52,712	08-21-01	4:04p	nm2n1402.min_info.txt
NM2N1402 TXT	3,332,738	11-15-01	8:31a	nm2n1402.txt
15 fil	le(s) 9,4	24,110 byt	es	

Directory of D:\Two-Stage

: •

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<DIR> 11-15-01 12:29p .

Attachment I

Page I-9 of I-11

	<dir></dir>	11-15-01 12:29p	
SCENAR~5	<dir></dir>	11-15-01 12:31p Scenario I	
SCENAR~7	<dir></dir>	11-15-01 12:35p Scenario II	Ι
	0 file(s)	0 bytes	

Directory of D:\Two-Stage\Scenario I

•	<dir></dir>	11-15-01	8:31a	
••	<dir></dir>	11-15-01	8:31a	••
NM1X1303 6I	38,545	07-16-01	7:35a	nmlx1303.6i
NM1X1303 60	3,664,654	07-16-01	7:41a	nm1x1303.60
NM1X1303 6P	34,824	07-16-01	7:41a	nm1x1303.6p
NM1X1~24 TXT	43,671	07-16-01	7:41a	nmlx1303.elem_aqu.txt
NM1X1~26 TXT	40,966	07-16-01	7:41a	nm1x1303.elem_min.txt
NM1X1~28 TXT	40,979	07-16-01	7:41a	nm1x1303.elem_tot.txt
NM1X1~30 TXT	67,345	07-16-01	7:41a	nm1x1303.min_info.txt
NM1X1403 6I	38,544	07-16-01	7:30a	nmlx1403.6i
NM1X1403 60	4,224,287	07-16-01	7:48a	nm1x1403.60
NM1X1403 6P	34,988	07-16-01	7:48a	nm1x1403.6p
NM1X1~50 TXT	46,751	07-16-01	7:48a	nmlx1403.elem_aqu.txt
NM1X1~52 TXT	43,854	07-16-01	7:48a	nm1x1403.elem_min.txt
NM1X1~54 TXT	43,867	07-16-01	7:48a	nm1x1403.elem_tot.txt
NM1X1~56 TXT	88,503	07-16-01	7:48a	nm1x1403.min_info.txt
SECOND~5	<dir></dir>	11-15-01	12:33p	second stage
14 fil	.e(s) 8,4	51,778 by	ces	

Directory of D:\Two-Stage\Scenario I\second stage

	<dir></dir>	11-15-01	12:40p	
••	<dir></dir>	11-15-01	12:40p	
NM2X1031 6I	40,418	07-16-01	12:38p	nm2x1031.6i
NM2X1031 60	1,183,740	07-16-01	12:39p	nm2x1031.60
NM2X1031 6P	40,405	07-16-01	12:39p	nm2x1031.6p
NM2X1~14 TXT	12,871	07-16-01	12:39p	nm2x1031.elem aqu.txt
NM2X1~16 TXT	12,086	07-16-01	12:39p	nm2x1031.elem min.txt
NM2X1~18 TXT	12,099	07-16-01	12:39p	nm2x1031.elem_tot.txt
NM2X1~20 TXT	22,629	07-16-01	12:39p	nm2x1031.min_info.txt
NM2X1332 6I	41,457	07-16-01	4:51p	nm2x1332.6i
NM2X1332 60	7,506,988	07-16-01	5:07p	nm2x1332.60
NM2X1332 6P	41,771	07-16-01	5:07p	nm2x1332.6p
NM2X1~52 TXT	75,626	07-16-01	5:07p	nm2x1332.elem_aqu.txt
NM2X1~54 TXT	70,929	07-16-01	5:07p	nm2x1332.elem_min.txt
NM2X1~56 TXT	70,942	07-16-01	5:07p	nm2x1332.elem_tot.txt
NM2X1~58 TXT	144,331	07-16-01	5:07p	nm2x1332.min_info.txt
NM2Y1031 6I	29,531	07-16-01	12:41p	nm2y1031.6i
NM2Y1031 60	357,876	07-16-01	12:41p	nm2y1031.60
NM2Y1031 6P	29,695	07-16-01	12:41p	nm2y1031.6p
NM2Y1~68 TXT	4,401	07 - 16-01	12:41p	nm2y1031.elem_aqu.txt
NM2Y1~70 TXT	4,144:	:07-16-01	12:41p	nm2y1031.elem_min.txt
NM2Y1~72 TXT				nm2y1031.elem_tot.txt
NM2Y1~74 TXT	7,627	07-16-01	12:41p	nm2y1031.min_info.txt
21 file	(s) 9,7	13,723 byt	tes	

Directory of D:\Two-Stage\Scenario II

<dir></dir>	11-15-01	12:33p	-
 <dir></dir>	11-15-01	12:33p	

NM1X1023	6I	44,527	07-12-01	5:32p	nmlx1023.6i
NM1X1023	60	10,068,668	07-12-01	5:55p	nm1x1023.60
NM1X1023	6P	41,220	07-12-01	5:55p	nmlx1023.6p
NM1X1~42	TXT	85,636	07-12-01	5:55p	nm1x1023.elem_aqu.txt
NM1X1~44	TXT	80,315	07-12-01	5:55p	nm1x1023.elem_min.txt
NM1X1~46	TXT	80,328	07-12-01	5:55p	nm1x1023.elem_tot.txt
NM1X1~48	TXT	149,609	07-12-01	5:55p	nmlx1023.min_info.txt
NM1X1032	61	44,527	07-16-01	11:40a	nmlx1032.6i
NM1X1032	60	2,591,200	07-16-01	11:48a	nm1x1032.60
NM1X1032	6P	41,302	07-16-01	11:48a	nm1x1032.6p
NM1X1032	6T	116,736	07-16-01	11:48a	nm1x1032.6t
NM1X1032	6TX	118,331	07-16-01	11:48a	nmlx1032.6tx
NM1X1~68	TXT	25,191	07-16-01	11:48a	nm1x1032.elem_aqu.txt
NM1X1~70	TXT	23,638	07-16-01	11:48a	nm1x1032.elem_min.txt
NM1X1~72	$\mathbf{T}\mathbf{X}\mathbf{T}$	23,651	07-16-01	11:48a	nm1x1032.elem_tot:txt
NM1X1~74	TXT	42,255	07-16-01	11:48a	nmlx1032.min_info.txt
NM1X1033	61	44,527	07-12-01	5:32p	nmlx1033.6i
NM1X1033	60	10,139,044	07-12-01	6:17p	nm1x1033.60
NM1X1033	6P	41,302	07-12-01	6:17p	nm1x1033.6p
NM1X~112	TXT	84,866	07-12-01	6:16p	nm1x1033.elem_aqu.txt
NM1X~114	TXT	79,593	07-12-01	6:16p	nm1x1033.elem_min.txt
NM1X~116	TXT	79,606	07-12-01	6:16p	nm1x1033.elem_tot.txt
NM1X~118	TXT	154,499	07-12-01	6:16p	nm1x1033.min_info.txt
SECOND~5		<dir></dir>	11-15-01	12:40p	second stage
	23 file	(s) 24,20	00,571 by	ces	

Directory of D:\Two-Stage\Scenario II\second stage

•		<dir></dir>	07-16-01	12:41p	
		<dir></dir>	07-16-01		
NM2X1302	61	32,920	07-16-01	2:47p	nm2x1302.6i
NM2X1302	60	8,420,000	07-16-01	-	nm2x1302.60
NM2X1302	6P	33,413	07-16-01	3:05p	nm2x1302.6p
NM2X1~38	TXT	66,386	07-16-01	3:05p	nm2x1302.elem_aqu.txt
NM2X1~40	TXT	62,265	07-16-01		nm2x1302.elem_min.txt
NM2X1~42	TXT	62,278	07-16-01	3:05p	nm2x1302.elem_tot.txt
NM2X1~44	TXT	90,003	07-16-01	3:05p	nm2x1302.min_info.txt
NM2X1303	6I	32,920	07-12-01	6:29p	nm2x1303.6i
NM2X1303	60	27,393,171	07-13-01	2:58a	nm2x1303.60
NM2X1303	6P	33,085	07-13-01	2:58a	nm2x1303.6p
NM2X~132	TXT	194,206	07-13-01	2:58a	nm2x1303.elem_aqu.txt
NM2X~136	TXT	182,117	07-13-01	2:58a	nm2x1303.elem_min.txt
NM2X~138	TXT	182,130	07-13-01	2:58a	nm2x1303.elem_tot.txt
NM2X~140	$\mathbf{T}\mathbf{X}\mathbf{T}$	288,249	07-13-01	2:58a	nm2x1303.min_info.txt
NM2X1323	61	33,817	07-12-01	6:24p	nm2x1323.6i
NM2X1323	60	27,310,618	07-13-01	1:58a	nm2x1323.60
NM2X1323	6P	34,064	07-13-01	1:58a	nm2x1323.6p
NM2X~230	TXT	191,896	07-13-01	1:57a	nm2x1323.elem_aqu.txt
NM2X~232		179,951	07-13-01	1:57a	nm2x1323.elem_min.txt
NM2X~234	TXT	179,964	07-13-01	1:57a	nm2x1323.elem_tot.txt
NM2X~236		267,941	07-13-01	1:57a	nm2x1323.min_info.txt
NM2Y1302		29,228	07-16-01	*	nm2y1302.6i
NM2Y1302		826,333	07-16-01	3:26p	nm2y1302.60
NM2Y1302		29,228	07-16-01	-	nm2y1302.6p
NM2Y~248		7,866	07-16-01		nm2y1302.elem_aqu.txt
NM2Y~250		7,393	07-16-01		nm2y1302.elem_min.txt
NM2Y~252	TXT	7,406	07-16-01	3:26p	nm2y1302.elem_tot.txt

Document Identifier: CAL-EDC-MD-000015 REV 00

NM2Y~254	TXT	14,349	07-16-01	3:26p	nm2y1302.min_info.txt
NM2Y1303	61	30,503	07-13-01	6:55a	nm2y1303.6i
NM2Y1303	60	30,205,779	07-13-01	2:23p	nm2y1303.60
NM2Y1303	6P	30,503	07-13-01	2:23p	nm2y1303.6p
NM2Y~350	TXT	243,871	07-13-01	2:23p	nm2y1303.elem_aqu.txt
NM2Y~354	TXT	228,686	07-13-01	2:23p	nm2y1303.elem_min.txt
NM2Y~356	TXT	228,699	07-13-01	2:23p	nm2y1303.elem_tot.txt
NM2Y~360	TXT	347,794	07-13-01	2:23p	nm2y1303.min_info.txt
NM2Y1323	61	31,482	07-13-01	6:54a	nm2y1323.6i
NM2Y1323	60	30,293,869	07-13-01	1:20p	nm2y1323.60
NM2Y1323	6P	31,482	07-13-01	1:20p	nm2y1323.6p
NM2Y~456	TXT	243,101	07-13-01	1:20p	nm2y1323.elem_aqu.txt
NM2Y~460	TXT	227,964	07-13-01	1:20p	nm2y1323.elem_min.txt
NM2Y~462	TXT	227,977	07-13-01	1:20p	nm2y1323.elem_tot.txt
NM2Y~464	TXT	319,735	07-13-01	1:20p	nm2y1323.min_info.txt
NM2Z1303	6I	30,503	07-16-01	6:47a	nm2z1303.6i
NM2Z1303	60	22,538,351	07-16-01	10:43a	nm2z1303.60
NM2Z1303	6P	30,421	07-16-01	10:43a	nm2z1303.6p
NM2Z~540	TXT	192,666	07-16-01	10:43a	nm2z1303.elem_aqu.txt
NM2Z~542	TXT	180,673	07-16-01	10:43a	nm2z1303.elem_min.txt
NM2Z~546	TXT	180,686	07-16-01	10:43a	nm2z1303.elem_tot.txt
NM2Z~548	TXT	243,295	07-16-01	10:43a	nm2z1303.min_info.txt
NM2Z1323	6I	31,480	07-16-01	12:46p	nm2z1323.6i
NM2Z1323	60	23,506,589	07-16-01	1:57p	nm2z1323.60
NM2Z1323	6P	31,400	07-16-01	1:57p	nm2z1323.6p
NM2Z~626	TXT	194,206	07-16-01	1:57p	nm2z1323.elem_aqu.txt
NM2Z~628	TXT	182,117	07-16-01	1:57p	nm2z1323.elem_min.txt
NM2Z~630	TXT	182,130	07-16-01	1:57p	nm2z1323.elem_tot.txt
NM2Z~634	TXT	245,423	07-16-01	1:57p	nm2z1323.min_info.txt
	56 file	(s) 176,6	54,582 by	ces	

Total files listed:

199 file(s) 529,787,814 bytes