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Supplement to the Disposal Criticality Analysis Methodology

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EXECUTIVE SUMMARY

The *Disposal Criticality Analysis Methodology Topical Report*, YMP/TR-0004Q (DOE 1998b) described a risk-informed methodology for postclosure criticality analyses in the potential repository at Yucca Mountain, Nevada. Various models contained in the methodology were described and a process for validating these models was presented. The topical report also committed to following this process in validating the models used for License Application. The *Supplement to the Disposal Criticality Analysis Methodology* discusses the data and analyses that will be used in model validation and included in validation reports. The validation reports will satisfy the commitments made in the topical report to support License Application and will also support Site Recommendation.

Neutronics

Two types of neutronic models are used for postclosure criticality evaluations – isotopic model and criticality model. The isotopic model discussed in this report is used for predicting actinide and fission product concentrations in commercial spent nuclear fuel (SNF) from either pressurized water reactors (PWRs) or boiling water reactors (BWRs). This includes concentrations resulting from both in-reactor irradiation and post-irradiation isotopic decay. Radiochemical assay data from commercial SNF is used for isotopic model validation. Laboratory critical experiments (LCEs) are used for criticality model validation. Commercial reactor criticality (CRC) data is used in addition to the LCE data in validating the criticality model for commercial reactor SNF. CRC data is also used in validating the isotopic model for commercial SNF and to confirm that the isotopic concentrations used in waste package design are conservative.

This report describes at a summary level the data and analyses to be used for validating the isotopic and criticality models. Radiochemical assay data and analyses are summarized for both BWR and PWR commercial reactor SNF. Half-life and branching fraction data and analyses are described for propagating the uncertainty associated with post-irradiation isotopic decay to an uncertainty in predicting k_{eff}. The process also checks for systematic errors introduced by the method. If systematic errors are found, these are added to the uncertainty as a method bias. The data and analyses of 504 LCEs are discussed at a summary level. The discussion includes potential characterizations of these experiments for repository applications. CRC data and analyses for 45 PWR statepoints (measured critical conditions) and 28 BWR statepoints are summarized. Finally, the validation process to be followed in the validation reports is discussed. The process includes quantifying the effects of approximations made in the neutronic models and establishing the applicability of the experimental data to repository conditions.

Probability

As explained in DOE 1998b, the probability of criticality is calculated by the mathematical process of taking the product of probabilities of individual events and processes that can lead to criticality and then summing (or averaging) over all possible values of the parameters characterizing these events and processes. Appendix C of that document illustrated the simulation of the mathematical process by the Monte Carlo technique using random sampling

from the distributions of the relevant parameters. This supplementary methodology discussion provides a list of the event and process parameters (more comprehensive than that given in DOE 1998b) and indicates how their individual probabilities (conditional and unconditional) are used as factors in the probability calculation. The extension of the probability calculation format to cover the calculation of risk is also given. The principal consequence measures used in the calculation of risk are identified for steady-state criticality as dose at the accessible environment and increase in radionuclide inventory, and for transient criticality as peak overpressure.

An example application of the methodology to the evaluation of old and new waste package designs is also illustrated. This preliminary analysis indicates that the new design results in a two order of magnitude lower probability of criticality for post emplacement times up to 100,000 years.

Consequences

The transient criticality consequence analysis reported in DOE (1998b) has been extended to consider the effect of reactivity insertion rate and the exit area on the primary impact measure, peak overpressure. Insertion rate is primarily determined by sudden events, seismic shaking is a likely example, but volcanism must also be considered. The exit area is the total area of the penetrations of the waste package barriers. It is found that peak overpressure will increase with decreasing exit area. Future calculations are expected to show that the probability of criticality will decrease with decreasing exit area, at a rate that is faster than the increase in peak overpressure, so that the overpressure risk (which is the product of probability and magnitude of peak overpressure) will show a net decrease with decreasing exit area.

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1. INTRODUCTION

The *Disposal Criticality Analysis Methodology Topical Report*, YMP/TR-0004Q (DOE 1998b) was provided to the United States Nuclear Regulatory Commission (NRC) on January 7, 1999. The topical report provides the methodology for evaluating criticality potential of high-level radioactive waste and spent nuclear fuel. Various models are applied in implementing the methodology. Additional analyses are required to support the model validation process described in the topical report. Model validation is required to support the use of this methodology in the Site Recommendation and License Application.

The *Technical Document Preparation Plan* (CRWMS M&O 1999a) for this report listed the title as *Supplement to the Disposal Criticality Analysis Methodology Topical Report*. This report is neither a revision nor an addendum to the topical report, therefore *Topical Report* has been removed from the title.

1.1 PURPOSE

The purpose of this report is to discuss data and analyses to be included in the validation reports that are required to support the use of the disposal criticality analysis methodology in the Site Recommendation and License Application. This includes describing at a summary level additional analyses performed since the topical report was issued and discussing other data and analyses that will be required to complete the validation reports.

1.2 OBJECTIVE

The objective of the *Supplement to the Disposal Criticality Analysis Methodology*, is to present additional information along with references that support the methodology presented in the *Disposal Criticality Analysis Methodology Topical Report*, YMP/TR-0004Q (DOE 1998b). This information will be used in validation reports and will also be used to assist in formulating responses to requests for additional information received from the United States Nuclear Regulatory Commission concerning the *Topical Report*.

1.3 SCOPE

This report summarizes and references additional neutronic, probability, and consequence information that will support the application of the disposal criticality analysis methodology. The application of the model validation process through validation reports is also described. These validation reports will support the use of the methodology in the License Application and will satisfy commitments made in the topical report.

1.4 QUALITY ASSURANCE

This report was prepared in accordance with the Civilian Radioactive Waste Management System (CRWMS) Management and Operating Contractor (M&O) Quality Administrative Procedures (QAPs). The information provided in the report is to be indirectly used in the evaluation of the Monitored Geologic Repository waste package and engineered barrier segment.

The waste package and engineered barrier segment have been identified as items important to radiological safety and waste isolation in the QAP-2-3 evaluation entitled *Classification of the Preliminary MGDS Repository Design* (CRWMS M&O 1999b, p. IV-11). The Waste Package Operations responsible manager has evaluated the report development activity in accordance with QAP-2-0 Conduct of Activities. The Activity Evaluation *Neutronics Methodology - SR* (CRWMS M&O 1999c) evaluation has determined the preparation and review of the document is subject to *Quality Assurance Requirements and Description* (QARD) (DOE 1998a) controls. There is no determination of importance evaluation developed in accordance with Nevada Line Procedure, NLP-2-0, since the report does not involve any field activity.

The results provided in this report are taken from various analyses, calculations, and evaluations developed in accordance with the CRWMS M&O QAPs. The information presented in this report is not design information that can be used in procurement, fabrication, or construction. Data from several references for this report should be considered to be verified (TBV) in that they are not considered accepted data sources per the retroactive procedural requirement of AP-SIII.2Q initiated by the July 27, 1999 issuance of the DOE Letter, "Accepted Data Call", from R. E. Spence to J. L. Yonker (DOE 1999). References to be considered TBV are as follows: CRWMS M&O 1998b, CRWMS M&O 1998c, CRWMS M&O 1998d, CRWMS M&O 1998e, CRWMS M&O 1998f, CRWMS M&O 1999f, CRWMS M&O 1999g, CRWMS M&O 1999j, and DOE 1998b. The "accepted data" classification of this data is pending receipt of a DOE rationale concurrence letter approving the classification (TBV-1349). Subsequent to the initiation of TBV-1349, DOE issued a concurrence letter (Mellington 1999) approving the request to identify information taken from the references specified above as "accepted data".

1.5 USE OF COMPUTER SOFTWARE

No computer software subject to the QARD was used in the development of this report. The results reported in this document were drawn from various documents, which did use software subject to the requirements of the QARD. The details of the computer software approved for quality affecting work used to generate the results, and the software controls used, are provided in the various individual documents referenced by this report.

2. NEUTRONICS

This section discusses the data and analyses that will be included in the validation reports for the neutronic models. These validation reports will satisfy commitments made in the topical report, and thus support the use of the methodology for the License Application.

2.1 ISOTOPIC MODEL

The commercial reactor spent nuclear fuel (SNF) isotopic model discussed in this report is applicable to two waste forms – pressurized water reactor (PWR) SNF and boiling water reactor (BWR) SNF. This model is used to calculate the change in isotopic inventory that results when the fuel is irradiated in a reactor. The change in isotopic inventory with irradiation (burnup) results in a change in the reactivity of the fuel. The fissile isotope content of the fuel changes with burnup. The ^{235}U concentration decreases, while ^{239}Pu and other fissile actinides are produced. Additionally, actinide neutron absorbers and fission-product neutron absorbers are produced. The isotopic concentration of burnable absorbers present in the fuel assembly will decrease with irradiation. The usual net result of burnup for PWR or BWR SNF contained inside a waste package is a reduction in the reactivity of the fuel. Taking credit for this reduction in reactivity is referred to as burnup credit. The amount of burnup credit taken is dependent upon two neutronic models. First, the isotopic model must be capable of predicting the isotopic inventory of the SNF. Second, the criticality model (discussed in Section 2.2) must be capable of predicting the reactivity of the SNF for a range of potential configurations inside the waste package.

The isotopic model is also used to predict the change in isotopic inventory that results from isotopic decay during the time period (cooling-time) since the fuel was last irradiated in the reactor. Potential biases in k_{eff} resulting from limitations in the ability of the model to accurately predict changes in isotopic concentrations resulting from fuel irradiation or post-irradiation isotopic decay are established during model validation.

Two types of isotopic data are used for the isotopic model validation. First, radiochemical assay data are used to establish the uncertainty in the calculated isotopic concentrations resulting from fuel irradiation in the reactor. Second, half-life and branching fraction uncertainty data from Appendix A of Hermann, Daniel, and Ryman (1998) and Brookhaven National Laboratory (BNL 1991) are used for post-irradiation isotopic decay. Commercial reactor criticality (CRC) data are also used in validating the isotopic model. The CRC data are used to confirm that the uncertainties established for the radiochemical assay data are contained in the critical limit values established during the criticality model validation. This confirmation is accomplished by accounting for compensating effects (with respect to k_{eff}) in individual isotopic concentration values used in establishing the critical limit values. In addition, the CRC data is used to confirm that the isotopic concentrations used for waste package design are conservative.

2.1.1 Radiochemical Assays

Analyses of radiochemical assay data from seven PWRs and three BWRs were referenced in the topical report. The predicted values for the isotopic concentrations for these analyses were

obtained with the SAS2H sequence of the SCALE-4.3 computer code system using the 44-energy group cross-section library (CSCI: 30011 V4.3, CRWMS M&O 1997a; ORNL 1995). The analyses included 54 PWR samples and 30 BWR samples.

2.1.1.1 BWR Fuel

Radiochemical assay data from 3 BWRs have been analyzed with SAS2H and the results are reported on pages 25, 29, 33, and 34 of Hermann and DeHart (1998). Six samples were analyzed from two fuel assemblies from the Cooper Nuclear Power Plant, operated by the Nebraska Public Power District. The samples were taken from General Electric fuel assemblies with a 7 x 7 pin lattice. Eight samples from two fuel assemblies with a 6 x 6 pin lattice from the Gundremmingen Nuclear Power Plant, operated by Kenkraftwerk RWE-Bayernwerk GmbH (KRB) were analyzed. Sixteen samples were analyzed from three fuel assemblies with a 6 x 6 pin lattice from the Japan Power Demonstration Reactor (JPDR), located at Tokai-mura, Ibaraki-ken. A summary of spent fuel characteristics for the fuel samples is presented in Table 2-1. The information in this table is from Tables 1, 16, 19, 21, and 22 of Hermann and DeHart (1998).

Table 2-1. Summary of BWR Spent Fuel Characteristics

No.	Unit Name	Test Assembly (Pin No.)	Initial Enrichment (wt% ^{235}U)	Axial Height[a] (cm)	Burnup (GWd/mtU)	Cooling Time (days)	Moderator Density[b] (g/cm^3)
1	Cooper	CZ346(B3)	2.939	351.7	18.96	1954	0.3446
2		CZ346(B3)		186.9	33.07	1954	0.4705
3		CZ346(B3)		131.0	33.94	1954	0.5736
4		CZ346(C3)		350.1	17.84	1929	0.3452
5		CZ346(C3)		290.7	29.23	1929	0.3723
6		CZ346(C3)		114.7	31.04	1929	0.6124
7	Gundremmingen	B23(A1)	2.530	44.0	25.73	1047	0.7378
8		B23(A1)		268.0	27.40	1053	0.3145
9		B23(B3)		268.0	21.24	1010	0.3145
10		B23(E3)		268.0	23.51	1244	0.3145
11		C16(A1)		44.0	20.30	1242	0.7460
12		C16(A1)		268.0	19.85	1244	0.3849
13		C16(B3)		268.0	14.39	1060.5	0.3849
14		C16(E5)		268.0	17.49	1004	0.3849
15	JPDR	A-14[c]	2.596	129.6	3.30	1092	0.6075
16		A-14		44.0	4.04	1039	0.7541
17		A-18[c]		129.6	2.71	1089	0.5629
18		A-18		80.7	4.25	1038	0.6708
19		A-20(A1)		117.4	7.01	1296	0.6719
20		A-20(A3)		31.8	6.15	1387	0.7642
21		A-20(A6)		117.4	6.95	1296	0.6719
22		A-20(A6)		44.0	6.51	1380	0.7600
23		A-20(C3)		141.8	2.65	1215	0.5232
24		A-20(C3)		117.4	5.09	1219	0.5688
25		A-20(C3)		92.9	6.08	1221	0.6276
26		A-20(C3)		56.2	6.04	1235	0.7305
27		A-20(C3)		31.8	5.06	1226	0.7534
28		A-20(C3)		7.3	2.16	1216	0.7701
29		A-20(E2)		117.4	5.60	1320	0.5688
30		A-20(E2)		31.8	5.38	1331	0.7534

[a] Height of sample above bottom of fuel.
[b] Estimated from a correlation between power and moderator density as a function of axial height.
[c] Pin identified only as in the center part of assembly.

Radiochemical isotopic analyses of the Cooper spent nuclear fuel were conducted by the Material Characteristics Center at Pacific Northwest National Laboratory. For the Gundremmingen spent nuclear fuel, radiochemical isotopic analyses were conducted at the Ispra (Italy) and Karlsruhe (German) facilities by the European Joint Research Center. Spent fuel samples from B23(A1) and C16(A1) were analyzed at Ispra only; all other sample analyses were performed at both facilities. For samples with two measurements, the average of the two was reported. The Japanese Atomic Energy Research Institute performed radiochemical analyses of the JPDR spent nuclear fuel. The percentage differences between measured and calculated isotopic composition for the spent fuel samples from the three BWR plants are summarized in Table 2-2. The information in this table is from Table 24 of Hermann and DeHart (1998) and shows only those isotopes from the Principal Isotope list (DOE 1998b, Table 3-1). The principal isotopes are 14 actinides and 15 fission products that were selected as part of the disposal criticality analysis methodology for commercial SNF burnup credit.

Table 2-2. Summary of Percentage Differences[a] between Measured and Calculated Isotopic Composition

Nuclide	No. of Cases	Percentage Difference			Standard Deviation
		Average	Maximum	Minimum	
^{99}Tc	6	12.1	14.6	7.0	3.1
^{143}Nd	16	0.4	1.8	-0.6	0.6
^{145}Nd	16	0.4	1.6	-0.4	0.5
^{234}U	22	-0.2	4.4	-6.1	2.6
^{235}U	30	-2.0	4.0	-11.7	3.3
^{236}U	30	-1.2	4.5	-7.8	2.7
^{238}U	30	-0.1	0.2	-1.5	0.4
^{237}Np	18	-1.1	17.3	-11.2	8.7
^{238}Pu	30	-7.0	45.3	-27.3	16.3
^{239}Pu	30	-2.1	8.8	-17.3	6.0
^{240}Pu	30	-0.9	6.9	-11.1	4.8
^{241}Pu	30	-4.5	17.1	-20.1	9.3
^{242}Pu	30	0.5	42.9	-17.5	12.6
^{241}Am	22	4.1	28.4	-11.1	11.5
^{242m}Am	12	2.3	88.1	-37.5	34.3

[a] (Calculated/Measured – 1) x 100%.

The radiochemical assay samples were each taken from single fuel pellets. The SAS2H model is for a fuel assembly of like pellets. This approximation made in the SAS2H model will introduce additional uncertainty into the analysis of the radiochemical assay data. The adequacy of the approximation will be established by examining the calculated neutron spectrum in the fuel pellet from which the assay sample is taken and the calculated average neutron spectrum in a fuel assembly of like pellets. The greater the difference between the two spectra, the larger the error introduced. The adequacy of this SAS2H approximation will be established using a two-dimensional lattice code.

2.1.1.2 PWR Fuel

Radiochemical assay data from 7 PWRs have been analyzed with SAS2H and the results are reported in CRWMS M&O (1997b). Nine samples from 3 fuel assemblies of Calvert Cliffs Unit 1 were analyzed. This plant is an 825 MWe Combustion Engineering (CE) PWR operated by

Baltimore Gas and Electric Company. The samples were taken from CE fuel assemblies with a 14 x 14 pin lattice. Six samples from the Obrigheim reactor in Germany were analyzed. The samples were taken from five assemblies (Siemens' 14 x 14 pin lattice) that were each split into halves and each half was dissolved separately. Four samples were analyzed from H.B. Robinson Unit 2. Carolina Power & Light Company operates this 683 MWe unit. The samples were taken from a Westinghouse 15 x 15 fuel assembly. Five samples were analyzed from Turkey Point Unit 3. This unit is operated by Florida Power & Light Company. The samples were taken from two Westinghouse 15 x 15 fuel assemblies. Fourteen samples from three fuel assemblies of the Trino Vercelles reactor in Italy were analyzed. This core has an unusual loading for a PWR. The fuel assemblies are a modified 15 x 15 pin lattice design with the reactor core also containing both cruciform control rod assemblies and cruciform fuel assemblies. Eight samples were analyzed from one fuel assembly of the Yankee Rowe reactor. Yankee Nuclear Corporation operated this reactor. Finally, nine samples were analyzed from 3 fuel assemblies (Westinghouse 15 x 15) of the Mihama-3 reactor in Japan. It was suggested in CRWMS M&O (1997b, p. 44) and justification was provided in DOE (1997, p. 2-19) that one of the samples (86g07) not be used for model validation.

A summary of the PWR spent fuel characteristics for the fuel samples is presented in Table 2-3. The information in this table is from Tables 3-1 through 3-7 of CRWMS M&O (1997b), with the exception that the cooling time for Trino Vercelles was taken from Table 2.1-13 of DOE (1997). Results from the analysis of these samples with the SAS2H sequence of SCALE-4.3 using the 44-energy group cross-section library are reported in Tables 4-1, 4-2, 4-5, and 4-8 through 4-11 of CRWMS M&O (1997b). A summary of percent differences between calculated and measured values is presented in Table 4-17 of CRWMS M&O (1997b). This summary also includes data from one BWR plant. Similar analyses of these PWR samples were performed with the SAS2H sequence of SCALE-4.2 using the 27BURNUPLIB cross-section library. Results from the SCALE-4.2 analyses of these samples are presented in Tables 2.1-5, 2.1-10, 2.1-16, 2.1-21, 2.1-27, 2.1-33, and 2.1-38 of DOE (1997). The analyses in DOE (1997) evaluated nine actinide isotopes, whereas the analyses in CRWMS M&O (1997b) evaluated the same nine actinide isotopes plus additional actinide and fission product isotopes. Trends in some, but not all, of the comparisons of calculated and measured data are similar for the two sets of analyses. Additional investigations are necessary to explain any differences in the observed trends between the two sets of evaluations. The adequacy of the SAS2H approximations for these evaluations will be tested using a two-dimensional lattice code.

Table 2-3. Summary of PWR Spent Fuel Characteristics

No.	Unit Name	Assembly (Pin No.)	Initial Enrichment (wt% ^{235}U)	Axial Height[a] (cm)	Burnup (GWd/mtU)	Cooling Time (days)
1	Calvert Cliffs	D047(MKP109)	3.038	13.20	27.35	1870
2				27.70	37.12	1870
3				165.22	44.34	1870
4		D101(MLA098)	2.720	8.90	18.68	2374
5				24.30	26.62	2374
6				161.70	33.17	2374
7		BT03(NBD107)	2.453	11.28	31.40	2447
8				19.92	37.27	2447
9				161.21	46.46	2447
10	Obrigheim	168	3.130	NA	28.40	10
11		170			25.93	10
12		171			29.04	10
13		172			26.54	10
14		176, batch 90			29.52	10
15		176, batch 91			27.99	10
16	H. B. Robinson	B05(N-9)	2.561	11.0	16.02	3936
17				26.0	23.81	3936
18				199.0	28.47	3631
19				226.0	31.66	3631
20	Turkey Point	D01(G09)	2.556	167.6	30.72	927
21		D01(G10)		167.0	30.51	927
22		D01(H09)		167.0	31.56	927
23		D04(G09)		167.6	31.26	927
24		D04(G10)		167.0	31.31	927
25	Trino Vercelles	509-104(M11)	3.870	79.2	12.042	10
26		509-032(E11)	3.130	158.5	15.377	10
27				79.2	15.898	10
28				26.4	11.529	10
29		509-069(E11)	3.130	237.7	12.859	10
30				211.3	20.602	10
31				158.5	23.718	10
32				79.2	24.304	10
33		509-069(E05)		158.5	23.867	10
34				79.2	24.548	10
35		509-069(L11)		158.5	23.928	10
36				79.2	24.362	10
37		509-069(L5)		158.5	24.330	10
38				79.2	24.313	10
39	Yankee Rowe	E6(C-f6)	3.400	220.22	15.95	281.5
40				138.94	30.39	717.0
41				57.66	31.33	281.5
42				17.02	20.19	281.5
43		E6(SE-c2)		138.94	32.03	281.5
44				57.66	31.41	281.5
45		E6(SE-e4)		138.94	35.97	281.5
46				57.66	35.26	281.5
47	Mihama-3	(sample 86b02)	3.208	-	8.30	1825
48		(sample 86b03)		-	6.92	1825
49		(sample 86g03)	3.203	-	21.29	1825
50		(sample 86g05)		-	15.36	1825
51		(sample 86c03)		-	29.50	1825
52		(sample 86c04)	3.210	-	32.20	1825
53		(sample 86c07)		-	33.71	1825
54		(sample 86c08)		-	34.32	1825

[a] Axial height from the bottom of the fuel rod.

2.1.2 Half-life and Branching Fractions

Radiochemical assay data will be used to establish the uncertainty in the calculated spent nuclear fuel isotopic concentrations resulting from fuel irradiation in a reactor. Additional data addressing the uncertainties in the half-life and branching fractions for post irradiation isotopic decay are discussed in this section. Both types of data will be used for isotopic model validation and for assuring that burnup credit is appropriately applied for the postclosure time period of the repository.

The ORIGEN-S code from SCALE-4.3 will be used to calculate post irradiation isotopic decay. The half-life and branching fraction data in the decay library have associated uncertainties. Half-life and branch fraction uncertainty data from Appendix A of Hermann, Daniel, and Ryman (1998) and BNL (1991) will be used along with ORIGEN-S and the CSAS1X module in SCALE-4.3 to establish the uncertainty in k_{eff} associated with post irradiation isotopic decay calculations. The method initially uses isotopic concentrations from the reactor irradiation evaluations and data from the decay library to perform isotopic decay calculations with ORIGEN-S for various post irradiation time intervals. The time intervals selected vary from the time immediately following reactor irradiation to several hundred thousand years. Base reactivity calculations are then performed using the CSAS1X module in SCALE-4.3 and the isotopic concentrations from ORIGEN-S established at the end of each time interval. The effects of uncertainties in the half-life and branching fractions on the isotopic concentrations for post irradiation time intervals are then evaluated by a statistical method (using Monte Carlo). This method is based on performing many ORIGEN-S calculations while allowing the half-life and branching fractions for each isotope to vary randomly over their uncertainty ranges. The isotopic concentrations from each set of ORIGEN-S calculations are used in reactivity evaluations with CSAS1X. Uncertainties in the k_{eff} resulting from uncertainties in the half-life and branching fractions are established for a range of enrichments, burnups, and decay times. The process also checks for systematic errors introduced by the method. If systematic errors are found, these are added to the uncertainty as a method bias.

Evaluations will be performed for both PWR and BWR waste forms and a bounding Δk_{eff} margin established for post irradiation decay uncertainty. These evaluations will be documented in the validation reports for PWR and BWR waste packages. An example evaluation has been performed using calculated irradiation data (SNF isotopic concentrations) from a fuel assembly present in the commercial reactor criticality evaluations (discussed in Section 2.2.2). This fuel assembly had an initial ^{235}U enrichment of 3.84 wt% and an assembly average burnup of 49.22 GWd/mtU. The results of this evaluation are listed in CRWMS M&O (1999d, Attachment II) and are summarized in Table 2-4.

Table 2-4. Example Reactivity Bias and Uncertainty Versus Post Irradiation Decay Time

Post Irradiation Decay Time (yr)	Reactivity Bias and Uncertainty[a]
100	0.00015
500	0.00015
1,000	0.00015
5,000	0.00019
10,000	0.00025
15,000	0.00030
20,000	0.00033
25,000	0.00036
30,000	0.00039
40,000	0.00045
50,000	0.00050
100,000	0.00060
200,000	0.00065

[a] Confidence limit of 95 percent with 99.5 percent of the population of the data set covered.

2.1.3 Validation

The isotopic model validation will be addressed in two validation reports. The first validation report will be completed and submitted to DOE by September 2000. This report will document the validation of the neutronic models for internal configurations of SNF in PWR waste packages. The second report will provide similar documentation for internal configurations of SNF in BWR waste packages. The isotopic model validation will address both the in-reactor irradiation component and the post irradiation decay component of the isotopic model that are used in taking burnup credit for internal configurations of SNF in waste packages.

Validation of the in-reactor irradiation component of the isotopic model will be based, in part, on the radiochemical assay data discussed in Section 2.1.1 and Requirement B (DOE 1998b, p. 4-9) of the topical report. For the analyses of SNF assay samples, burnup history parameters such as power densities, moderator temperatures and densities, fuel temperatures, and soluble boron concentrations (for PWRs) affect the neutron spectrum that the fuel sample experiences. This in turn will affect the isotopic concentrations of the fuel sample. Thus, fuel samples with insufficient burnup history information should not be used.

Radiochemical assay samples are generally taken from a single fuel pellet in a burned fuel assembly. This fuel pellet may not be representative of the many fuel pellets contained in the fuel assembly. Thus, models such as the SAS2H model may contain large errors because of the limited capability to represent individual fuel pellets and the neutron spectrum associated with fuel pellet samples. This limitation and the limitation resulting from the potential sparsity of the design and burnup history information are addressed in Requirement B of the topical report. This requirement states that "... bounding reactor parameters will be used to predict isotopic concentrations that, when compared to best-estimate isotopic predictions of the measured radiochemical assay data or the measured radiochemical data itself, must produce values for k_{eff} that are conservative." This requirement is very stringent since it requires the selection of bounding burnup history parameters to overcome potentially large errors resulting from the sparseness of design and burnup history information, as well as data from fuel samples that are not representative of the fuel assembly from which they were taken.

[Note: Requirement B should be rewritten to read "Bounding reactor parameters will be used to predict isotopic concentrations that, when used in criticality evaluations must produce values for k_{eff} that are conservative when compared to similar criticality evaluations using either measured radiochemical assay data or best-estimate isotopic concentrations."]

Burnup history for fuel samples is limited to the information that is available. Best-estimate assembly operating history data will be used with accompanying documentation of the assumptions made in the process. The accuracy of this data will vary for the different fuel samples analyzed. However, sensitivity analyses may be performed to illustrate variations in the calculated isotopic concentrations resulting from variations in selected operating history parameters (CRWMS M&O 1997b; Hermann and DeHart 1998). Information from sensitivity analyses can then be used to ensure that operating history parameters are chosen for waste package design that will produce conservative values for k_{eff}, thus satisfying Requirement B for isotopic model validation in the topical report.

Limitations in the capability of the SAS2H model to appropriately represent the fuel samples in the radiochemical assays will be addressed through the use of a more detailed isotopic model. A two-dimensional lattice code (e.g., CASMO – Edenius and Forssen 1989) will provide a more accurate representation of the fuel sample. (CASMO models all of the relevant actinide isotopes contained in the Principal Isotope list and most of the fission products.) Although SAS2H may be limited in some of its modeling capabilities, these can be overcome through the use of a lattice code to quantify these limitations and developing means to overcome them. SAS2H has other features that are desirable for the repository evaluations. It carries a complete set of isotopes during its depletion/decay analyses. Existing lattice codes don't, which limits these codes for postclosure analyses. Thus, the lattice code provides an interim step in the model validation.

The radiochemical assays will be analyzed with a two-dimensional lattice code to establish the uncertainty in the calculated isotopic concentrations. A code-to-code validation between the two-dimensional lattice code and the SAS2H code system will then be performed on a fuel assembly basis, which is the way SAS2H is being used for burnup credit. This establishes the uncertainty in isotopic concentrations calculated with SAS2H on a fuel assembly basis relative to the two-dimensional lattice code. The uncertainties established for the lattice code relative to measured assay data and the uncertainties established for SAS2H relative to the lattice code are combined to provide the uncertainties in isotopic concentrations calculated with SAS2H. The best-estimate isotopic concentrations used to satisfy Requirement B in the topical report will then be based on the code-to-code validation with allowances made for the established uncertainties. This code-to-code validation will not exceed the range of parameters (e.g., assembly type, ^{235}U initial enrichment, and burnup) covered by the radiochemical assay database.

2.2 CRITICALITY MODEL

The criticality model is used for evaluating configurations of fissionable material in the potential repository. A configuration is defined by a set of parameters that characterize the amount and physical arrangement of materials that affect criticality (e.g., fissionable, neutron absorbing, moderating, and reflecting materials). A set of similar configurations whose composition and

geometry are defined by specific parameters that distinguish them from other configurations is referred to as a configuration class. Identification of a potentially critical configuration starts with degradation scenarios from the Master Scenario List presented in Section 3.1 of DOE (1998b). Degradation analyses are performed to define parameter ranges and values for configurations in each configuration class. Parametric criticality evaluations are performed for configurations in each class using the criticality model as illustrated in Figure 2-1. (Figure 2-1 is a suggested revision of Figure 3-3 in the topical report [DOE 1998b]).

A critical limit (CL) is placed on the calculated value of k_{eff} for the configurations analyzed. The CL is the value of k_{eff} at which a configuration is considered potentially critical as characterized by statistical tolerance limits. The CL accounts for the criticality analysis method bias and uncertainty. The method bias and uncertainty are obtained from analyzing experimental systems with a range of neutronic parameters that are representative of those used in the parametric criticality evaluations. As illustrated in Figure 2-1, the range of neutronic parameters covered by the experimental data in estimating the method bias and uncertainty define the range of applicability of the CL. If the range of neutronic parameters for the parametric criticality evaluations is beyond the range of applicability of the experimental data, either additional experiments must be evaluated or a k_{eff} penalty must be applied to the CL. The procedure for extending the range of applicability and applying a k_{eff} penalty will be described in each of the validation reports. This procedure will require examining the bias and potentially compensating biases that may occur with individual changes in materials, geometry, or neutron spectrum. Alternative calculational methods will also be used as an independent check of the bias in the extended range. The process of satisfying the range of applicability criterion also identifies the applicable CL criterion for the configuration class.

Values of k_{eff} from the parametric criticality evaluations are compared with the CL criterion. This comparison separates configuration classes based on their potential for criticality. For configurations where the peak k_{eff} may exceed the CL criterion over some portion of the parameter range of a configuration class, multivariate regressions for k_{eff} are developed as a function of parameters that significantly affect criticality. Since a finite number of parametric criticality evaluations are performed in establishing the potential for the peak k_{eff} to exceed the CL criterion, an additional margin (Δk_m) is subtracted from the CL prior to developing the multivariate regressions (i.e., a screening criterion, CL-Δk_m, is used). A margin value of 0.05 is proposed to assure that a peak k_{eff} value larger than the CL will not be missed. The adequacy of this margin value will be established and documented in the validation reports.

Parameters that may significantly affect k_{eff} include the amounts of fissionable material, absorber material, moderator and reflector material, and degradation products. The multivariate regressions are developed from criticality calculations for representative configurations and values of these parameters. The standard error of regression is established during the development of the regression and added to the predicted k_{eff} values for comparison with the CL criterion. The range of parameters and parameter values covered by the regression is checked against the range of applicability criterion and a conservative margin applied if the trended CL data must be extrapolated. Configuration classes satisfying the CL criterion are acceptable for disposal. For those configurations exceeding the CL criterion, potential design options are

identified for reducing k_{eff} and an estimate of the likelihood (probability) of configurations showing potential for criticality is made.

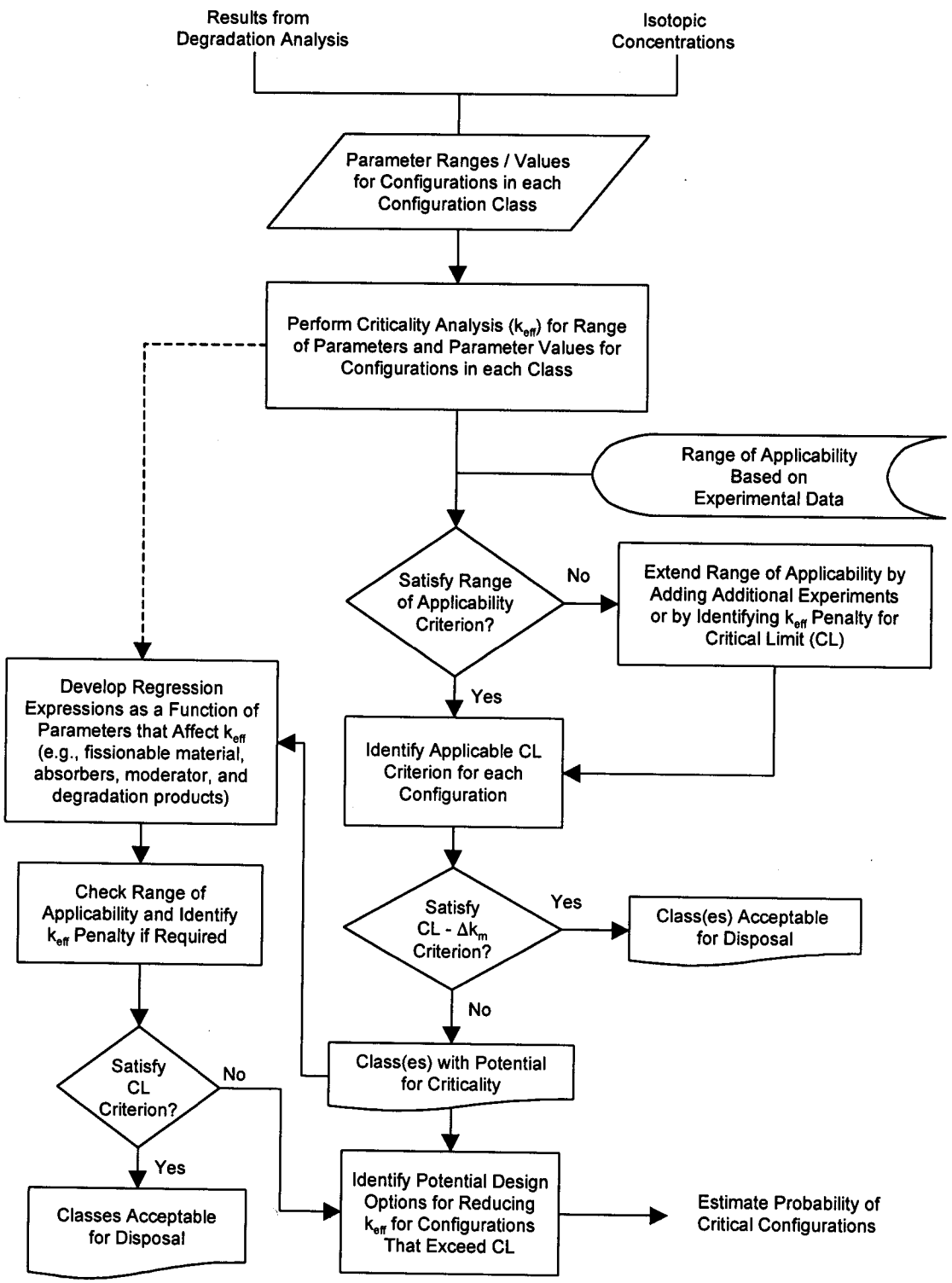

Figure 2-1. Criticality Analysis Methodology

Critical limit values are established as part of model validation and will be documented in validation reports. Two types of experimental data will be used for criticality model validation. Laboratory critical experiments (LCEs) will be used in model validation for all waste forms, but not for all principal isotopes. Commercial reactor criticals (CRCs) will be used along with LCEs in model validation for waste packages containing SNF from BWRs and PWRs. The LCEs and CRCs analyzed to date are summarized in Sections 2.2.1 and 2.2.2. The neutronic model validation process is discussed in Section 2.2.3.

2.2.1 Laboratory Critical Experiments

Laboratory critical experiments will be used to benchmark the criticality model for a range of fissionable materials, enrichments of fissile isotopes, moderator and reflector materials, and absorber materials. These include bare and reflected experiments, as well as experiments with homogeneous and heterogeneous geometry. The applicability of these experiments to repository configurations will be demonstrated in the validation reports.

A total of 504 LCEs were analyzed during the past year using MCNP (CSCI: 30033 V4B2LV, CRWMS M&O 1998a; Briesmeister 1997). These analyses are summarized in CRWMS M&O (1999e). The LCE experiments are divided into two major categories: homogeneous/array systems (331 experiments) and lattice systems (173 experiments). The LCE database contains 10 of the 14-actinide isotopes from the Principal Isotope list. The remaining actinides and the 15-fission product isotopes are contained in the CRCs.

The LCE experiments are further characterized according to the range of fissile isotope enrichment (weight-percent of fissile isotope) and the range of the calculated value for average energy of neutrons causing fission (AENCF). These LCE characterizations are summarized in Table 2-5. The characterization of these experiments in Table 2-5 is an example of potential characterizations that will be examined in developing the validation reports. This example characterization does not imply that AENCF will be used as a trending parameter. The characterizations presented in Table 2-5 for the homogeneous/array systems category are from Table 2.1-1 of CRWMS M&O (1999e), and the characterizations for the lattice systems category are from Table 2.2-1 of the same reference. The number of experiments for each type of system is shown in parentheses in Table 2-5.

LCE data will be included in establishing critical limit values for configurations of fissionable material both inside and outside of waste packages. The applicability of these experiments to repository conditions will be established during model validation.

Table 2-5. Summary of LCE Characterizations

Type of System	Parameter	Minimum	Maximum
Homogeneous/Array Systems (331)			
Mixed plutonium and natural uranium (34)	^{235}U Enrichment (wt%)[a]	0.44	2.29
	^{239}Pu Enrichment (wt%)	91.10	93.95
	AENCF (MeV)	0.0038	0.0596
Plutonium (85)	^{239}Pu Enrichment (wt%)	88.6	99.46
	AENCF (MeV)	0.0025	1.9188
High-enriched uranium, ^{235}U (120)	^{235}U Enrichment (wt%)	89.04	94.0
	AENCF (MeV)	0.0022	1.5979
Intermediate-enriched uranium, ^{235}U (39)	^{235}U Enrichment (wt%)	16.0	55.38
	AENCF (MeV)	0.0455	1.4403
Low-enriched uranium, ^{235}U (37)	^{235}U Enrichment (wt%)	1.01	10.0
	AENCF (MeV)	0.0114	0.2541
High-enriched uranium, ^{233}U (16)	^{233}U Enrichment (wt%)	97.67	99.70
	AENCF (MeV)	0.0030	1.7740
Lattice Systems (173)			
Mixed plutonium and natural uranium fuel pins (25)	^{235}U Enrichment (wt%)	0.71	0.71
	^{239}Pu Enrichment (wt%)	86.15	91.84
	AENCF (MeV)	0.0609	0.3776
High-enriched uranium, ^{235}U, fuel pins (26)	^{235}U Enrichment (wt%)	62.4	96.0
	AENCF (MeV)	0.0229	0.2422
Intermediate-enriched uranium, ^{235}U, fuel pins (2)	^{235}U Enrichment (wt%)	20.0	20.0
	AENCF (MeV)	0.0236	0.0240
Low-enriched uranium, ^{235}U, fuel pins (69)	^{235}U Enrichment (wt%)	1.15	5.74
	AENCF (MeV)	0.0886	0.4085
High-enriched uranium, ^{235}U, fuel plates (23)	^{235}U Enrichment (wt%)	93.17	93.17
	AENCF (MeV)	0.0097	0.0147
High-enriched uranium, ^{235}U, cruciform fuel rods (28)	^{235}U Enrichment (wt%)	80.0	90.0
	AENCF (MeV)	0.0106	0.0919

[a] Enrichment is expressed as weight-percent (wt%) of fissile isotope.

2.2.2 Commercial Reactor Criticals

The CRCs represent commercial SNF in known critical configurations. CRC data will be used to supplement LCE data for criticality model validation where configuration classes inside both PWR and BWR waste packages are represented. This validation will be documented in two validation reports – one for PWR waste packages and the other for BWR waste packages. The validation reports will be discussed further in Section 2.2.3.

CRC evaluations for PWRs were discussed in Section 4.1 of the topical report (DOE 1998b). A total of 45 CRC experiments were evaluated and the results from these evaluations were used in Section 4.1.3.4.1 of the topical report to illustrate trending of criticality data when establishing CL values. A summary of burnup and initial enrichment data for the 45 CRC statepoints

(measured critical conditions at zero-power) for the PWRs is presented in Table 2-6. The coolant temperatures for these statepoints ranged from 555 K to 566 K. The burnup data in this table are from Table 2.3-2 of CRWMS M&O (1999e).

Table 2-6. Summary of Pressurized Water Reactor CRC Statepoint Parameters

Plant	Number of Statepoints	Maximum Core Average Burnup[a] (GWd/mtU)	Maximum Assembly Burnup[a] (GWd/mtU)	Enrichment (wt% ^{235}U)
Crystal River Unit 3	33	33	49	1.93 – 4.17[b]
TMI Unit 1	3	14	28	2.06 – 3.05[c]
Sequoyah Unit 2	3	19	34	2.10 – 3.80[d]
McGuire Unit 1	6	23	38	2.11 – 3.75[e]

[a] The maximum core average and assembly burnups are for the statepoint with the largest core average value.
[b] Data from Table 3-1 of CRWMS M&O (1998b).
[c] Data from Table 3-1 of CRWMS M&O (1998c).
[d] Data from Table 3-1 of CRWMS M&O (1998d).
[e] Data from Table 3-1 of CRWMS M&O (1998e).

Trending results from evaluations of the 45 statepoints with MCNP were presented in Section 4.1.3.4.1 of DOE (1998b). Additional CRC data will be analyzed for the PWR neutronic model validation report that will expand the initial ^{235}U enrichment range to 4.96 wt%. These statepoints will also include fuel assemblies with axial blanket fuel and fuel rods with Gd_2O_3 as a burnable absorber.

CRC evaluations for BWRs are currently being performed. A total of 28 CRC experiments are being evaluated and the results from these evaluations will be presented in the BWR validation report. These statepoints included fuel assemblies with axial blanket fuel and fuel rods with Gd_2O_3 as a burnable absorber. The fuel assemblies also contained variable ^{235}U enrichments (zone-loaded) both radially and axially. The radial zone loading of enrichments was modeled with a lattice average enrichment (i.e., average of all fuel rod segment enrichments for a given axial segment). The axial zone loading of enrichments was modeled with the lattice average enrichment for each particular axial segment. A summary of burnup and initial enrichment (assembly average) data for 12 CRC statepoints for the BWRs is presented in Table 2-7. The data in Table 2-7 was taken from CRWMS M&O (1999f) and CRWMS M&O (1999g). The coolant temperature for all of the BWR statepoints range from 317 K to 481 K.

Table 2-7. Summary of Boiling Water Reactor CRC Statepoint Parameters

Plant	Number of Statepoints	Maximum Core Average Burnup[a] (GWd/mtU)	Maximum Assembly Burnup[a] (GWd/mtU)	Enrichment (wt% ^{235}U)
Quad Cities Unit 2	7	24.56	40.07	2.88 – 3.17
LaSalle Unit 1	5	23.61	39.94	3.01 – 3.43

[a] The maximum core average and assembly burnups are for the statepoint with the largest core average value.

The largest assembly average enrichment for the BWR statepoints currently being analyzed is 3.56 wt%. The largest lattice average enrichment for this assembly was 4.06 wt% with the largest pin segment enrichment being greater than 4.5 wt%. The degree of variability in axial and radial enrichments within BWR fuel assemblies coupled with other operational heterogeneous effects (e.g., control blade operation and large moderator density variations) make BWR fuel assemblies more challenging to model than PWR assemblies. The BWR neutronic model validation report will address these modeling concerns and the adequacy of the current BWR database.

A preliminary evaluation of the characteristics of LCEs, CRCs, and waste packages is presented in CRWMS M&O (1999j). This evaluation considered the geometry of construction, materials of construction (including fissionable materials), and the inherent neutron spectrum affecting the fissionable material. These are the three fundamental parameters that according to NUREG/CR-6361 (Lichtenwalter et al. 1997, p. 179) should be considered in the selection of suitable experiments for use in the evaluation of transportation and storage package designs. The neutron spectrum from a selected PWR CRC statepoint evaluation was compared with the neutron spectrum of a waste package that contained 21 fuel assemblies removed from the CRC. These comparisons were made for the entire core and waste package and for selected fuel assemblies at various axial heights. Comparisons were also made of the effect of temperature on reactivity with 300 K cross sections and 587 K cross sections in both a CRC and a waste package environment. The criticality model validation will expand on the types of evaluation presented in CRWMS M&O (1999j) in establishing the applicability of the experiments to waste package conditions.

2.2.3 Validation

The criticality model validation will be documented in the neutronic model validation reports. There will be one validation report for each waste package design covering all applicable internal configurations. All applicable external configurations for all waste forms will be covered in a single neutronic model validation report. LCE data will be included for criticality model validation in all of these reports. The neutronic model validation reports for PWR and BWR SNF waste packages will use radiochemical assay data for the isotopic model validation. Both LCE and CRC data will be used for the criticality model validation in the PWR and BWR reports. CRC data will also be used in validating the isotopic model for commercial SNF and to confirm that the isotopic concentrations used in waste package design are conservative.

The validation reports will start with the identification of the initial experimental database to be used for configuration classes from each applicable degradation scenario from the Master Scenario List (DOE 1998b, Section 3.1). This database will be used to establish critical limit values that are applicable for the range of parameters identified for each configuration class.

The initial experimental database will be characterized and grouped into subsets based on MCNP tallies (e.g., flux spectrum, fission spectrum, or reaction rates), material type, and geometry (where applicable). The database will then be evaluated for trends within each subset and CL values will be established following the process described in Section 4.1.3.2 of the topical report. The applicability of the CL values to configurations within each configuration class will be

established as described in Section 4.1.3.3 of the topical report. These CL values will be documented in the neutronic model validation reports.

As noted in Section 2.1.3, the first neutronic model validation report will be for configurations of SNF inside PWR waste packages. First, degradation scenarios from the Master Scenario List will be examined to establish parameter ranges for the configuration classes identified for criticality model validation. Next, the applicability of subsets of the LCE data to model validation for the range of specific parameters defined for the configuration classes will be established. This includes the range of fissile isotope concentrations, moderator and reflector material concentrations, neutron absorber isotope concentrations, and the geometry of these materials. Finally, MCNP tallies characterizing the neutron spectrum and leakage for the LCE evaluations will be compared with similar evaluations for the waste package configurations. Trending analyses will be performed for calculated k_{eff} values from the LCE evaluations, CL values will be established, and the range of applicability of the CLs for PWR waste package configurations will be identified.

The evaluation process performed with the LCE data will then be repeated using CRC data. The fuel isotopic concentrations for the LCE experiments are from design and fabrication specifications. The SNF isotopic concentrations for the CRC experiments are calculated values obtained from burnup calculations using the isotopic model. Thus, additional uncertainty exists for the isotopic concentrations used in the CRC evaluations.

The uncertainty in the calculated isotopic concentrations will be established during the isotopic model validation using radiochemical assay data. The isotopic model validation is limited by the availability of reactor operating history data, approximations made by the model in representing the fuel sample during in-reactor irradiation, and is restricted to those isotopes that were assayed. As discussed in Section 2.1.3 of this report, the effects of these limitations will be evaluated, in part, by code-to-code comparisons to a two-dimensional lattice-depletion code and SNF assay samples. These evaluations will be used along with Requirement B in Section 4.1.3.1.4 (p. 4-9) of the topical report to provide assurance that bounding operating history parameters will be used in waste package design to calculate commercial SNF isotopic concentrations.

Further assurance in the adequacy of the isotopic model is provided by Requirement A in the topical report (Section 4.1.3.1.4, page 4-9). This requirement states that "Reactor operating histories and conditions must be selected together with axial burnup profiles such that the isotopic concentrations used to represent commercial SNF assemblies in waste package design shall produce values for k_{eff} that are conservative in comparison to any other expected combination of reactor history, conditions, or profiles." This will be demonstrated in the PWR neutronic model validation report by performing numerical experiments using CRC statepoint data (both calculated and measured). The database available for numerical experiments from the 45 PWR CRC statepoints analyses is summarized in Table 2-8.

Table 2-8. PWR Database from CRC Analysis for Selecting Numerical Experiments

Plant Type	Number of Burned Fuel Assemblies	Number of Unique Burned Fuel Assemblies[a]
177 Fuel Assembly Core	5358[b]	878
193 Fuel Assembly Core	1131[c]	182

[a] Burned fuel assembly in center of core counts as one experiment, 4 burned fuel assemblies on a quarter core axis count as one experiment, and 8 burned fuel assemblies in eighth-core symmetry locations count as one experiment.
[b] Based on information from Table 3-2 and Figures 3-3 through 3-11 of CRWMS M&O (1998b), and Table 3-2 and Figure 3-5 of CRWMS M&O (1998c).
[c] Based on information from Table 3-2 and Figures 3-6 and 3-7 of CRWMS M&O (1998d), and Table 3-2 and Figure 3-3 of CRWMS M&O (1998e).

For any burnup and enrichment combination, the most limiting commercial SNF assembly relative to criticality potential is the assembly that experienced the hardest neutron spectrum during in-reactor irradiation. The harder neutron spectrum during in-reactor irradiation converts more of the ^{238}U isotope into ^{239}Pu. The increased ^{239}Pu inventory provides additional fissile material for fissioning and helps conserve ^{235}U. The net result is to maximize the fissile isotope (^{235}U and ^{239}Pu) content. The PWR CRC database was chosen to include fuel assemblies with control rod histories, axial power shaping rod histories, and burnable absorber rod histories. Control rod histories, as used in this context, means that control rods were more than 50 percent inserted for some portion of the fuel assembly's irradiation lifetime. Axial power shaping rods (Figures 2-10 and 2-11 of CRWMS M&O 1998b) are part length (either 3 feet or 5.25 feet long) control rods that are inserted for an entire fuel cycle. Burnable absorber rods are typically inserted in fresh (unburned) fuel assemblies and remain in the reactor for an entire fuel cycle. PWR SNF assemblies that contain these types of absorber rods during their in-reactor irradiation lifetime will have a higher k_{eff} than similar (same enrichment and burnup) SNF assemblies that did not contain absorber rods. Additional in-reactor, irradiation history effects (e.g., moderator density or fuel temperature) that alter the isotopic concentration distribution will be analyzed to demonstrate the adequacy of the commercial SNF isotopic model when applied in criticality evaluations. These analyses will be summarized in the validation reports for commercial SNF.

The reactivity effect of past in-reactor irradiation history for individual fuel assemblies (selected from the PWR database summarized in Table 2-8) will be quantified with the numerical experiments. For example, an individual fuel assembly that is being evaluated will be modeled assuming two or more neutron absorber histories for in-reactor irradiation. For each case analyzed, the remaining fuel assemblies will contain isotopic concentrations from the best-estimate isotopic model used in the original CRC statepoint evaluations. Since the original statepoint evaluations compare best-estimate calculations to measurements, the numerical experiments are comparing small, localized perturbations of this model to measurements. This in turn provides a direct comparison of the calculated parameter being investigated (e.g., neutron absorber history effect, but will also be applied for other parameters) to measurements. The effect on k_{eff} is then quantified and documented in the validation report. MCNP tallies (flux spectrum, etc.) that were performed during the original CRC statepoint evaluations are repeated for the numerical experiments for comparison with similar MCNP tallies for waste package configurations.

The PWR CRC experiments are at hot-zero-power conditions. The temperatures inside the reactor core are at isothermal conditions and vary from 555 K to 566 K for the 45 CRC experiments. The temperatures of the PWR SNF in the repository will be closer to 294 K at the time when criticality is a concern. Any additional bias introduced in extending the range of applicability of critical limit values established using CRC data to repository conditions (temperatures) will be quantified. Additional reactor startup information (e.g., reactivity deficit in going from cold shutdown condition to hot-zero-power condition) will be obtained and used in establishing the temperature bias. In addition, alternative calculational methods will be used to provide an independent estimate of the bias at repository conditions.

The next neutronic model validation report will be for configurations of SNF inside BWR waste packages. The validation process described for the PWR validation report will be followed for the BWR validation report. However, additional validation is required for BWR SNF because of approximations made in modeling the fuel assemblies for in-reactor irradiation. BWR fuel assemblies are more heterogeneous than PWR fuel assemblies. Fuel enrichments are zone loaded both axially and radially. Control blade operation and large variations in moderator density produce additional heterogeneous effects. Thus, the SAS2H model used for fuel assembly burnup calculations contains approximations that are more severe for BWR fuel. A two-dimensional lattice-depletion code will be used for evaluating the approximations made for the one-dimensional, point-depletion SAS2H model. The accuracy of the approximations made for using a single enrichment to represent a radial lattice of variable enrichments will be evaluated. The approximations made in modeling control blades and Gd_2O_3 will be evaluated. Finally, the radiochemical assay data will be evaluated with the two-dimensional lattice-depletion code, which is more capable of representing the assay samples. This will be followed by a code-to-code validation with SAS2H. The radiochemical assay evaluations will be performed for both PWR and BWR assay samples. All BWR evaluations will be documented in the BWR neutronic model validation report.

Critical limit values will be established with both LCE and CRC data and presented in the neutronic model validation reports. The range of applicability of the sets of CL data will then be applied, as appropriate, to criticality evaluations for the repository.

Neutronic model validation for other waste forms will only include criticality model validation. Isotopic concentrations for these waste forms will generally be waste form fabrication values. However, as noted in Section 4.1 of DOE (1998b), it must be confirmed that this composition is conservative for a range of potential scenarios (e.g., fuel where significant plutonium has been generated, and a scenario where the plutonium and uranium may be separated). A method for confirming this conservatism will provided in the validation reports. LCEs will be used for criticality model validation of these waste forms. The neutronic model validation reports for these waste forms will be completed after the reports for commercial SNF are completed.

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3. PROBABILITY

This section will describe the additional analyses and evaluations for the probability and scenario/configuration class development parts of the methodology.

3.1 ELABORATION OF THE METHODOLOGY FOR CALCULATING CRITICALITY PROBABILITY

The probability of criticality is calculated by the mathematical process of taking the product of probabilities of individual events and processes that are included in scenarios leading to potentially critical configurations, and then summing (or averaging) over all possible values of the parameters characterizing these events and processes, as described in the *Disposal Criticality Analysis Methodology Topical Report* (DOE 1998b). In practice, this mathematical process is simulated by the Monte Carlo technique (random sampling from the distributions of the relevant parameters), as illustrated by the examples in Appendix C of DOE (1998b).

The purpose of this supplementary methodology discussion is to provide a more comprehensive list of all of the event and process parameters and to indicate their dependence on each other. The principal unconditional probabilities involved in the events or processes are the following:

- Climate: $Pr\{climate_i\}$
- Corrosion rate of the carrier of the neutron absorber, such as borated stainless steel, determined by M&O-developed experimental data: $Pr\{corrosion\ rate\ for\ BSS_p\}$
- Corrosion rate of structural material. There will generally be at least two variants, one for the basket material, and one for the spacer grids of the assembly: $Pr\{corrosion\ rate\ for\ structural\ material_v\}$
- Disruptive events, such as earthquake or volcano: $Pr\{disruptive\ event_x\}$

Human error events, such as misloading of the waste package or human intrusion into the repository, have not been explicitly included in the methodology at this time because there is no way to construct a probability distribution for such events. Such events can be incorporated into the methodology if suitable probability models are developed.

Principal conditional probabilities involved in the events or processes are the following:

- Drip rate per unit area of the waste package (projected onto the horizontal plane), determined by the hydrothermal model and the fracture focussing model: $Pr\{drip\ rate\ per\ unit\ area_j \mid climate_i\}$. Note that the vertical bar (|) in the Pr{} denotes that the parameter, or event, preceding the | is conditioned on the event or parameter following the |.
- Area of opening (penetration) in the top of the waste package, projected onto the horizontal plane. In general, a higher drip rate will lead to a larger penetration area. The probability distribution of this parameter will be determined by abstraction of results from the waste package degradation simulation code (currently WAPDEG version 3.09, CRWMS M&O 1998h, which properly accounts for any dependencies among the corrosion related parameters): $Pr\{area\ of\ opening_k \mid drip\ rate\ per\ unit\ area_j\}$

- Drip rate into package, given drip rate per unit area onto the waste package: Pr{drip rate into package$_n$ | drip rate$_j$, area of opening$_k$}
- Time of breach (start of corrosion of components inside the waste package, particularly the carrier of the neutron absorber, such as borated stainless steel); determined using WAPDEG: Pr{time of breach$_t$ | drip rate per unit area$_j$}
- Duration of water ponding in the waste package (called bathtub) and water level when there is ponding; determined using WAPDEG: Pr{duration of bathtub$_{tt}$ | drip rate per unit area$_j$}
- Parameter representing the retention or loss of the neutron absorber. For example, this could be the thickness of the borated stainless steel plate remaining. A variation of this parameter could be the solubility of the neutron absorber. Solubility is dependent on other parameters, such as the pH of the waste package solution, which would then need to be included in the parameter set. Pr{absorber loss$_q$ | breach time$_t$, corrosion rate$_p$}
- Moderator displacement material amount generally, and its distribution, which would require the use of several related parameters, so the index r could represent several related, or refinement, parameters: Pr{moderator displacer$_r$ | breach time$_t$, corrosion rate$_p$}
- Characteristics of the SNF, particularly initial enrichment and burnup (with appropriate credit for the latter). The dependence of criticality probability on these factors will generally include an explicit dependence on the amount of neutron absorber, since these parameters (amount of absorber, burnup, and initial enrichment) are the ones most directly affecting neutronics calculations. For the commercial PWR SNF criticality summarized in DOE 1998b, the probability took the form of a multivariate normal distribution, with mean specified by a regression of k_{eff} on these parameters (both linearly and as products up to the third power), and with an appropriately determined standard deviation. The general form of the dependence is best expressed as Pr{criticality$_m$ | burnup$_b$, enrichment$_e$, neutron absorber remaining}.
- Geometric factor for fissile material. For commercial SNF one useful measure is pitch/separation between fuel pins, as the assembly goes through various stages of collapse.
- Loss of reactor-generated neutron absorbers initially in the SNF (fission products and actinides). In the analyses thus far the dependence of criticality on this parameter is not part of the principal regression mentioned in the previous item. It is added on as a change in k_{eff}. The general probability dependence for this term is best represented by: Pr{criticality$_m$ | reactor generated neutron absorbers remaining$_s$, corrosion rate for structural material$_v$}

The following is a summary of the subscript index variables representing a range of values for uncertain parameters. They are intended for illustrative purposes only. The actual use of variable symbols will be chosen as appropriate for the case being analyzed.
Climate: i
Drip rate per unit area: j
Area of opening in the upper surface of the waste package: k
Criticality: m
Drip rate into the waste package: n
Corrosion rate of carrier of neutron absorber: p
Parameter characterizing retention (adsorption) or removal (solubility) of neutron absorber: q

Parameter characterizing the effective amount of moderator displacing material: r
Neutron absorbers remaining in the SNF (out of the total permitted by burnup credit): s
Time of waste package breach: t
Duration of bathtub: tt
Peak overpressure in a transient criticality: u
Corrosion rate of structural material: v
Increment in radionuclide inventory determined by the power level and duration of the criticality: w
Disruptive event: x
Reactivity insertion rate: y
Burnup and enrichment: b, e

Refinements, or subdivisions, of these parameter categories may be represented by multiple subscripts. For example, the thickness of borated stainless steel remaining could be represented by qq.

The probability of criticality is the product of the following factors, summed over the distributions of the indicated indices:

$Pr\{\text{drip rate per unit area}_j \mid \text{climate}_i\}\ Pr\{\text{climate}_i\}$
$Pr\{\text{area of opening}_k \mid \text{drip rate per unit area}_j\}$
$Pr\{\text{drip rate into package}_n \mid \text{drip rate}_j, \text{area of opening}_k\}$
$Pr\{\text{time of breach}_t \mid \text{drip rate per unit area}_j\}$
$Pr\{\text{duration of bathtub}_{tt} \mid \text{drip rate per unit area}_j\}$
$Pr\{\text{absorber loss}_q \mid \text{breach time}_t, \text{corrosion rate}_p\} \times Pr\{\text{corrosion rate for BSS}_p\}$
$Pr\{\text{moderator displacer}_r \mid \text{breach time}_t, \text{corrosion rate}_p\}$
$Pr\{\text{criticality}_m \mid \text{burnup}_b, \text{enrichment}_e, \text{added neutron absorber loss}_q, \text{moderator displacer}_r, \text{neutron absorbers remaining in the SNF}_s\}$

The steady-state criticality risk is the product of the criticality probability factors, multiplied by $Pr\{\text{radionuclide inventory increment}_w \mid \text{drip rate into pkg}_n, \text{other factors}\}$ and by the factor (radionuclide inventory increment_w) and summed over all values of the indices. As mentioned above, the mathematical summation is simulated by the Monte Carlo technique.

The transient criticality risk is the product of the criticality probability factors, multiplied by $Pr\{\text{peak overpressure}_u \mid \text{exit area}_k, \text{insertion rate}_y\} \times Pr\{\text{insertion rate}_y \mid \text{disruptive event}_x\} \times Pr\{\text{disruptive event}_x\}$ and by the factor (peak overpressure_u) and summed over all values of the indices.

3.2 EXAMPLE

3.2.1 Background

As a result of the *License Application Design Study* (CRWMS M&O 1999o), the waste package baseline design has been changed to reduce the probability of aqueous penetration. An important consequence of reduction in the probability of aqueous penetration is a corresponding reduction

in the probability of criticality. The purpose of this section is to summarize the calculation of the probability distribution (as a function of time) of criticality for the new design, which has been designated as EDA II. The details of this calculation are given in CRWMS M&O (1999m); the methodology is similar to that used for the previous baseline design (called the VA design, for Viability Assessment), which was reported in the *Disposal Criticality Analysis Methodology Topical Report* (DOE 1998b, Appendix C). In addition to the comparison of the new design (EDA II) with the previous design (VA), this calculation also incorporates the incremental effect of assembly collapse and loss of fission product neutron absorbers.

3.2.2 Implementation of the Methodology for this Example

The likely internal degradation scenario for the commercial PWR SNF waste package is shown in six stages in Figure 3-1. The first stage (Figure 3-1A) is the intact configuration, which is assumed to exist just prior to breach of the waste package irrespective of the time to breach. The water breaching the waste package will fill the waste package to the level of the breach. For several hundred years following the filling of the waste package, the dominant degradation process will be the corrosion of the carbon steel and aluminum components. The first structural components to fail will be the carbon steel side guides and corner guides (Figure 3-1B). Following those failures, the rest of the structural material and thermal shunts will fail, leading to the fully collapsed basket configuration (Figure 3-1C).

The Monte Carlo simulation process tracks the corrosion of borated stainless steel (with consequent loss of boron) following the attainment of the fully collapsed basket configuration of Figure 3-1C, which implies the approximation that all of the carbon steel has corroded before the start of stainless steel corrosion. In other words the progression from the initial configuration to the fully collapsed basket (Figure 3-1A to Figure 3-1C) is instantaneous. This approximation is justified by the much faster corrosion rate of carbon steel with respect to borated stainless steel. The approximation is slightly non-conservative because it will result in having all the iron corrosion product of the carbon steel available for criticality control when the loss of boron begins. However, there can be no criticality until nearly all the borated stainless steel has corroded (CRWMS M&O 1996, Section 7.6), so this non-conservatism is inconsequential. The remaining configurations (Figure 3-1 D through F) show the end results of the degradation of the borated stainless steel, the zircaloy assembly spacer grids, and the zircaloy cladding, respectively. In actuality, these components will degrade simultaneously, but the borated stainless steel will degrade at a much faster rate than the zircaloy (DOE 1998b, Appendix C, Section 1.4.3), so the scenario is very likely to pass through a configuration resembling Figure 3-1D. Since the zircaloy spacer grids are not as thick as the zircaloy fuel pin cladding (Toledo Edison 1998, Volume 6, Table 4.2-1 and CRWMS M&O 1998f, Table 3-1), and since the spacer grids are exposed to corrosion from both sides while the cladding is only exposed to corrosion from one side, the assemblies are more likely to collapse (Figure 3-1E) before significant degradation of the fuel matrix itself (Figure 3-1F).

There are several levels of conservatism in this analysis of fission product loss and assembly collapse. The major conservatism is the assumption that the zircaloy failure (cladding and spacer grids) can occur before 100,000 years. In actuality, zircaloy is so slowly corroding that these components will have average lifetimes much longer than 100,000 years (DOE 1998b, Appendix

C, Section 1.4.3). The secondary conservatism is that the nominal Monte Carlo simulation assumes that the collapse and fission product loss can occur simultaneously, or have overlapping durations. The discussion in the previous paragraph shows that the more likely condition will have the spacer grids collapsing much before the loss of cladding. A further elaboration on this conservatism is provided by the comparison case that assumes that the collapse occurs after the fission product loss. One conservatism that has not been applied is loss of iron oxide from the waste package. The code for implementing the Monte Carlo methodology has the capability to simulate the effect of such a process, and that capability has been tested on sensitivity studies. However, such calculations will not be published until evidence is found for a significant loss mechanism.

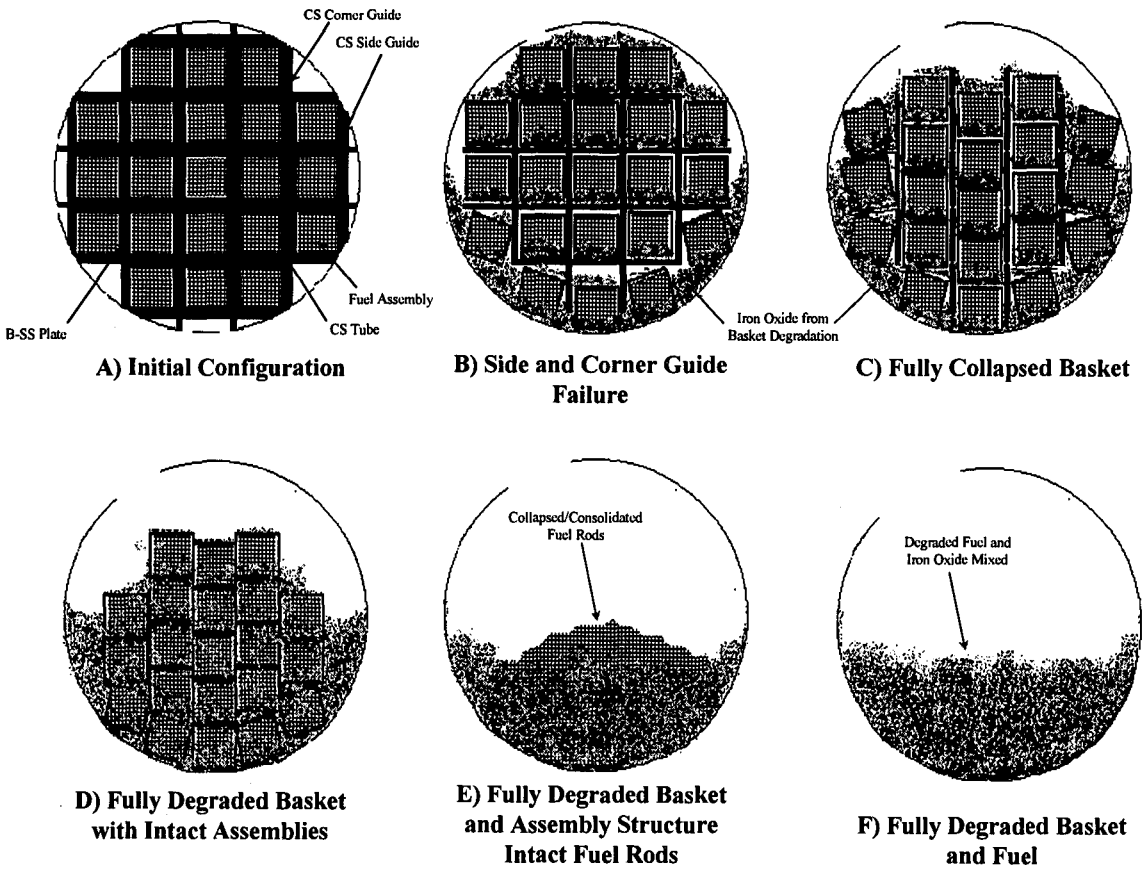

Figure 3-1. Degradation Sequence for the 21 PWR Absorber Plate Waste Package (DOE 1998b, Appendix C, Figure C-15)

The degradation scenario described above can be related to the exhaustive list of parameters and probabilities given in Section 3.1. Of the four unconditional probabilities listed at the beginning of the section, climate has been incorporated into the WAPDEG calculation of the distribution of breach times (Figure 3-2) and bathtub duration times (Figure 3-3). The corrosion rate of borated stainless steel is used in this calculation. The corrosion rate of the structural material is used implicitly, but there is no need for a probability distribution of values since the carbon steel

degrades so much faster than the other components that it can all be assumed to have degraded before the simulation starts. The fourth, and last of the unconditional probabilities, a disruptive event has not been included because preliminary analysis shows that neither earthquake nor volcano can lead to a more reactive configuration than those considered here. (This preliminary observation will be demonstrated in the License Application.)

Of the conditional probabilities listed in Section 3.1, the first two (drip rate per unit area and area of opening in the top of the waste package) have been incorporated into the WAPDEG calculation. The remaining ones are all included in the Monte Carlo simulation described herein.

The Monte Carlo technique is implemented by a software routine (MONTECARLO.C, CRWMS M&O 1999m, Attachment II) that builds the expected criticality statistics from a file of expected assembly receipts at the repository. In this file, the assemblies are grouped in batches from 1 to 50 assemblies representing common reactor histories. Each batch is characterized by a set of parameters; the ones most important for criticality are burnup and initial enrichment. The first step in the processing of each batch is to screen for criticality potential; only those batches with criticality potential above a specified threshold are then subject to the large number of Monte Carlo realizations. The number of realizations used for this calculation is 500. Each Monte Carlo realization begins with a random selection of whether the package is dripped on and whether the package is breached on the top before it is breached on the bottom. For realizations that satisfy both conditions, the time before breach and the time between first top breach and first bottom breach (duration of waste package "bathtub" configuration) are randomly generated. Also generated at this time are the parameters for the distribution of rates of assembly collapse and fission product loss (which results from the degradation of the fuel matrix).

For each time step of the numerical integration of a Monte Carlo realization, the following parameters are also calculated or generated randomly from a specified distribution: decrement in thickness of borated stainless steel, quantity of boron lost from the waste package, degree of assembly collapse, and quantity of fission products lost from the fuel matrix. The k_{eff} of the remaining configuration is then calculated, using a regression as a function of the following: time since irradiation, burnup, initial enrichment, and parameters describing the degree of degradation of the borated stainless steel and the boron loss from the waste package. This regression is based on over 1000 criticality calculations using MCNP4A: the process for its development is summarized in Appendix C of the topical report (DOE 1998b). The regression has been extended to include a parameter characterizing the degree of assembly collapse and a parameter characterizing the loss of neutron absorbing fission products from the fuel matrix. This extension is based on an additional 400 criticality calculations, as described in CRWMS M&O (1999n, Sections 5.3, 5.4, and 6).

If the adjusted $k_{eff} \geq CL$, then a criticality will be recorded. For this purpose the total number of criticalities is incremented by the number of assemblies in the batch. The total number of criticalities is also apportioned according to the time of occurrence of the criticality using an array of bins, with one bin for each time step. For this purpose, the bin corresponding to this time step is also incremented by the number of assemblies in the batch. The simulation then moves to the next realization. If, on the other hand, the adjusted $k_{eff} < CL$, then the simulation

moves to the next time step. If the time steps reach to the duration of the bathtub, the realization is considered to have had no criticality, and the next realization will begin.

3.2.3 Computation of Probabilities (of Individual Events and Processes)

3.2.3.1 Probability that Waste Package is Located Under a Dripping Fracture

The probability that a waste package is located under a dripping fracture has been taken to be 0.26. This is consistent with the mean seepage fraction used for TSPA-VA for the long-term average climate (DOE 1998c, Table 3-5 and Figure 3-13).

3.2.3.2 Time of Waste Package Breach

Information on the distribution of waste package breach times for packages under dripping fractures was developed as described in CRWMS M&O (1999k), using the WAPDEG v3.09 code. The WAPDEG output for each case lists the times that first penetrations occur on the top and bottom of the package both for parts of the package under the drip and parts not under the drip. Each output contains this information for a sample of 400 waste packages. Since breaches on the top of the package are required to allow dripping water to enter, the earliest time of any top penetration was used as the waste package breach time. This is conservative as only top breaches under a drip would be expected to allow significant amounts of water to enter the waste package. A least-squares fit of the above data to a three-parameter Weibull distribution was performed using Excel 97. The probability density function (pdf) of the Weibull distribution is given by:

$$f(t) = \frac{\beta}{\alpha}\left(\frac{t-\theta}{\alpha}\right)^{\beta-1} \exp\left[-\left(\frac{t-\theta}{\alpha}\right)^{\beta}\right]$$

where α , β , and θ represent the scale, shape, and location (distribution minimum value) parameters respectively (all > 0) and $t \geq \theta$. It should be noted that the variable t actually represents the natural log of time (in years) for convenience of calculation. The associated Weibull cumulative distribution function (CDF) is given by:

$$F(t) = 1 - \exp\left[-\left(\frac{t-\theta}{\alpha}\right)^{\beta}\right]$$

for $t \geq \theta$. For values of $t < \theta$, both f(t) and F(t) equal zero. For this application, θ was adjusted until the best fit to the lower part of the distribution (smaller values of t) was achieved. The lower part of the distribution is the portion of interest for this calculation.

The Weibull distribution was chosen for this application because of its ability to fit a wide variety of distribution shapes. The resulting Weibull parameters are given in Table 3-1 for degradation of the EDA II waste package design (CRWMS M&O 1999k); the corresponding values for the VA design are given for comparison. Figure 3-2 shows the Weibull CDF for the

waste package breach time for the EDA II design, and the data points used in the fit. Because the emphasis is on fitting the lower portion of the curve, the fit on the upper portion is not as good. This calculation is not concerned with time beyond 250,000 years, at which point the fit is still quite good.

Table 3-1. Weibull Parameters for WP Breach Time for VA and EDA II Design

Case	Alpha	Beta	Theta
VA	12.099	16.425	0.000
EDA II	2.347	4.810	10.820

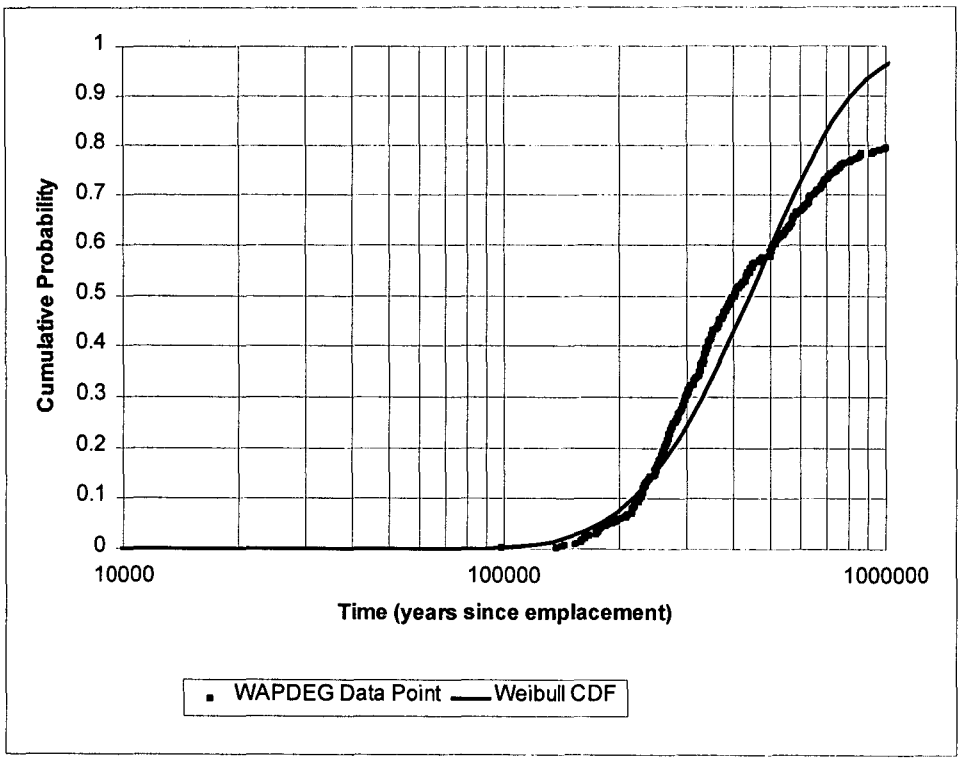

Figure 3-2. Cumulative Distribution for EDA II Waste Package Breach Time (CRWMS M&O 1999k, Figure 5.1.2-2)

3.2.3.3 Probability and Duration of Waste Package Flooding

As indicated above, the WAPDEG output contains information on the time of penetration of both the top and bottom surfaces of the waste package. In order for the waste package to be capable of accumulating water, it must be penetrated on the top surface, and not on the bottom surface. To obtain a distribution for the possible duration of this condition, the Δt between the earliest top penetration, and the earliest bottom penetration, was calculated for each of the 400 waste package Monte Carlo simulations in the WAPDEG analysis. Approximately half the packages had a negative Δt, indicating that they were penetrated on the bottom first. At the time of top breach, these packages would be incapable of collecting the water necessary for criticality, since they would have already been breached from the bottom. It is recognized that this approximation

is not conservative because it may be possible for the waste package to plug an initial hole in the bottom, and then fill with water. The most likely agent for such plugging is clay, which is a likely degradation product in codisposal canisters, which have a large amount of silica present in the form of glass. It is possible for a significant amount of clay to form in a commercial SNF waste package, using the silica from the incoming water, but it would take upwards of several hundred thousand years. This possibility will be more carefully evaluated for License Application, particularly if there is an interest in criticality at such long times. The fraction of packages with positive Δt's are indicated in Table 3-2, as probability of waste packages flooding, for the EDA II design. For comparison, the VA design is also given.

A least-squares fit to a three-parameter Weibull distribution was then performed in the same manner as discussed above for breach time. The Weibull CDF was found to provide a good fit to the data. The resulting Weibull parameters are given in Table 3-2, with the parameters for the VA design for comparison (CRWMS M&O 1999k, p. 13). Figure 3-3 shows the Weibull CDF (resulting from the the EDA II parameters) for the duration of flooding for waste packages that are capable of accumulating water, and the data points used in the fit. It should be noted that the time in Figure 3-3 is measured from the first breach, when it should be measured from the time of first filling, which would be at least several years later. This approximation is used because WAPDEG does not consider flooding, only the occurrence of penetrations. This approximation is conservative because it leads to a longer duration of flooding.

Table 3-2. Weibull Distribution Parameters and Probability of Flooding: EDA II Design

Case	Flooding Duration Weibull Parameters			Probability of WP Flooding
	Alpha	Beta	Theta	
VA	10.849	8.228	0.000	0.4775
EDA II	11.881	10.218	0.000	0.4125

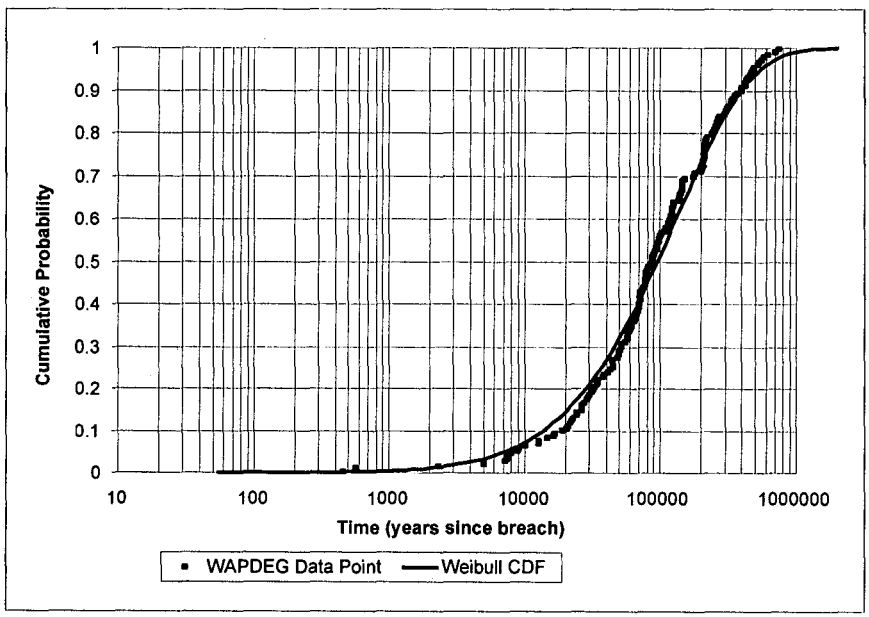

Figure 3-3. Cumulative Distribution for EDA II Waste Package Duration of Flooding (CRWMS M&O 1999k, Figure 5.1.3-2)

3.2.3.4 Borated Stainless Steel Corrosion Rate

The analysis of stainless steel corrosion rates, and the estimation of an appropriate probability distribution to represent the uncertainty, are given in Section 5.1.6 of CRWMS M&O (1998g). The resulting Weibull parameters are: $\alpha = 4.852$, $\beta = 4.041$, and $\theta = 4.605$. A chi-squared test showed a good fit to the data. Figure 3-4 shows the Weibull fit to the complementary cumulative distribution function, CCDF, for the stainless steel corrosion rate. The CCDF is the probability that the parameter (in this case the corrosion rate of 304/316 stainless steel) is greater than the specified value. The CCDF is used in this case because it provides a more convenient fit to the data.

The corrosion rate for borated stainless steel has yet to be well characterized, but it will be higher than the values represented in Figure 3-4. The analysis of CRWMS M&O (1998g, Section 5.1.6) considered the available data and concluded that it was most appropriate to increase the corrosion rate from that of unborated stainless steel by using a multiplicative "boron factor". In CRWMS M&O (1998g, p. 13), this boron factor was sampled from a uniform distribution ranging from 1 to 4. For the present calculation only a mean value of 2.5 is used.

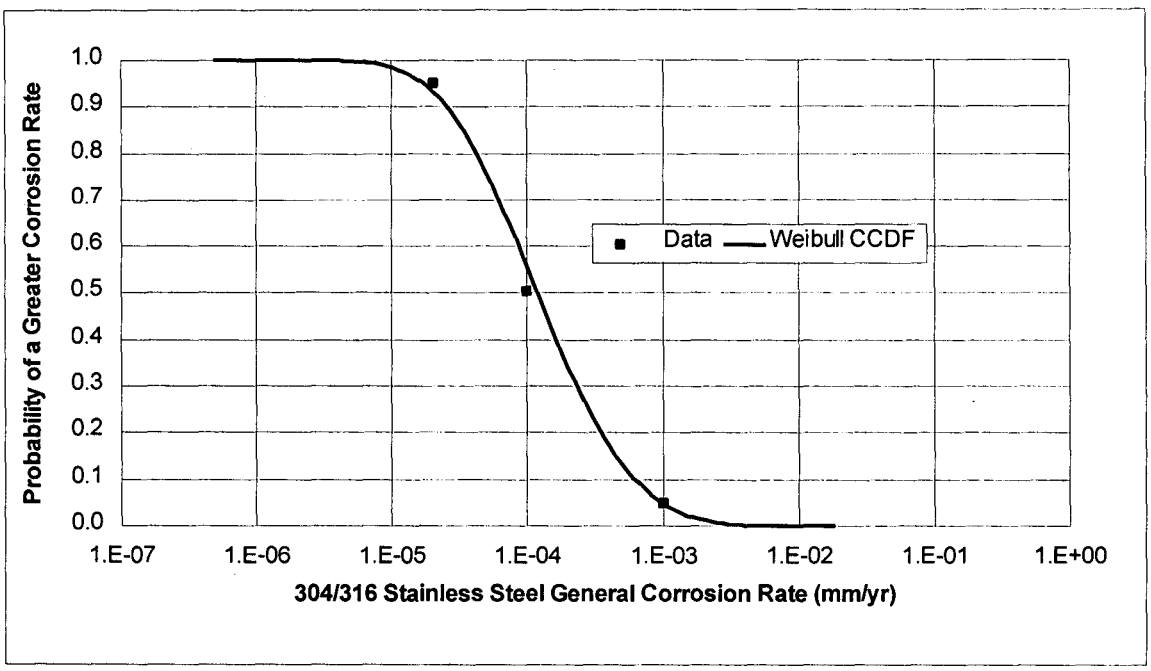

Figure 3-4. Stainless Steel General Corrosion Rate Weibull CDF (DOE 1998b, Appendix C Figure C-14)

The average flooding duration is approximately 100,000 years (Figure 3-3), and the expected lifetime of the borated stainless steel is only 14,000 years (7 mm thickness/(0.00025 mm/yr)/2 (for corrosion from both sides of the plate)). Therefore, a bias of 10% - 20% in the lifetime of the borated stainless steel, measured in tens of thousands of years, will not significantly effect the earliest time to criticality, measured in hundreds of thousands of years. An appropriately developed distribution will be used for the borated stainless steel corrosion rate for the License Application.

3.2.4 Calculation Results (Expected Number of Criticalities)

The results are summarized for representative years in Table 3-3 (CRWMS M&O 1999m), and for all years up to 249,000 in Figure 3-5.

The delayed collapse variations (cases 2 and 4) have the assembly collapse delayed until most of the fission products have been dissolved and removed from the waste package. In this way much of the neutron absorber material is removed from the waste package, while the assemblies are still in their nearly optimum spacing; therefore, the k_{eff} for these variations would be expected to be larger than for the nominal case, as is observed in Table 3-3 and Figure 3-5.

Table 3-3. Comparison of Representative Cases

Case	Expected Number of Criticalities	
	100,000 years	249,000 years
1. VA Design, nominal	2.39	6.51
2. VA Design, delayed collapse of assembly	2.83	7.59
3. EDA2 Design, nominal	0.00276	1.32
4. EDA2 Design, delayed collapse of assembly	0.00924	1.62

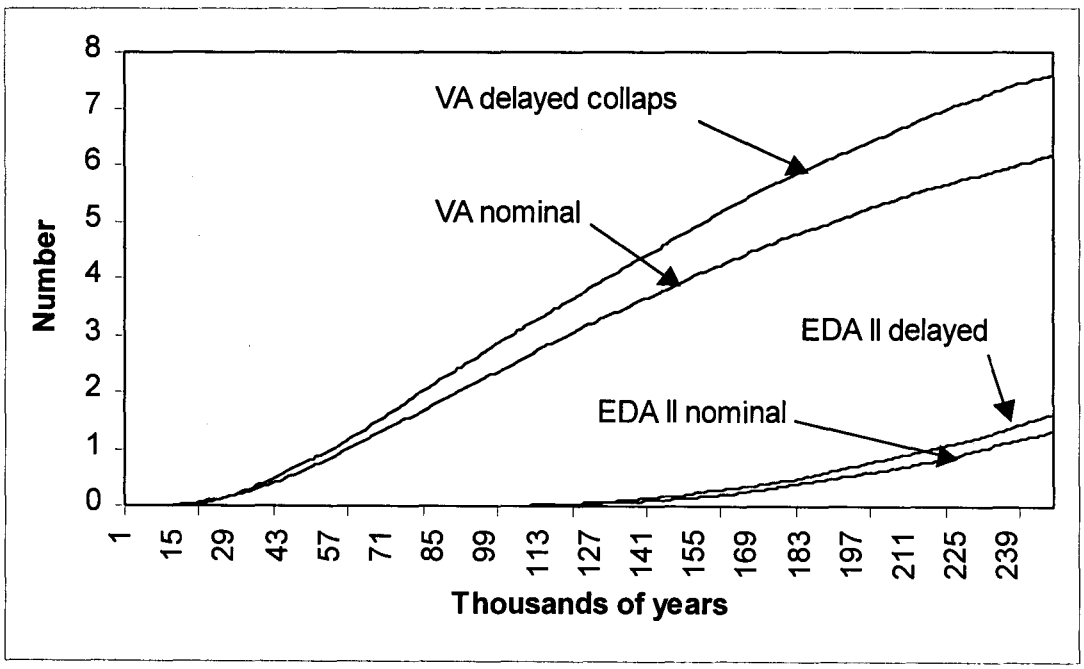

Figure 3-5. Conservative Estimate of the Expected Number of Criticalities for all PWR Waste Packages: VA and EDA II Designs Compared (CRWMS M&O 1999m, Figure 6.2-6)

It should be noted that the EDA2 cases show no criticalities at 10,000 years and very few even at 100,000 years. The ratio between expected number of criticalities for 249,000 and 100,000 years is much larger for EDA2 than for VA because 100,000 years is the threshold of waste package breach time for the EDA2 alternative (CRWMS M&O 1999k, Attachment I). Therefore, the

expected number of criticalities at 100,000 years is very low. By contrast, the VA calculation has a significant number of criticalities occurring before 100,000 years and the rate continuing fairly constant thereafter, as can be seen from Figure 3-5.

4. CONSEQUENCES

For steady-state criticality, the primary consequence measure is dose at the accessible environment, with an intermediate consequence measure of increase in radionuclide inventory. As explained in Section 3.6 of DOE (1998b), the dose can only be calculated by the total system performance assessment (TSPA) process, so it cannot be conveniently incorporated entirely within this methodology. However, the increment in radionuclide inventory can be computed directly from the parameters described here (either deterministically or probabilistically). The increment in radionuclide inventory is principally dependent on the power level of the criticality and its duration, both of which are strongly determined by the drip rate. It is also a function of many other parameters effecting the criticality. Therefore, it is appropriate to represent this relationship by Pr{radionuclide inventory increment$_w$ | drip rate into pkg$_n$, other factors}.

For the transient criticality there is no primary consequence measure. All parameters directly related to potential damage (to WP barriers or SNF cladding) will be considered. Peak overpressure is a likely candidate. This parameter is primarily determined by the reactivity insertion rate and the exit area (defined as the total area of penetrations of the waste package). The former is determined by sudden events, seismic shaking is a likely example, but volcanism will also be considered. The exit area is similar to the area of the opening identified above, but without the projection onto the horizontal plane. The appropriate representation for this relation is Pr{peak overpressure$_u$ | exit area$_k$, disruptive event$_x$}

The remainder of this section summarizes the additional analyses that have been performed to extend the range of applicability of the transient criticality methodology. Particular emphasis is given to the time history of overpressure and mass flow rate. These analysis are described in further detail throughout CRWMS M&O (1999l), which also gives other consequence measures, including the time history of temperature, reactor power, and neutron flux. Beta and gamma flux are also available from the computer program output.

4.1 SENSITIVITY OF TRANSIENT CRITICALITY CONSEQUENCES TO WASTE PACKAGE EXIT FLOW AREA

The major parameters of a transient criticality have been analyzed previously (CRWMS M&O 1997c), for a somewhat arbitrary hole size in a waste package at the time of criticality (assuming that such a criticality did occur). These results were also summarized as a demonstration of the transient criticality consequence analysis methodology (DOE 1998b, Appendix C, Section 5.1). The conclusion was that the peak overpressure was too small to cause significant damage to the waste package, or even to the SNF assembly fuel pins. The purpose of the present analysis is to show that even at smaller hole areas, the peak overpressure is not sufficient to cause damage.

Of course, a very small hole area could cause sufficient confinement to lead to a significant overpressure, that could cause damage to the SNF fuel pins. However, as the hole area decreases, the probability of sufficient water entering to cause criticality also decreases. The analysis methodology for transient criticality will define a risk measure as the product of the peak overpressure multiplied by the probability of criticality, and averaged over all possible transient criticalities. This calculation will be performed when the distribution of hole sizes is

available from the WAPDEG waste package corrosion model, and the distribution of drip frequency (per unit drift area or length) and drip magnitude is available from the repository thermo-hydrology model. Since these models are not available at the present time, it is useful to do an evaluation of the sensitivity of peak overpressure to hole size. The present analysis shows that for a hole size larger than 0.25 cm^2, the peak overpressure is not sufficient to cause damage to the fuel pins.

The following is an explanation of the most significant processes involved in the transient criticality:

> If the area through which water drips into the WP is sufficiently small, inflow rates will be restricted, lengthening the time required to flood the WP. This, in turn, will delay potential criticality events, which require flooded conditions. If a criticality event does occur, the increase in temperature and pressure will cause water vapor to be ejected, which limits the criticality through the negative void coefficient. If the total penetration area (which could be larger than the area through which water is dripping) is small enough the ejection of water vapor may be restricted, thereby reducing the negative void effect, increasing the peak pressure and temperature resulting from the transient criticality.

The purpose of the analysis summarized in this document (CRWMS M&O 1999l) is to determine the relation between reduction in the exit area and increase in peak pressure and temperature for a transient criticality. The previous analyses (CRWMS M&O 1997c) considered the possible mechanisms for generating a short-term increase in reactivity (k_{eff}) and characterized the range of mechanisms by two extremes: slow insertion rate and rapid insertion rate. The most appropriate mechanism found for a slow insertion rate was a sudden increase in drip rate that could be caused by a large storm at the surface above the repository, with subsequent flow focused onto the waste package by a fracture network. In CRWMS M&O (1997c), a likely maximum insertion rate for this mechanism was estimated as 0.0004 $/sec.

A possible mechanism for a more rapid reactivity insertion could be a shaking due to seismic disturbance. Such a shaking could free iron oxide particles clinging to the surfaces of the stacked assemblies. Once freed, the particles could settle leaving a more reactive configuration. Such a settling could leave some fraction of the fuel pins with no more iron oxide in their vicinity, so that they could be surrounded by more water for moderation. In other words, an initially under-moderated configuration would become more moderated, thereby increasing k_{eff}. The increase in k_{eff} due to the small amount of assembly that becomes completely uncovered by iron oxide more than compensates the smaller decrease in k_{eff} due to the higher density of iron oxide in the rest of the pile of assemblies in the waste package (CRWMS M&O 1997d, Sections 7.3 and 7.4). For purposes of conservatism the analysis of CRWMS M&O (1997c, Section 7) assumed that the worst case settling would occur in 30 seconds, although the actual calculations of the physical settling process indicated the minimum time is over 2 minutes. For this more precise analysis discussed in this document, the time period of 90 seconds was used, leading to an insertion rate of 0.158 $/sec, which is only one-third the value used on page 28 of CRWMS M&O (1997c).

Events capable of producing faster insertion rate have been conceptualized. For example, the re-shuffling of the fuel by a seismic event was considered a plausible scenario, but it was not used as a model for transient criticality because there was no physically possible shuffled configuration that produced a significant increase in k_{eff}. These preliminary analyses have not been published, but will be documented as part of the License Application.

4.2 SLOW INSERTION RATE RESULTS

It should be noted that changes do not generally take place rapidly in nature; the accumulation of water or the removal of neutron absorber would be expected to take place so slowly that only a steady-state criticality would result. The hypothetical conditions discussed above leading to transient criticality are quite improbable.

For sufficiently slow events, where the Doppler and bulk void reactivity feed back effects can terminate the criticality event without large void generation due to boiling, the exit area has little effect on the criticality consequences. This non-sensitivity is demonstrated by the criticality event evaluation for the slow insertion rate, 0.0004 \$/sec, with variation of the exit area. The results are shown in Figures 4-1 and 4-2, which give the time dependence of pressure and temperature respectively, for two cases having a large difference in the exit flow area (0.1 cm^2 and 5 cm^2). For both figures, the difference between the two cases with different exit areas is so small as to make the two curves indistinguishable. Not only is there very little difference between the two cases, but the magnitude of the overpressure peak given in Figure 4-1 is only a small fraction of the normal atmospheric pressure (100,000 Pa). It should be noted that the peak flow rates in Figure 4-2 occur slightly later than the peak pressures in Figure 4-1. This is because the high flow rate immediately relieves the high pressure.

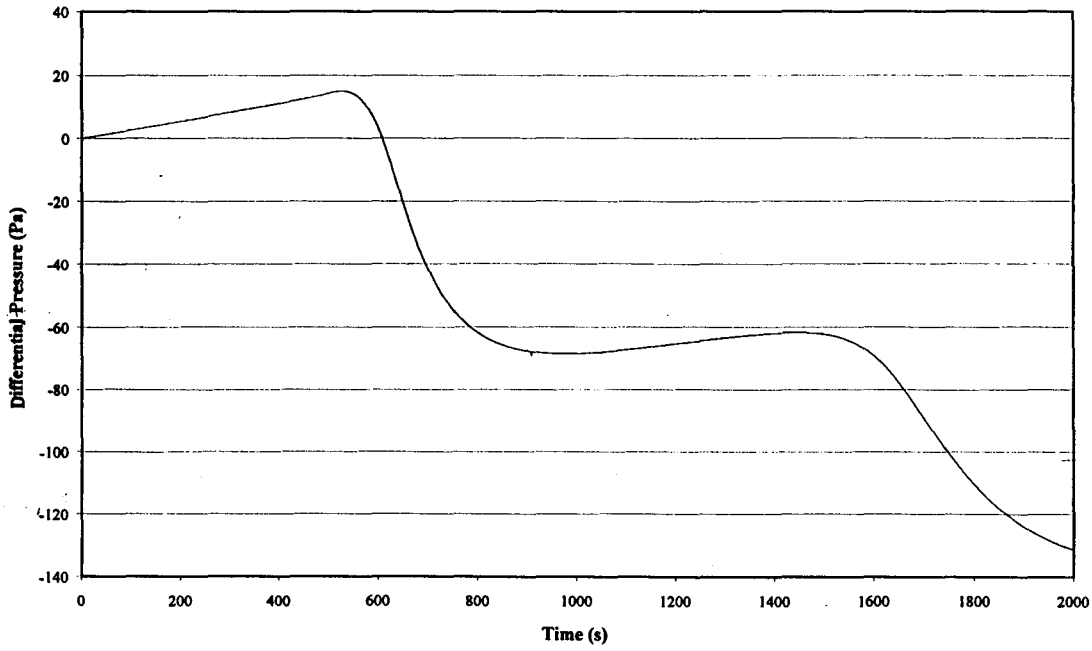

Figure 4-1. Differential Pressure Histories within Waste Package for 0.1 and 5.0 cm^2 Exit Areas and a 0.0004 \$/sec Reactivity Insertion Rate (CRWMS M&O 1999l, Figure 6.2-6)

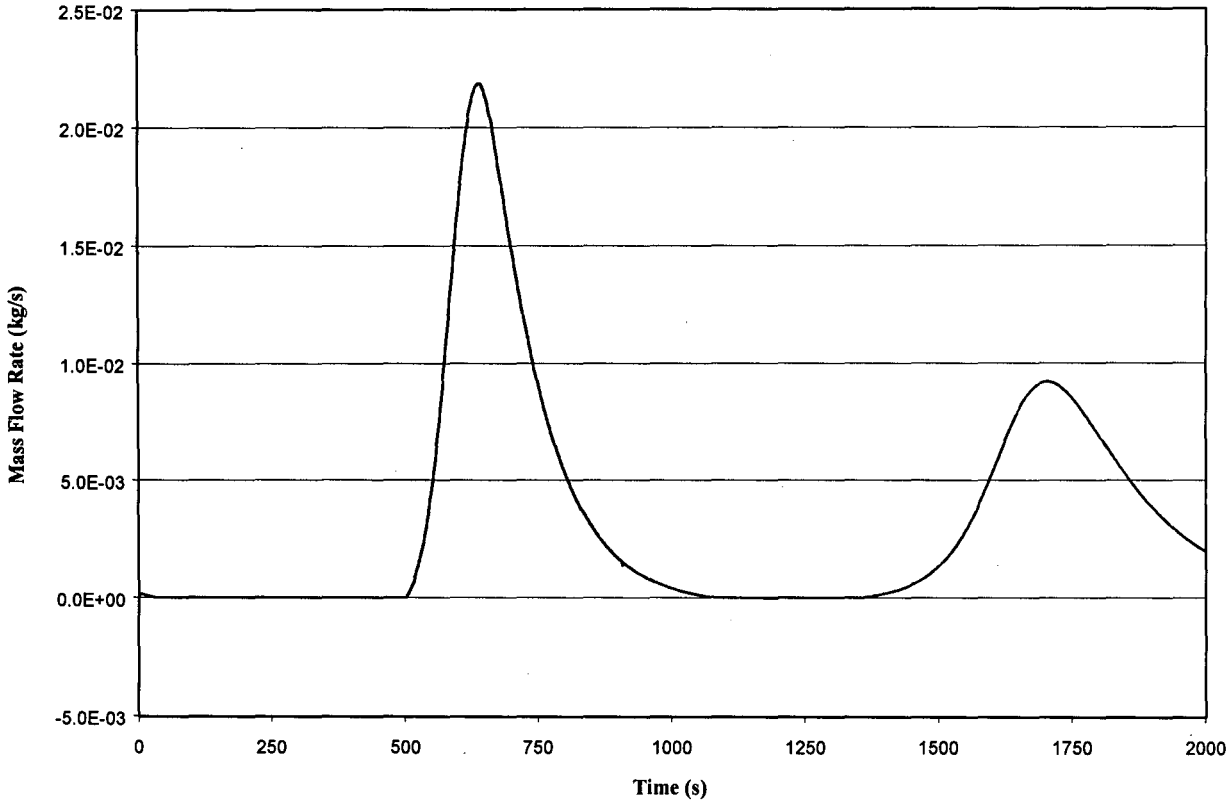

Figure 4-2. Exit Flow Rate for Slow (0.0004 $/sec) Reactivity Insertion Criticality Event for both 0.1 and 5.0 cm^2 Exit Area (CRWMS M&O 1999l, Figure 6.2-5)

4.3 RAPID INSERTION RATE

In contrast to the slow reactivity insertion, the rapid reactivity insertion does show significant sensitivity to the magnitude of the exit area. This is shown by the plots of overpressure as a function of time for a family of 6 different exit areas shown in Figure 4-3. Restrictions of exit flow forces the system to higher pressures and temperatures to compensate for the excess reactivity through Doppler and void reactivity mechanisms. Ultimately, the loss of mass to the drift region will cause the negative void reactivity to bring the waste package back below critical. The loss of mass is shown in Figure 4-4. As with the slow insertion rate, the peak flow rates are seen to occur slightly after the peak pressure.

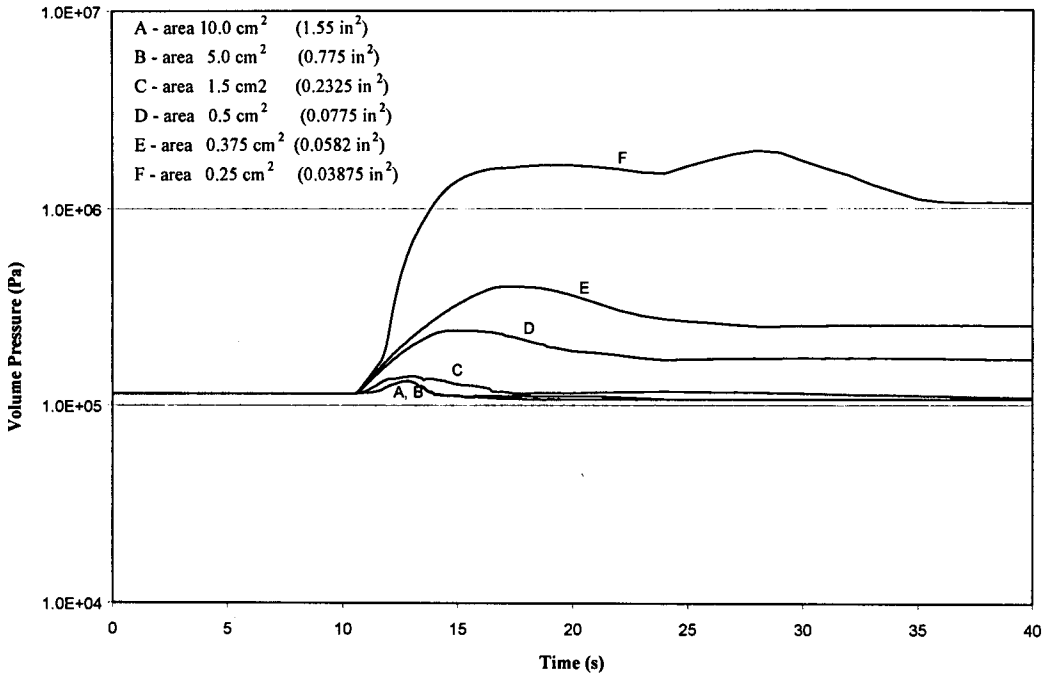

Figure 4-3. Waste Package Internal Pressure for a Range of Exit Areas for the High Insertion Rate (0.158 $/sec) (CRWMS M&O 1999l, Figure 6.1-3)

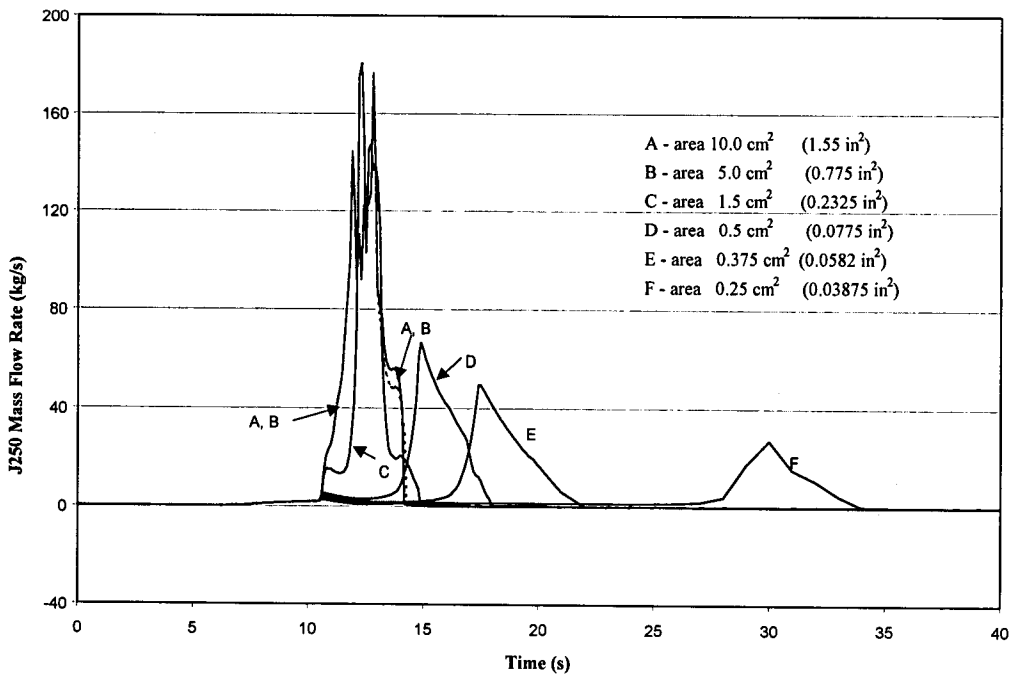

Figure 4-4. Waste Package Exit Mass Flow Rate Histories for the High (0.158 $/sec) Reactivity Insertion Rate Parameterized by Exit Area (CRWMS M&O 1999l, Figure 6.1-9)

The effects of exit area shown in Figure 4-3, are most conveniently summarized by tabulations of temperature and overpressure peaks in Table 4-1 (CRWMS M&O 1999l). To further illustrate the exit area dependence, the overpressure peaks are plotted as a function of exit area in Figure 4-5.

Table 4-1. Maximum Temperature and Pressure Values for 0.158 $/sec Reactivity Insertion Rate

Exit Area (cm^2)	Temperature		Pressure	
	(K)	(F)	(Pa)	(psi)
10.0	437.3	327.5	1.326E+05	19.2
5.0	437.3	327.5	1.326E+05	19.2
1.5	437.3	327.5	1.405E+05	20.4
0.5	437.4	327.7	2.399E+05	34.8
0.375	440.5	333.2	4.005E+05	58.1
0.25	505.9	451.0	1.951E+06	283.0

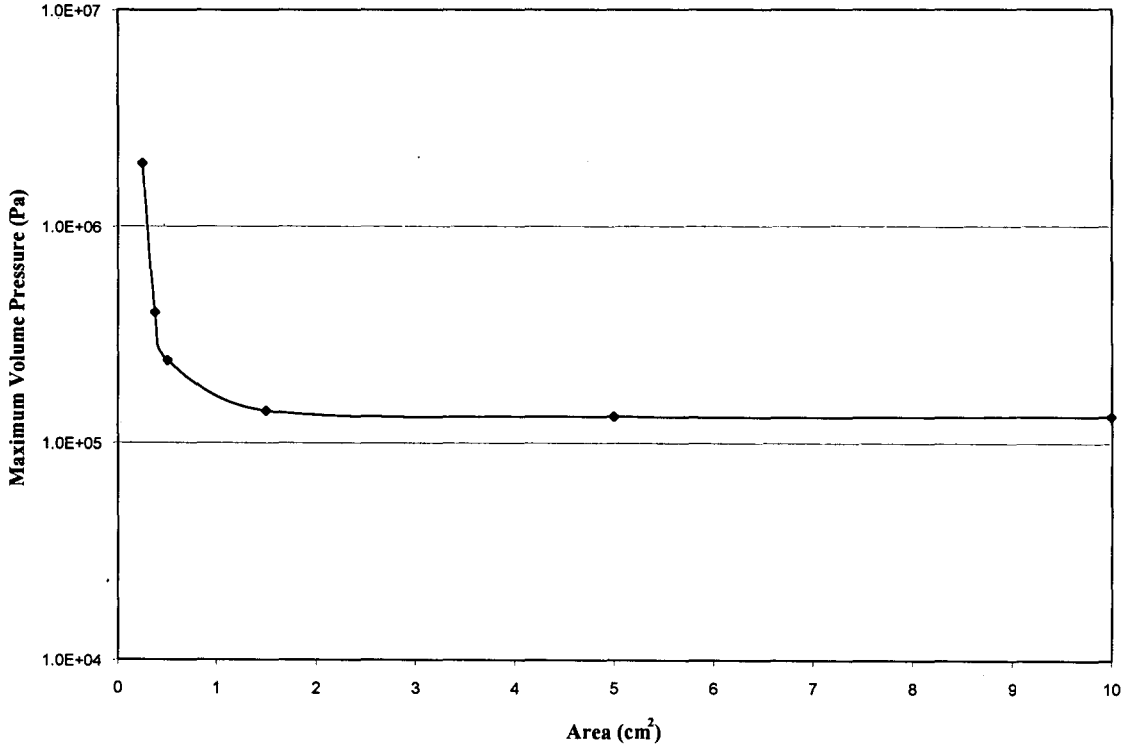

Figure 4-5. Peak Internal Pressure as a Function of Exit Area for the Rapid Insertion Rate of (0.158 $/sec) (CRWMS M&O 1999l, Figure 6.1-1)

The maximum overpressure is approximately 13 times normal atmospheric pressure of 100,000 Pa. This is less than the pressure experienced in the reactor, so it is unlikely to cause damage to the fuel pins. Of course, Figure 4-5 also suggests that decreasing the exit area below 0.25 cm^2 will result in still higher peak overpressures. However, future calculations are expected to show that the probability of criticality will decrease with decreasing exit area, at a rate that is faster than the increase in peak overpressure, so that the overpressure risk (which is the product of probability and magnitude of peak overpressure) will show a net decrease with decreasing exit area.

5. CONCLUSIONS

The methodology for evaluating criticality potential for high-level radioactive waste and spent nuclear fuel after the repository is sealed and permanently closed is described in the *Disposal Criticality Analysis Methodology Topical Report* (DOE 1998b). The topical report provides a process for validating various models that are contained in the methodology and states that validation will be performed to support License Application. The *Supplement to the Disposal Criticality Analysis Methodology* provides a summary of data and analyses that will be used for validating these models and will be included in the model validation reports. The supplement also summarizes the process that will be followed in developing the model validation reports. These reports will satisfy commitments made in the topical report, and thus support the use of the methodology for Site Recommendation and License Application.

It is concluded that this report meets the objective of presenting additional information along with references that support the methodology presented in the topical report and can be used both in validation reports and in answering request for additional information received from the Nuclear Regulatory Commission concerning the topical report. The data and analyses summarized in this report and presented in the references are not sufficient to complete a validation report. However, this information will provide a basis for several of the validation reports.

Data from several references in this report have been identified with TBV-1349. Release of the TBV governing this data is required prior to its use in quality affecting activities and for use in analyses affecting procurement, construction, or fabrication. Subsequent to the initiation of TBV-1349, DOE issued a concurrence letter (Mellington 1999) approving the request to identify information taken from the references specified in Section 1.4 as "accepted data".

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APPENDIX A: ACRONYMS AND ABBREVIATIONS

AENCF	Average Energy of Neutrons Causing Fission
BNL	Brookhaven National Laboratory
BWR	Boiling Water Reactor
CASMO	Name of a computer program
CDF	Cumulative Distribution Function
CE	Combustion Engineering
CL	Critical Limit
CRC	Commercial Reactor Critical
CRWMS	Civilian Radioactive Waste Management System
CSAS1X	Name of a computer program, part of SCALE
DOE	Department of Energy
Gd_2O_3	Gadolinium Oxide
JPDR	Japan Power Demonstration Reactor
K	Kelvin
LCE	Laboratory Critical Experiment
M&O	Management and Operating Contractor
MCNP	Name of a computer program
NRC	Nuclear Regulatory Commission
ORNL	Oak Ridge National Laboratory
pdf	Probability Distribution Function
PWR	Pressurized Water Reactor
QAP	Quality Administrative Program
QARD	Quality Assurance Requirement and Description
ORIGEN-S	Name of a computer program, part of SCALE
RSIC	Radiation Shielding Information Center
SAS2H	Name of a computer program, part of SCALE
SCALE	Name of a computer program
SNF	Spent Nuclear Fuel
TSPA	Total System Performance Assessment
VA	Viability Assessment

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APPENDIX B: GLOSSARY

Average energy of neutrons causing fission (AENCF) is the average of the energies at which neutrons cause fission.

Burnup is the amount of exposure a nuclear fuel assembly receives, in a power production mode, expressed in units of gigawatt days per metric ton of uranium (GWd/mtU) initially loaded into the assembly.

Burnup credit is an approach used in criticality evaluations, which accounts for the reduction in criticality potential associated with spent nuclear fuel relative to that of fresh fuel. Burnup credit reflects the net depletion of fissionable isotopes and the creation of neutron absorbing isotopes during reactor operations. Burnup credit also accounts for variations in the criticality potential of spent nuclear fuel produced by radioactive decay since the fuel was discharged from a reactor. For geologic disposal, burnup credit (if accepted by the NRC) will account for the reduction in reactivity associated with 29 isotopes (Principal Isotopes) from commercial light water reactor spent nuclear fuel. This credit applies specifically to the ceramic form of commercial spent nuclear fuel.

Configuration is the relative disposition of the parts or elements of a scenario.

Configuration class is a set of similar configurations whose composition and geometry is defined by specific parameters that distinguish one class from another. Within a class the configuration parameters may vary over a given range.

Critical limit is a limiting value of k_{eff} at which a configuration is considered potentially critical, as characterized by statistical tolerance limits.

Criticality analysis is a mathematical estimate, usually performed with a computer, of the neutron multiplication factor of a system or configuration that contains material capable of undergoing a self-sustaining chain reaction.

Cross section is the extent to which neutrons interact with nuclei. It is the proportionality factor that relates the rate of a specified nuclear reaction to the product of the number of neutrons per second impinging normally onto a unit area of a thin target and the number of target nuclei per unit area.

Cumulative distribution function (CDF) is a function that gives the probability that a random variable (representing some physical parameter) is less than the value of the argument of the function.

Disposal is the isolation of radioactive wastes from the accessible environment (10 CFR 60.2). Disposal means the emplacement in a repository of high-level radioactive waste, spent nuclear fuel, or other highly radioactive material with no foreseeable intent of recovery, whether or not such emplacement permits the recovery of such waste (10 CFR 961.11) Nuclear Waste Policy Amendment (NWPA Section 2[9]).

Enrichment is the weight-percentage of ^{233}U or ^{235}U in uranium, or ^{239}Pu in plutonium.

Fissile materials are those materials which will fission with slow neutrons (e.g., ^{235}U, ^{239}Pu).

Fissionable materials are those materials, which will fission if neutrons have enough energy. Note all fissile materials are fissionable, but not all fissionable materials are fissile. "Fissionable" is used in most places in this report instead of "fissile," although fissile may be applicable for most configurations from commercial SNF.

Geologic repository is a system which is intended to be used for, or may be used for, the disposal of radioactive wastes in excavated geologic media. A geologic repository includes (1) the geologic repository operations area, and (2) the portion of the geologic setting that provides isolation of the radioactive waste (10 CFR 60.2).

Insertion rate is the rate of change in reactivity, which is defined as the fractional change in k_{eff} divided by the delayed neutron fraction, per unit time.

k_{eff} is the effective neutron multiplication factor for a system. It provides a measure of criticality potential for a system ($k_{eff} = 1.0$ for criticality).

Methodology, as used in this document, refers to the systematic procedures proposed to evaluate the risk of criticality in the repository. Specific computer programs and mathematical procedures are not part of the methodology, but rather are tools used to execute individual procedures in the methodology.

Moderating material is material that "slows down," or lowers the energy state of neutrons.

Over-moderated is a state of a system in which removing moderating material increases the reactivity of the system, while adding moderator decreases the reactivity of the system.

Postclosure means the period of time after the permanent closure of the geologic repository.

Probability density function (pdf) is a function that is used to compute the probability that a random variable (representing some physical parameter) falls within an interval specified by the argument of the function and a multiplier specifying the length of interval in units of the argument of the function. The probability in question is the product of the probability density function and the interval multiplier. The probability density function has the units of reciprocal of its argument, and it is computed as the derivative of the cumulative distribution over the range of argument for which the cumulative distribution function is continuous.

Reactivity is the relative deviation of the neutron multiplication factor of the system from unity (i.e., reactivity = $(k_{eff} - 1)/k_{eff}$). Reactivity is dimensionless, and the units are usually referred to as $.

Repository is any system licensed by the U.S. Nuclear Regulatory Commission that is intended to be used for, or may be used for, the permanent deep geologic disposal of high-level radioactive waste and spent nuclear fuel, whether or not such system is designed to permit the recovery, for a limited period during initial operation, of any materials placed in such system. Such term includes both surface and subsurface areas at which high-level radioactive waste and spent nuclear fuel handling activities are conducted (NWPA 1987).

Risk is the product of the probability of a given process or event and a measure of its consequences.

Spectral parameter is a neutronic parameter that provides an index that may be used to characterize a neutron in system.

Spent nuclear fuel (SNF) is fuel which has been withdrawn from a nuclear reactor following irradiation, the constituent elements of which have not been separated by reprocessing. (Specifically in this document, SNF includes (1) intact, non-defective fuel assemblies; (2) failed fuel assemblies in canisters; (3) fuel assemblies in canisters; (4) consolidated fuel rods in canisters; (5) non-fuel assembly hardware inserted in PWR fuel assemblies, including, but not limited to, control rod assemblies, burnable poison assemblies, thimble plug assemblies, neutron source assemblies, instrumentation assemblies; (6) fuel channels attached to boiling water reactor fuel assemblies; and (7) non-fuel assembly hardware and structural parts of assemblies resulting from consolidation in canisters.) (NWPA Section 2(23)) (10 CFR 961.11) The specific types of SNF discussed in the disposal criticality analysis methodology include:

> **Intact (Waste form or fuel)**. Retaining the initial geometry and chemical composition (except for radioactive decay).
>
> **Degraded (Waste form or fuel)**. Material that was initially part of a waste form/fuel that is no longer intact. The spectrum of such material ranges from intact fragments of partially degraded waste forms/fuel to elements in solution to elements in minerals that have precipitated (either interior or external to the waste package). Except for the intact fragments, this material is more specifically referred to as degradation products.
>
> **Degradation product**. Material that was part of a waste form, but has become part of a solution or a precipitate.

Steady-state criticality is a criticality event that is stable or maintained over a long period of time as nearly time-independent.

Transient criticality is a criticality event that is time-dependent.

Under-moderated is a state of a system in which adding moderating material increases the reactivity of the system, while removing moderating material decreases the reactivity of the system.

Waste form is the radioactive waste materials and any encapsulating or stabilizing matrix (10 CFR 60.2). A loaded multi-purpose canister is a canistered waste form. (YMP 1998)

Waste package means the waste form and any containers, shielding, packing and other absorbent materials immediately surrounding an individual waste container (10 CFR 60.2).

Waste package degradation model (WAPDEG) is the model developed as part of the total system performance assessment process to predict the degradation of waste packages.