OCRWM	MODEL COVER SHEET	1. QA: QA Page 1 of 84

2. Type of Mathematical Model:

☒ Process Model ☐ Abstraction Model ☐ System Model

Describe Intended Use of Model:

To provide a process for evaluating the criticality potential of configurations of fissionable materials.

3. Title:

Criticality Model Report

4. DI (including Rev. No. and Change No., if applicable):

MDL-EBS-NU-000003 REV 01 ICN 01

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ENCLOSURE 2

2. Title:

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3. DI (including Rev. No. and Change No., if applicable):

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4. Revision / Change Number:	5. Description of Revision/Change:
00	Initial Issue
00 / 01	Entire document modified for formatting, style, and editorial corrections. Changed lines are indicated by vertical lines in the margin.
01	Document modified to insert Executive Summary. Sections modified to tie Model Report to Disposal Criticality Analysis Methodology Topical Report (YMP 2003) and to clarify overall process, but no changes made to technical content. Most changes made to Sections 1, 2, 6, and 7. Entire model documentation was revised because changes were too extensive to indicate changed lines with vertical lines in the margin.
01 / 01	Document modified to incorporate comments from DOE AP-6.28Q review. Changed lines are indicated by a black vertical line in the margin. Modifications were made in the following areas: Executive Summary, Sections 1, 2, 3.2, 4.1, 4.2, 4.3, 4.4.1, 4.4.2, 6, 6.2, 7.2.4, 7.3, 9.1, and 9.2. As well as the footer and the Table of Contents.

EXECUTIVE SUMMARY

Disposal Criticality Analysis Methodology Topical Report[1] describes a methodology for performing postclosure criticality analyses within the repository at Yucca Mountain, Nevada. An important component of the methodology is the criticality model. This model report documents the criticality model and its validation. The validation uses current data for pressurized water reactor spent nuclear fuel and provides a validated model that may be updated as additional data becomes available.

The criticality model is to be used for evaluating the criticality potential of configurations of fissionable materials. The criticality model uses the MCNP, Monte Carlo computer code to analyze the geometry and materials that define a configuration, and to calculate the effective neutron multiplication factor (k_{eff}). The criticality model is validated so that the range of applicability covers the various configurations of intact and degraded fuel that could occur in the repository over the preclosure and postclosure time periods.

This model report addresses three open items (13, 15, and 17) from "Safety Evaluation Report for Disposal Criticality Analysis Methodology Topical Report, Revision 0[2]". These open items are as follows:

> Open Item 13: "The DOE should address the types of criticality uncertainties and biases, which is based on ANSI/ANS-8.17, presented by the staff."
>
> Open Item 15: "The DOE is required to include the isotopic bias and uncertainties as part of Δk_c if not included as isotopic correction factors."
>
> Open Item 17: "The DOE should subject the method used for extending the trend to the procedures defined in ANSI/ANS-8.1-1998, C4(a) and C4(b)."

This model report provides a description of the model and validation process, the intended use of the model, the limitations of the model, and a discussion of how the criticality model fits within the overall methodology from *Disposal Criticality Analysis Methodology Topical Report*[1]. This model report also provides a data example of the application.

Based on applicable pressurized water reactor spent nuclear fuel benchmark experiment results, this report concludes that the criticality model is valid for determining criticality potential for the various pressurized water reactor spent nuclear fuel waste package configurations that may exist over time in the repository. This model report recommends that the criticality model be implemented for pressurized water reactor spent nuclear fuel.

---

[1] Yucca Mountain Site Characterization Project 2003. *Disposal Criticality Analysis Methodology Topical Report.* YMP/TR-004Q, Rev. 02D. Las Vegas, Nevada: Yucca Mountain Site Characterization Office. ACC: MOL.20030617.0322. TBV-5072.

[2] Reamer, C.W. 2000. "Safety Evaluation Report for Disposal Criticality Analysis Methodology Topical Report, Revision 0." Letter from C.W. Reamer (NRC) to S.J. Brocoum (DOE/YMSCO), June 26, 2000, with enclosure. ACC: MOL.20000919.0157.

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ACRONYMS

AENCF	average energy of a neutron causing fission
ALF	average lethargy of a neutron causing fission
ANS	American Nuclear Society
ANSI	American National Standards Institute
B&W	Babcock & Wilcox
CC	configuration class applicability
CL	critical limit
CR3	Crystal River Unit 3
CRC	commercial reactor critical
DOE	U.S. Department of Energy
EFPD	effective full power days
EPRI	Electric Power Research Institute
EROA	extension of the range of applicability
LCE	laboratory critical experiment
LUTB	lower uniform tolerance band
MOX	mixed oxide
NDTL	normal distribution tolerance limit
PNL	Pacific Northwest Laboratory
PWR	pressurized water reactor
ROA	range of applicability
ROP	range of parameters
SNF	spent nuclear fuel

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1. PURPOSE

The scope of this model report is to document the criticality model and its validation. The criticality model will be used for evaluating the criticality potential of configurations of fissionable materials within the proposed repository at Yucca Mountain, Nevada. The methodology is applicable to any waste package configuration in the preclosure or postclosure period. The criticality model is a component of the methodology presented in *Disposal Criticality Analysis Methodology Topical Report* (YMP 2003). How the criticality model fits in the overall disposal criticality analysis methodology is illustrated in Figure 1. The specific methodology steps related to the criticality model are highlighted in Figure 1. The criticality model will not provide a direct input to the total system performance assessment for license application. It is to be used as necessary to determine the criticality potential of configuration classes as determined by the configuration probability analysis of the configuration generator model (BSC 2003a).

An example application of the criticality model for potential pressurized water reactor (PWR) waste form configuration classes is provided in Section 7 of this model report. This is shown for example only. Actual applications of the criticality model will be performed on a case-by-case basis dependent upon the results of the configuration generator model (BSC 2003a) application.

The criticality model limitations are as follows:

- Trending parameters characterizing system leakage, spectrum, interstitial poison effects, and benchmark applicability not included in the model.
- Currently, the validation is only applicable to commercial PWR spent nuclear fuel (SNF).

This model report addresses specific Open Items 13, 15, and 17 from "Safety Evaluation Report for Disposal Criticality Analysis Methodology Topical Report, Revision 0" (Reamer 2000, Section 4) which are as follows:

- Open Item 13: "The DOE [U.S. Department of Energy] should address the types of criticality uncertainties and biases, which is based on ANSI/ANS-8.17-1984, presented by the staff." (Addressed in Section 6.2)
- Open Item 15: "The DOE is required to include the isotopic bias and uncertainties as part of Δk_c if not included as isotopic correction factors." (Addressed in Section 6.2.1)
- Open Item 17: "The DOE should subject the method used for extending the trend to the procedures defined in ANSI/ANS-8.1-1998, C4(a) and C4(b)." (Addressed in Section 6.2.1.2)

The activity of developing *Criticality Model Report* is defined in *Technical Work Plan for: Risk and Criticality Department* (BSC 2002).

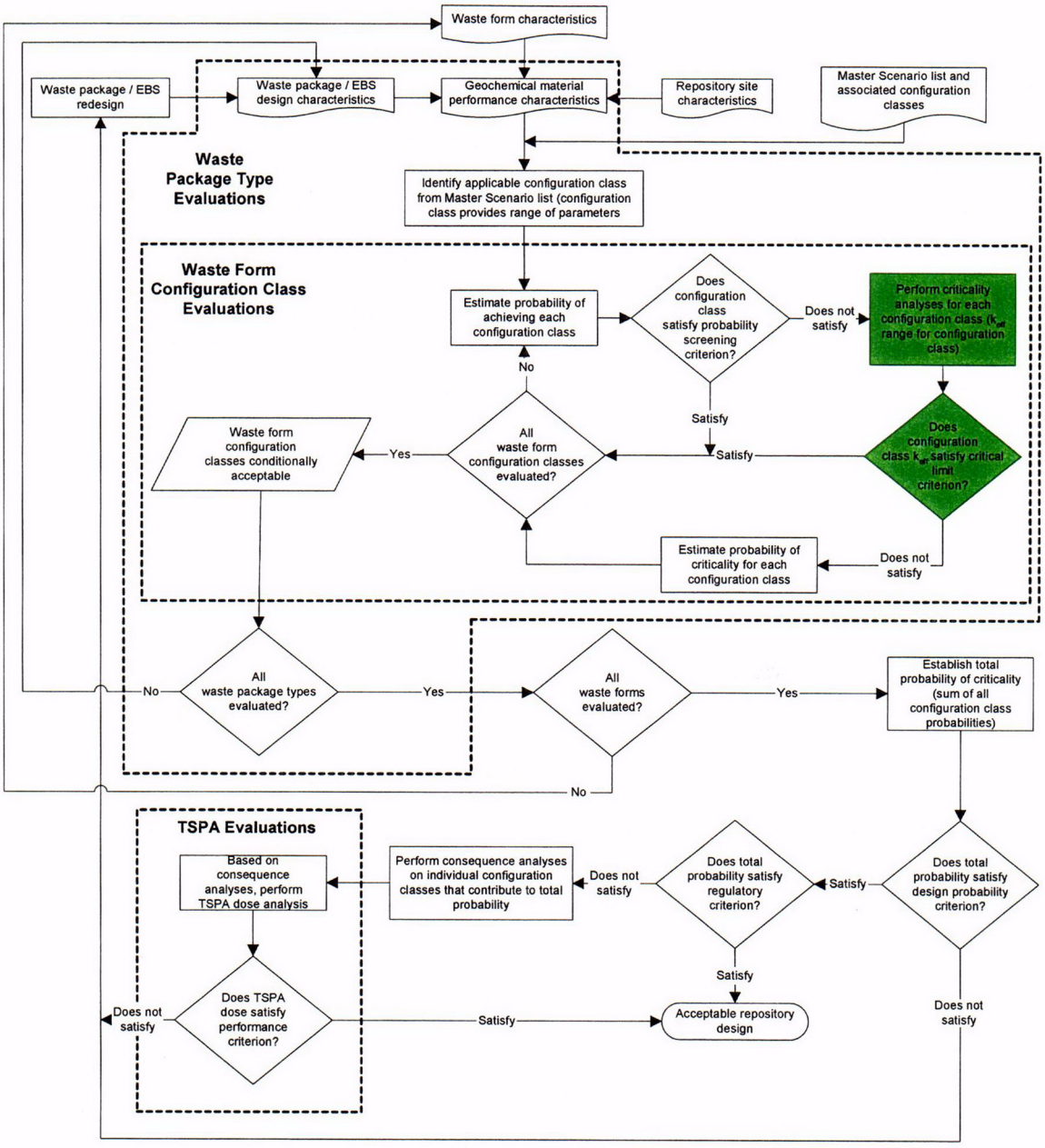


Figure 1. Disposal Criticality Analysis Methodology

2. QUALITY ASSURANCE

Development of this model report and the supporting modeling activities have been determined to be subject to the Yucca Mountain Project's quality assurance program in Section 8 of *Technical Work Plan for: Risk and Criticality Department* (BSC 2002). Approved quality assurance procedures identified in the technical work plan (BSC 2002, Section 4) have been used to conduct and document the activities described in this model report. The technical work plan also identifies the methods used to control the electronic management of data (BSC 2002, Section 8) during the modeling and documentation activities.

This model report concerns engineered barriers that are included in the *Q-List* (YMP 2001) as "Quality Level - 1" items important to waste isolation. The report contributes to the analysis and modeling data used to support performance assessment; however, the conclusions do not directly impact engineered features important to safety, as defined in AP-2.22Q, *Classification Analyses and Maintenance of the Q-List.*

3. USE OF SOFTWARE

This model report references software codes that are used in the supporting calculations and/or analyses, but these software products were not necessarily used in the development of the model itself. The details of the computer software approved for quality affecting work used to generate the results are provided in the various individual documents referenced by this report. The software used or referenced in this report include the following:

3.1 MCNP

The baselined MCNP code (MCNP 4B2LV, CSCI: 30033 V4B2LV) was used in the supporting documentation for k_{eff} calculations. In addition, it was used in this report to duplicate several evaluations documented in Sections 7.1.1 and 7.1.2 to generate output file tally edits for spectral characteristics. The software specifications are as follows:

- Software Title: MCNP
- Version/Revision Number: Version 4B2LV
- Status/Operating System: Qualified/HP-UX B.10.20
- Software Tracking Number: 30033 V4B2LV (Computer Software Configuration Item Number)
- Computer Type: Hewlett Packard 9000 Series Workstations
- Computer Processing Unit number: 700887.

The MCNP software was not used for any k_{eff} calculation in this report, but only for generating edits of fission and absorption rates. The input and output files for the MCNP calculations are documented in Attachment III (Attachment III provides a listing of the files contained on compact disc [Attachment IV]) such that an independent repetition of the software use could be performed.

The MCNP software used was (1) appropriate for the application of k_{eff} calculations, and spectral characteristic calculations, (2) used only within the range of validation as documented throughout *MCNP-A General Monte Carlo N-Particle Transport Code* (Briesmeister 1997) and *Software Qualification Report for MCNP Version 4B2, A General Monte Carlo N-Particle Transport Code* (CRWMS M&O 1998a), and (3) obtained from Software Configuration Management in accordance with appropriate procedures.

3.2 CLREG

The CLREG software code (CLREG. V1.0, STN: 10528-1.0-01) was used to calculate the lower bound tolerance limit for the benchmark experiments included in this report and extend the range of applicability for the critical limit (CL). The software specifications are as follows:

- Software Title: CLREG
- Version/Revision Number: V1.0
- Status/Operating System: Qualified/Windows 2000
- Software Tracking Number: 10528-1.0-01
- Computer Type: DELL OPTIPLEX GX240 Personal Computer
- Computer Processing Unit number: 150527.

CLREG is a computer program that calculates sets of lower bound tolerance limits (lower bound tolerance limit functions) for waste packages under certain conditions. Each lower bound tolerance limit represents the value of k_{eff} at which a configuration is considered potentially critical. This value accounts for the criticality analysis method bias and uncertainty of the calculated k_{eff} values for a set of critical experiments that represent the waste package, as determined by linear regression trending.

The input and output files for the CLREG calculations are documented in Attachment III (Attachment III provides a listing of the files contained on compact disc [Attachment IV]) such that an independent repetition of the software use could be performed. The CLREG software used was: (1) appropriate for the calculation of lower bound tolerance limits, (2) used only within the range of validation as documented in the CLREG documentation (BSC 2001), and (3) obtained from Software Configuration Management in accordance with appropriate procedures.

4. INPUTS

4.1 DATA AND PARAMETERS

No direct input was used in the development of this model. Input sources for the demonstration of the model are listed in Section 4.4.

4.2 CRITERIA

This report complies with the Yucca Mountain Project's quality assurance program as stated in Section 3 of *Technical Work Plan for: Risk and Criticality Department* (BSC 2002), is in accordance with Bechtel SAIC Company, LLC management directives, and in compliance with Bechtel SAIC Company, LLC's Planning and Control Processes Program.

The applicable requirement(s) come from *Project Requirements Document* (Canori and Leitner 2003), and is as follows:

- "The methodology defined in the *Disposal Criticality Analysis Methodology Topical Report* (YMP 2003) shall be used to demonstrate acceptable criticality control for canisters and the waste packages in which they are disposed." (Canori and Leitner 2003, PRD-013/T-016).

Applicable Safety Evaluation Report (Reamer 2000, pp. 77 to 79) open items addressed by this work include numbers 13, 15, and 17, which are as follows:

> Open Item 13: "The DOE should address the types of criticality uncertainties and biases, which is based on ANSI/ANS-8.17-1984, presented by the staff."

Open Item 15: "The DOE is required to include the isotopic bias and uncertainties as part of Δk_c if not included as isotopic correction factors."

Open Item 17: "The DOE should subject the method used for extending the trend to the procedures defined in ANSI/ANS-8.1-1998, C4(a) and C4(b)."

4.3 CODES AND STANDARDS

The following standard(s) are used for the bases of this report:

- ANSI/ANS-8.1-1998. *Nuclear Criticality Safety in Operations with Fissionable Material Outside Reactors.*
- ANSI/ANS-8.17-1984. *Criticality Safety Criteria for the Handling, Storage, and Transportation of LWR Fuel Outside Reactors.*

4.4 INPUT PARAMETERS

4.4.1 Material Cross Sections

Nuclear cross section data are available from several source evaluations (data libraries). Utilizing the appropriate material cross sections in a criticality calculation is essential to obtaining credible results. The cross sections are used to describe the physical interactions of neutrons with the materials of the SNF and waste package as the nuclear chain reaction process is simulated. The MCNP neutron interaction tables are processed from either the ENDF/B-V, ENDF/B-VI, LLNL, LANL:T-2, or LANL:XTM evaluations. The sources for the neutron interaction tables are listed by material in *MCNP-A General Monte Carlo N-Particle Transport Code* (Briesmeister 1997, Appendix G). The cross section evaluations are performed for elements or isotopes at a specific temperature; some evaluations contain evaluations of materials at multiple temperatures. The reason for using multiple temperature cross sections is because not all cross section libraries are available at the benchmark experiment temperatures.

For a particular table, the cross sections for each reaction are given on one energy grid that is sufficiently dense that linear-linear interpolation between points reproduces the evaluated cross sections within a specified tolerance that is generally within 1 percent or less of the evaluated data (Briesmeister 1997, p. 2-18).

Neutron interaction table designations are included as part of the material composition input to MCNP. Each material composition is composed of one or more elements or isotopes designated by a ZAID identifier. The ZAID identifier takes the form "ZZZAAA.nnC" where *ZZZ* represents the atomic number of the element (*ZZZ* may be one or two digits), *AAA* represents the elemental isotope (*AAA* must be three digits incorporating leading zeros), *nn* represents the neutron interaction table designation, and C indicates continuous-energy reaction tables. A more complete description of the ZAID nomenclature is available in *MCNP-A General Monte Carlo N-Particle Transport Code* (Briesmeister 1997, Appendix G).

Calculations involving transport through the resonance region use the most detailed neutron interaction tables available unless there is a valid reason to do otherwise, such as the availability of more appropriate temperature-dependent cross sections. Table 1 contains a listing of elements and isotopes selected and validated for use in the criticality model. The cross section libraries were selected for use in *Selection of MCNP Cross Section Libraries* (CRWMS M&O 1998b). The criteria for the cross sections selected included use of standard versions of ENDF/B (ENDF/B-VI and ENDF/B-V, which contains evaluations at the elevated temperatures found in an operating reactor) whenever possible. It should be noted that the calculations of isotopic concentrations by the isotopic model (BSC 2003b) are performed at elevated reactor temperatures, as are the commercial reactor criticals (CRCs). Calculations using the criticality model for repository applications are performed using room-temperature cross sections since the temperatures for preclosure and postclosure conditions are lower than reactor temperatures, and it is conservative to use the lowest temperature cross section evaluations for the repository environment. The cross section sets selected including elevated reactor temperatures are used in Section 7.1.1 and the cross section sets selected at room temperature are used in Section 7.1.2.

Table 1. Selected MCNP ZAIDs for Various Elements and Isotopes

Element	Isotope	Cross Section Library ZAID[a]	Element	Isotope	Cross Section Library ZAID[a]
Hydrogen	H-1	1001.50c	Barium	Ba-138	56138.50c
	H-2	1002.55c	Praseodymium	Pr-141	59141.50c
	H-3	1003.50c	Neodymium	Nd-143	60143.50c
Helium	He-3	2003.50c		Nd-145	60145.50c
	He-4	2004.50c		Nd-147	60147.50c
Lithium	Li-6	3006.50c		Nd-148	60148.50c
	Li-7	3007.55c	Promethium	Pm-147	61147.50c
Beryllium	Be-7	4007.35c		Pm-148	61148.50c
	Be-9	4009.50c		Pm-149	61149.50c
Boron	B-10	5010.50c	Samarium	Sm-147	62147.50c
	B-10	5010.53c		Sm-149	62149.50c
	B-11	5011.56c		Sm-150	62150.50c
Carbon	C (natural)	6000.50c		Sm-151	62151.50c
	C-12	6012.50c		Sm-152	62152.50c
	C-13	6013.35c	Europium	Eu-151	63151.55c
Nitrogen	N-14	7014.50c		Eu-152	63152.50c
	N-15	7015.55c		Eu-153	63153.55c
Oxygen	O-16	8016.50c		Eu-154	63154.50c
	O-16	8016.53c		Eu-155	63155.50c
	O-16	8016.54c	Gadolinium	Gd-152	64152.50c
	O-17	8017.60c (B-VI.0)		Gd-154	64154.50c
Fluorine	F-19	9019.50c		Gd-155	64155.50c
Sodium	Na-23	11023.50c		Gd-156	64156.50c
Magnesium	Mg (natural)	12000.50c		Gd-157	64157.50c
Aluminum	Al-27	13027.50c		Gd-158	64158.50c
Silicon	Si (natural)	14000.50c		Gd-160	64160.50c
Phosphorous	P-31	15031.50c	Holmium	Ho-165	67165.55c
Sulfur	S (natural)	16000.60c (B-VI.0)	Thulium	Tm-169	69169.55c
	S-32	16032.50c	Hafnium	Hf (natural)	72000.50c
Chlorine	Cl (natural)	17000.50c	Tantalum	Ta-181	73181.50c
Argon	Ar (natural)	18000.59c		Ta-182	73182.60c (B-VI.0)
Potassium	K (natural)	19000.50c	Tungsten	W (natural)	74000.55c
Calcium	Ca (natural)	20000.50c		W-182	74182.55c
	Ca-40	20040.21c		W-183	74183.55c
Scandium	Sc-45	21045.60c (B-VI.2)		W-184	74184.55c
Titanium	Ti (natural)	22000.50c		W-186	74186.55c
Vanadium	V (natural)	23000.50c	Rhenium	Re-185	75185.50c
Chromium	Cr-50	24050.60c (B-VI.1)		Re-187	75187.50c
	Cr-52	24052.60c (B-VI.1)	Iridium	Ir (natural)	77000.55c
	Cr-53	24053.60c (B-VI.1)	Platinum	Pt (natural)	78000.35c
	Cr-54	24054.60c (B-VI.1)	Gold	Au-197	79197.50c
Manganese	Mn-55	25055.50c	Lead	Pb (natural)	82000.50c
Iron	Fe-54	26054.60c (B-VI.1)		Pb-206	82206.60c (B-VI.0)
	Fe-56	26056.60c (B-VI.1)		Pb-207	82207.60c (B-VI.1)
	Fe-57	26057.60c (B-VI.1)		Pb-208	82208.60c (B-VI.0)
	Fe-58	26058.60c (B-VI.1)	Bismuth	Bi-209	83209.50c
Cobalt	Co-59	27059.50c	Thorium	Th-230	90230.60c (B.VI.0)
Nickel	Ni-58	28058.60c (B-VI.1)		Th-231	90231.35c
	Ni-60	28060.60c (B-VI.1)		Th-232	90232.50c
	Ni-61	28061.60c (B-VI.1)		Th-233	90233.35c
	Ni-62	28062.60c (B-VI.1)	Protactinium	Pa-231	91231.60c (B-VI.0)
	Ni-64	28064.60c (B-VI.1)		Pa-233	91233.50c

Table 1. Selected MCNP ZAIDs for Various Elements and Isotopes (Continued)

Element	Isotope	Cross Section Library ZAID[a]	Element	Isotope	Cross Section Library ZAID[a]
Copper	Cu-63	29063.60c (B-VI.2)	Uranium	U-232	92232.60c (B-VI.0)
	Cu-65	29065.60c (B-VI.2)		U-233	92233.50c
Gallium	Ga (natural)	31000.50c		U-234	92234.50c
Arsenic	As-74	33074.35c		U-235	92235.50c
	As-75	33075.35c		U-235	92235.53c
Bromine	Br-79	35079.55c		U-235	92235.54c
	Br-81	35081.55c		U-236	92236.50c
Krypton	Kr-78	36078.50c		U-237	92237.50c
	Kr-80	36080.50c		U-238	92238.50c
	Kr-82	36082.50c		U-238	92238.53c
	Kr-83	36083.50c		U-238	92238.54c
	Kr-84	36084.50c		U-239	92239.35c
	Kr-86	36086.50c		U-240	92240.35c
Rubidium	Rb-85	37085.55c	Neptunium	Np-235	93235.35c
	Rb-87	37087.55c		Np-236	93236.35c
Yttrium	Y-88	39088.35c		Np-237	93237.50c
	Y-89	39089.50c		Np-238	93238.35c
Zirconium	Zr (natural)	40000.60c (B-VI.1)		Np-239	93239.60c (B-VI.0)
	Zr-93	40093.50c	Plutonium	Pu-236	94236.60c (B-VI.0)
Niobium	Nb-93	41093.50c		Pu-237	94237.35c
Molybdenum	Mo (natural)	42000.50c		Pu-238	94238.50c
	Mo-95	42095.50c		Pu-239	94239.55c
Technetium	Tc-99	43099.50c		Pu-240	94240.50c
Ruthenium	Ru-101	44101.50c		Pu-241	94241.50c
	Ru-103	44103.50c		Pu-242	94242.50c
Rhodium	Rh-103	45103.50c		Pu-243	94243.60c (B-VI.2)
	Rh-105	45105.50c		Pu-244	94244.60c (B-VI.0)
Palladium	Pd-105	46105.50c	Americium	Am-241	95241.50c
	Pd-108	46108.50c		Am-242m	95242.50c
Silver	Ag-107	47107.60c (B-VI.0)		Am-243	95243.50c
	Ag-109	47109.60c (B-VI.0)	Curium	Cm-241	96241.60c (B-VI.0)
Cadmium	Cd (natural)	48000.50c		Cm-242	96242.50c
Indium	In (natural)	49000.60c (B-VI.0)		Cm-243	96243.35c
Tin	Sn (natural)	50000.35c		Cm-244	96244.50c
Iodine	I-127	53127.60c (T-2)		Cm-245	96245.35c
	I-129	53129.60c (B-VI.0)		Cm-246	96246.35c
	I-135	53135.50c		Cm-247	96247.35c
Xenon	Xe (natural)	54000.35c		Cm-248	96248.60c (B-VI.0)
	Xe-131	54131.50c	Berkelium	Bk-249	97249.60c (B-VI:XTM)
	Xe-134	54134.35c	Californium	Cf-249	98249.60c (B-VI:XTM)
	Xe-135	54135.50c		Cf-250	98250.60c (B-VI.2))
	Xe-135	54135.53c		Cf-251	98251.60c (B-VI.2)
	Xe-135	54135.54c		Cf-252	98252.60c (B-VI.2)
Cesium	Cs-133	55133.50c			
	Cs-134	55134.60c (B-VI.0)			
	Cs-135	55135.50c (B-VI.0)			
	Cs-136	55136.60c (B-VI.0)			
	Cs-137	55137.60c (B-VI.0)			

Source: CRWMS M&O 1998b

NOTE: [a] Information in parentheses "()" for the ENDF/B-VI cross sections indicate release number.

4.4.2 Criticality Benchmark Experiments

Criticality benchmark experiments were selected from a group of experiments that include laboratory critical experiments (LCEs) and CRCs. Numerous references were used as indicated in Section 7 along with descriptions of pertinent information regarding each of the experiments. LCEs are used to validate the criticality model for un-irradiated, fresh fuel in various configurations representative of the range of potential configurations anticipated in the repository. CRCs are used to validate the criticality model for irradiated, burned SNF in an intact lattice geometry. The criticality benchmark experiments that were selected provide a range of enrichments, lattice geometries, and fuel rod spacings typical of commercial PWR fuel in an intact configuration. The LCEs also contain homogeneous solution criticality benchmark experiments that are representative of degraded waste form configurations. These criticality benchmark experiment configurations cover the span of potential configurations possible over time in the repository. The CRCs provide a range of fuel enrichments in actual reactor geometries and conditions. CRCs are described in Section 7.1.1 and LCEs are described in Section 7.1.2. The criticality benchmark experiment sources are technical information and are not direct input data, but used for descriptions of experiment parameters. The rationale for their use is provided in Table 2.

The following sources were used to demonstrate applicability as part of the model validation process. They were used to take previously evaluated benchmark experiment MCNP input cases and add a tally output edit that illustrates the neutron spectral characteristics. The results of these tallies are illustrated in Section 7.3. The MCNP input and output files for the tally calculations are documented in Attachment III (Attachment III provides a listing of the files contained on compact disc [Attachment IV]) such that an independent repetition of the software use could be performed.

- *Waste Package, LCE, CRC, and Radiochemical Assay Comparison Evaluation* (CRWMS M&O 1999b) (cases crc2 and wp2 referred to as crc and wp, respectively in Section 7.3)
- *Laboratory Critical Experiment Reactivity Calculations* (CRWMS M&O 1999c) (case exp22e5 referred to as exp22 in Section 7.3)
- *LCE for Research Reactor Benchmark Calculations* (CRWMS M&O 1999d) (cases ssr48.i and ssr53.i referred to as ssr48 and ssr53, respectively in Section 7.3).

Table 2. Rationale for Use of Experiment Sources

Source	Rationale for Use
Critical Experiments with 4.31 Wt% ^{235}U Enriched UO_2 Rods in Highly Borated Water Lattices (Durst et al. 1982)	Applicable to PWR SNF in waste package configurations
Critical Experiments on 10% Enriched Uranyl Nitrate Solution Using a 60-cm-Diameter Cylindrical Core (Miyoshi et al. 1997)	Applicable to PWR SNF in waste package configurations
Urania-Gadolinia: Nuclear Model Development and Critical Experiment Benchmark (Newman 1984)	Applicable to PWR SNF in waste package configurations
International Handbook of Evaluated Criticality Safety Benchmark Experiments (NEA 1998)	Applicable to PWR SNF in waste package configurations
Analysis of Fresh Fuel Critical Experiments Appropriate for Burnup Credit Validation (ORNL 1995)	Applicable to PWR SNF in waste package configurations
Saxton Plutonium Program, Critical Experiments for the Saxton Partial Plutonium Core (Taylor 1965)	Applicable to PWR SNF in waste package configurations
K Basin Criticality Evaluation for Irradiated Fuel Canisters in Sludge (Wittekind 1992)	Applicable to PWR SNF in waste package configurations
Criticality Experiments with Low Enriched UO_2 Fuel Rods in Water Containing Dissolved Gadolinium (Bierman et al. 1984)	Applicable to PWR SNF in waste package configurations
Criticality Experiments with Subcritical Clusters of 2.35 Wt% and 4.31 Wt% 235U Enriched UO2 Rods in Water with Uranium or Lead Reflecting Walls; Undermoderated Water-to-Fuel Volume Ration of 1.6 (Bierman et al. 1981)	Applicable to PWR SNF in waste package configurations
Critical Separation Between Subcritical Clusters of 2.35 Wt% 235U Enriched UO2 Rods in Water with Fixed Neutron Poisons (Bierman et al. 1977)	Applicable to PWR SNF in waste package configurations
Criticality Experiments with Subcritical Clusters of 2.35 Wt% and 4.31 Wt% 235U Enriched UO2 Rods in Water with Steel Reflecting Walls (Bierman and Clayton 1981)	Applicable to PWR SNF in waste package configurations
Criticality Experiments with Neutron Flux Traps Containing Voids (Bierman 1990)	Applicable to PWR SNF in waste package configurations
Critical Experiments Supporting Close Proximity Water Storage of Power Reactor Fuel (Baldwin et al. 1979)	Applicable to PWR SNF in waste package configurations
Summary Report of Commercial Reactor Critical Analyses Performed for the Disposal Criticality Analysis Methodology (CRWMS M&O 1998c)	Monitored PWR critical systems
Summary Report of Laboratory Critical Experiment Analyses Performed for the Disposal Criticality Analysis Methodology (CRWMS M&O 1999a)	Applicable to PWR SNF in waste package configurations

5. ASSUMPTIONS

None used.

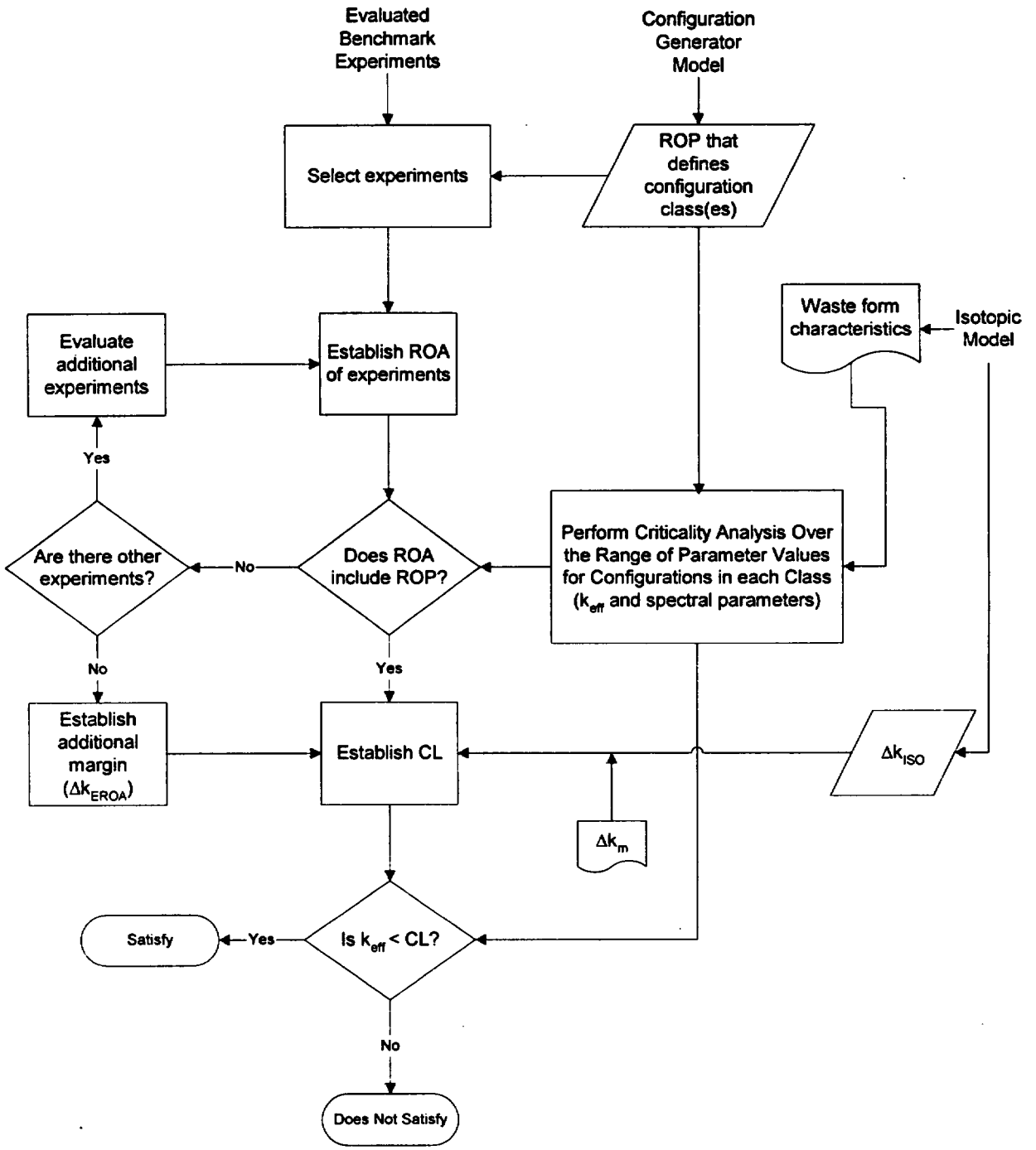
6. MODEL DISCUSSION

The criticality model is the process of establishing criticality potential for configurations of fissionable materials within the proposed repository at Yucca Mountain, Nevada. 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.

An overview of the criticality model is presented in Figure 2. As shown in Figure 2, k_{eff} evaluations are performed over the range of parameters and parameter values for configurations in each class, as determined by the configuration generator model (BSC 2003a). The isotopic model provides information to the criticality model in the form of an isotopic penalty for the CL calculation (Δk_{ISO}) and provides commercial SNF isotopic compositions to the waste form characteristics. Based on benchmark experiment evaluations, a range of applicability is established and an allowable limit (or CL) is calculated for a given configuration class. This CL, which is the value of k_{eff} at which a configuration is considered potentially critical, accounts for the criticality analysis method bias and uncertainty. The range of parameters and parameter values applied to the k_{eff} evaluations are checked against the range of parameters and parameter values that were used in establishing the CL. The process for establishing CL values is discussed in Section 6.1.1. A description of the process for defining the range of applicability of the CL values based on the experimental database used in establishing the CL values is presented in Section 6.1.1.1. A CL is established that is applicable to the range of parameter values that are used in the k_{eff} evaluation(s) so that a comparison can be made to assess the criticality potential of the configuration(s). If the calculated k_{eff} is less than the CL for all configurations within a class, the configuration class is acceptable for disposal. A configuration class with one or more configurations that have calculated k_{eff} values that are greater than or equal to the CL has the potential for criticality.

In this approach, criticality benchmark experiments are selected from a group of experiments that include LCEs and CRC measurements. The selected experiments are used to determine the bias and uncertainty associated with analysis of the experiments. The range of certain physical characteristics of these experiments is used to establish the ROA of the experiments. Acceptance criteria are determined using tolerance limits and margins (where applicable). The term "margin" is used to denote any further reductions in the tolerance limits.



NOTES: Δk_{EROA} = penalty for extending the range of applicability

Δk_{ISO} = penalty for isotopic composition bias and uncertainty

Δk_m = an arbitrary margin ensuring subcriticality for preclosure and turning the CL function into an upper subcritical limit function (it is not applicable for use in postclosure analyses because there is no risk associated with a subcritical event)

Figure 2. Criticality Model Overview

A listing of corroborating/supporting data, models, or information used to complete the model development activities, along with their sources is provided as follows in Table 3.

Table 3. Supporting Information and Sources for Model Development Activities

Description	Source
Overview of Monte Carlo methodology	Briesmeister 1997
Principal isotopes for application	CRWMS M&O 1998d
Disposal criticality analysis methodology	YMP 2003
CRC SNF isotope evaluation	CRWMS M&O 1998c

6.1 COMPUTATIONAL METHOD

The criticality model applies the Monte Carlo simulation method (implemented by MCNP) along with ENDF/B material cross section data in calculating the k_{eff} for potential waste package configurations. The Monte Carlo simulation method for representing neutron transport can best be described by the Neutron Transport Equation shown in Equation 1 (Duderstadt and Hamilton 1976, p. 113).

$$\frac{\partial n}{\partial t} + v\Omega \cdot \nabla n + v\Sigma_t n(r,E,\Omega,t) = \int_{4\pi} d\Omega' \int_0^\infty dE' v' \Sigma_s (E' \rightarrow E, \Omega' \rightarrow \Omega) n(r,E',\Omega',t) + s(r,E,\Omega,t) \quad \text{(Eq. 1)}$$

where (a complete description of all variables is provided by Duderstadt and Hamilton [1976, pp. 103 to 114])

- r = coordinates in space (x, y, z)
- Ω = Θ and Φ
- t = time
- E = energy
- $n()$ = neutron density specification
- $s()$ = neutron source specification
- v = velocity.

MCNP is a general purpose Monte Carlo N-Particle code that can be used for neutron, photon, electron, or coupled neutron/photon/electron transport including the capability to calculate eigenvalues for various systems. The code treats an arbitrary three-dimensional configuration of materials in geometric cells bounded by first- and second-degree surfaces and fourth-degree elliptical tori (Briesmeister 1997, p. ix). The Monte Carlo method is used to theoretically duplicate a statistical process. The individual probabilistic events that comprise a process are simulated sequentially. The probability distributions governing these events are statistically sampled to describe the total phenomenon (Briesmeister 1997, p. 1-3).

The Monte Carlo method allows explicit geometrical modeling of material configurations. The appropriate material cross section data, as described in Section 4.1.1, is used. The accuracy of the Monte Carlo method for criticality calculations is limited only by the accuracy of the material cross section data, a correct explicit modeling of the geometry, and the duration of the computation. The

accuracy of the method and cross section data is established by evaluating critical experiments as shown in Section 7.1.1 (CRCs) and Section 7.1.2 (LCEs).

MCNP calculates three k_{eff} estimates for each cycle in a given problem:

1. The collision estimate
2. The absorption estimate
3. The track length estimate.

A detailed description of the three k_{eff} estimates may be found in *MCNP-A General Monte Carlo N-Particle Transport Code* (Briesmeister 1997, Chapter 2, Section VIII, Part B). The k_{eff} estimate used in the criticality analyses and in the bias value determination is the statistical combination of all three k_{eff} estimates.

6.2 ESTABLISHING CRITICALITY ACCEPTANCE CRITERIA

The acceptance criteria are determined by the final comparison of a configuration's k_{eff} with the applicable CL. This will determine which configuration classes have a potential for criticality. In equation notation the acceptance criteria for a waste package system is as follows:

$$k_S + \Delta k_S < CL \qquad \text{(Eq. 2)}$$

where

k_s = calculated k_{eff} for the system

Δk_s = an allowance for

(a) statistical or convergence uncertainties, or both in the computation of k_s

(b) material and fabrication tolerances, and

(c) uncertainties due to the geometric or material representations used in the computational method

(Note: b and c above can be obviated through the use of bounding representations)

CL = the value of k_{eff} at which a configuration is considered potentially critical, accounting for the criticality analysis method bias and uncertainty, and any additional uncertainties (i.e., Δk_{EROA} and/or Δk_{ISO})

The criticality model provides a means for calculating k_s and Δk_s using the Monte Carlo method and ENDF/B cross section libraries as implemented by MCNP. The criticality model also provides a means for determining the penalty for extending the range of applicability (EROA) (Δk_{EROA}) in the CL calculation, and allows the determination of whether a configuration has the potential for criticality. Additional uncertainty arising from isotopic composition calculations will be propagated to the CL calculation through the isotopic model (BSC 2003b).

6.2.1 Determining the Critical Limit

An essential element of the criticality model used for calculating k_{eff} for a waste form configuration is the determination of the CL. The CL is derived from the bias and uncertainties associated with the criticality code and modeling process. The CL for a configuration class is a limiting value of k_{eff} at

which a configuration is considered potentially critical. The CL is characterized by statistical tolerance limits that account for biases and uncertainties associated with the criticality code trending process, and any uncertainties due to extrapolation outside the range of experimental data, or limitations in the geometrical or material representations used in the computational method.

In equation notation the CL is represented as:

$$CL(x) = f(x) - \Delta k_{EROA} - \Delta k_{ISO} - \Delta k_m \quad \text{(Eq. 3)}$$

where

- x = a neutronic parameter used for trending
- $f(x)$ = the lower bound tolerance limit function accounting for biases and uncertainties that cause the calculation results to deviate from the true value of k_{eff} for a critical experiment, as reflected over an appropriate set of critical experiments
- Δk_{EROA} = penalty for extending the range of applicability
- Δk_{ISO} = penalty for isotopic composition bias and uncertainty
- Δk_m = an arbitrary margin ensuring subcriticality for preclosure and turning the CL function into an upper subcritical limit function (it is not applicable for use in postclosure analyses because there is no risk associated with a subcritical event)

A CL is associated with a specific type of waste package and its state (intact or various stages of degradation described by the Master Scenarios [YMP 2003, Figures 3-2a and 3-2b]). The CL is characterized by a representative set of benchmark criticality experiments. This set of criticality experiments also prescribes the basic range of applicability of the results.

The steps that need to be completed in establishing a CL are as follows: (1) selection of benchmark experiments; (2) establishment of the range of applicability of the benchmark experiments (identification of physical and spectral parameters that characterize the benchmark experiments); (3) establishment of a lower bound tolerance limit; and (4) establishment of additional uncertainties due to extrapolations or limitations in geometrical or material representations.

6.2.1.1 Range of Applicability

In ANSI/ANS-8.1-1998 (p. 1), the term "area of applicability" means "the limiting ranges of material compositions, geometric arrangements, neutron energy spectra and other relevant parameters (such as heterogeneity, leakage, interaction, absorption, etc.) within which the bias of a calculational method is established." The term "area of applicability" and ROA are used interchangeably here.

When evaluating biases and uncertainties and choosing parameters (or areas) for which a bias would exhibit a trend, there are three fundamental areas (Lichtenwalter et al. 1997, p. 179) that should be considered:

1. Materials of the waste package and the waste form, especially the fissionable materials
2. The geometry of the waste package and waste forms
3. The inherent neutron energy spectrum affecting the fissionable materials.

There are substantial variations within each of these categories that require further considerations. These are discussed by Lichtenwalter et al. (1997, p. 180). Quantifying the various categories of parameters is complicated and generally requires approaches that use benchmark experiments that are characterized by a limited set of physical and computed neutron parameters that are then compared with the neutronic parameters of a waste package. In this case, the application is a particular waste package in various forms of degradation as defined by the Master Scenarios (YMP 2003, Figures 3-2a and 3-2b).

In the general practice of characterizing biases and trends in biases, one would first look at those fundamental parameters that might create a bias. That is, what are the main parameters that could be in error and have the most significant effect on the accuracy of the calculation? Important areas for evaluating criticality are the geometry of the configuration, the concentration of important materials (reflecting materials, moderating materials, fissionable materials, and significant neutron absorbing materials), and the nuclear cross sections that characterize the nuclear reaction rates that will occur in a system containing fissionable and absorbing materials.

It is desirable that the range of the fundamental parameters of the benchmark critical experiments (ROA) and the range of the fundamental parameters of the system (ROP) evaluated are identical. This is not usually practical, and for those parameters that do not show a bias, it is acceptable to use critical benchmark experiments that cover most, but not all, of the ROP of the system under evaluation. In these situations, expert judgement may be used to determine if there is a reasonable assurance that the two are sufficiently close.

6.2.1.2 Extension of the Range of Applicability

This section describes a process for extending the ROA. The means used to extend the ROA will depend on a number of factors. Some of these are: 1) the nature of the critical experiments used to determine the ROA and trends with biases; 2) the particular waste form involved; and 3) the availability of other proven computer codes or methods used to evaluate the situation.

The process described in ANSI/ANS-8.1 (1998, p. 18, C4) is used for the extension of the range of applicability:

> The area (or areas) of applicability of a calculational method may be extended beyond the range of experimental conditions over which the bias is established by making use of correlated trends in the bias. Where the extension is large, the method should be:
>
> - Subjected to a study of the bias and potentially compensating biases associated with individual changes in materials, geometries or neutron spectra. This will allow changes, which can affect the extension to be independently validated. In practice, this can be accomplished in a step wise approach; that is, benchmarking for the validation should be chosen (where possible) such that the selected experiments differ from previous experiments by the addition of one new parameter so the effect of only the new parameter, on the bias can be observed.
>
> - Supplemented by alternative calculational methods to provide an independent estimate of the bias (or biases) in the extended area (or areas) of applicability.

If a ROA is extended, where there is a trend in the data, without the use of additional experiments, additional penalty will be added to the acceptance criteria used to determine if a system is critical. The penalty for EROA (Δk_{EROA}), will be subtracted from the lower bound tolerance limit, as part of establishing a CL for a prescribed parameter range. The following techniques for extending the ROA when there are trends may be used to determine the additional penalty: 1) expert judgement (an evaluation by someone skilled, by training and experience, in criticality analysis); 2) sensitivity analysis; 3) statistical evaluation of the importance of these parameters; or 4) comparison with other credible methods (code-to-code comparisons).

For situations where a bias (trend) is not established, there are two options for extending the ROA. If the extension of the ROA is small and the understanding of the performance of the criticality code for these parameter ranges is also understood, it would be appropriate to use the established lower bound tolerance limit and an appropriate penalty. If the extension is not small, then more data, covering the ROA, will be necessary. When more data are obtained, the process of Figure 2 must be applied to the new data set. This applies when the ROA for fundamental parameters (material concentrations, geometry, or nuclear cross sections) does not cover the ROP of the waste package configuration and no trend is exhibited.

6.2.1.3 Lower Bound Tolerance Limit

A lower bound tolerance limit function may be expressed as a regression-based function of neutronic and/or physical variable(s). In application, a lower bound tolerance limit function could also be a single value, reflecting a conservative result over the range of applicability for the waste form characterized.

Geometric modeling and inputs for computing the k_{eff} for a critical experiment with a criticality code often induce bias in the resulting k_{eff} value. Bias is a measure of the systematic differences between the results of a calculational method and experimental data. Uncertainty is a measure of the random error associated with the difference between the calculated and measured result. These k_{eff} values deviate from the expected result ($k_{eff} = 1$) of benchmark sets of critical experiments. The experimental value of k_{eff} for some benchmarks may not be unity (some are extrapolations to critical); however, this value is used for purposes of calculating errors.

The application of statistical methods to biases and uncertainties of k_{eff} values is determined by trending criticality code results for a set of benchmark critical experiments that will be the basis of establishing lower bound tolerance limits for a waste form. This process involves obtaining data on various neutronic parameters that are associated with the set of critical experiments used to model the code-calculated values for k_{eff}. These data, with the calculated values of k_{eff}, are the basis of the calculation of the lower bound tolerance limit function.

The purpose of the lower bound tolerance limit function is to translate the benchmarked k_{eff} values from the criticality code to a design parameter for a waste form/waste package combination. This design parameter is used in acceptance criteria for criticality. The lower bound tolerance limit definition addresses biases and uncertainties that cause the calculation results to deviate from the true value of k_{eff} for a critical experiment, as reflected over an appropriate set of critical experiments.

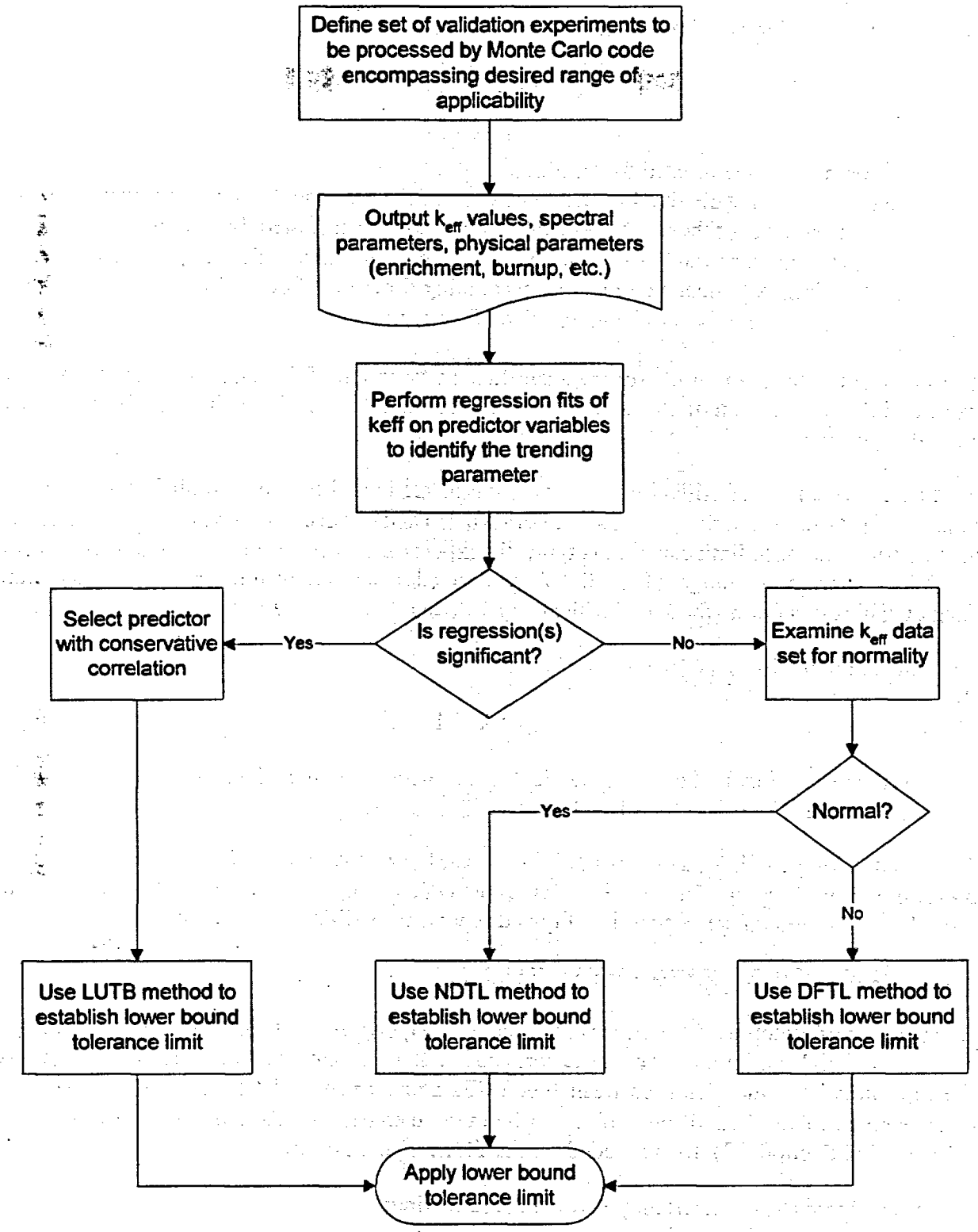
Figure 3 displays two general processes for establishing lower bound tolerance limit functions. These two processes are as follows: (1) regression-based methods reflecting criticality code results over a set of critical experiments that can be trended and (2) random sample based methods that apply when trending is not an appropriate explanation of criticality code calculations.

The regression approach addresses the calculated values of k_{eff} as a trend of neutronic and/or physical parameters. That is, regression methods are applied to the set of k_{eff} values to identify trending with such parameters. The trends show the results of systematic errors or bias inherent in the calculational method used to estimate criticality. In some cases, a data set may be valid, but might not cover the full range of parameters used to characterize the waste form. The area (or areas) of applicability of a calculational method may be extended beyond the range of the experimental conditions of the data set over which the bias is established by making use of correlated trends in the bias.

If no trend is identified, a single value may be established for a lower bound tolerance limit that provides the desired statistical properties associated with the definition of this quantity. The data are treated as a random sample of data (criticality code values of k_{eff}) from the waste form population of interest and straightforward statistical techniques are applied to develop the lower bound tolerance limit. For purposes of differentiation, this technique will be described as "non-trending." The normal distribution tolerance limit (NDTL) method and the distribution-free tolerance limit method, discussed in *Disposal Criticality Analysis Methodology Topical Report* (YMP 2003, Sections 3.5.3.2.8 and 3.5.3.2.9), are "non-trending" methods.

The regression or "trending" methods use statistical tolerance values based on linear regression techniques to establish a lower bound tolerance-limit function. Trending in this context is linear regression of k_{eff} on the predictor variable(s). Statistical significance of trending is determined by the test of the hypothesis that the regression model mean square error is zero (YMP 2003, Section 3.5.3.2.6). Here the predictor variable(s) may be a parameter such as burnup or a parameter that indicates the distribution of neutrons within the system such as the average energy of a neutron that causes either fission or absorption. Where multiple candidates are found for trending purposes, each regression model will be applied and the conservative model may be used to determine the value of the lower bound tolerance limit. The lower uniform tolerance band (LUTB) method, discussed in *Disposal Criticality Analysis Methodology Topical Report* (YMP 2003, Section 3.5.3.2.7), trends a single parameter against k_{eff}. Multiple regression methods that trend multiple parameters against k_{eff} may also be used to establish the lower bound tolerance limit function. In either single or multiple situations, the regression trend that produces the lowest lower bound tolerance limit is defined to be the more conservative regression.

In all calculations of lower bound tolerance limit functions, the concept described as the "no positive bias" (Lichtenwalter et al. 1997, p. 160) rule must be accommodated. This rule excludes benefits for raising the lower bound tolerance limit for cases in which the best estimate of the bias trend would result in a lower bound tolerance limit greater than 1.0. The treatment of this element is discussed below in the context of each method used to establish the basic lower bound tolerance limit function.



NOTES: DFTL = distribution free tolerance limit

Figure 3. Process for Calculating Lower Bound Tolerance Limits

The lower bound tolerance limit function is defined as,

$$f(x) = k_C(x) - \Delta k_C(x) \quad \text{(Eq. 4)}$$

where

x = parameter vector used for trending.

k_C (x) = the value obtained from a regression of the calculated k_{eff} of benchmark critical experiments or the mean value of k_{eff} for the data set if there is no trend.

Δk_C (x) = the uncertainty of k_C based on the statistical scatter of the k_{eff} values of the benchmark critical experiments, accounting for the confidence limit, the proportion of the population covered, and the size of the data set.

The statistical description of the scatter quantifies the variation of the data set about the expected value and the contribution of the variability of the calculation of the k_{eff} values for the benchmark critical experiments.

Based on a given set of critical experiments, the lower bound tolerance limit is estimated as a function (f [x]) of a parameter(s). Because both Δk_C (x) and k_C (x) can vary with this parameter, the lower bound tolerance limit function is typically expressed as a function of this parameter vector, within an appropriate range of applicability derived from the parameter bounds, and other characteristics that define the set of critical experiments.

The calculational bias, β, is defined as

$$\beta = k_C - 1 \quad \text{(Eq. 5)}$$

and thus the uncertainty in the bias is identical to the uncertainty in k_C (i.e., $\Delta k_C = \Delta\beta$). This makes the bias negative if k_C is less than 1 and positive if k_C is > 1.

To prevent taking credit for a positive bias, the lower bound tolerance limit is further reduced by a positive bias adjustment. The positive bias adjustment sets k_C = 1.0 when k_C exceeds 1.0. This provides further assurance of subcriticality and represents additional conservatism.

6.3 DISCUSSION OF UNCERTAINTIES

Due to a lack of prototypic SNF criticality benchmark experiments (LCEs using SNF), and the wide range of potential configurations of waste package internal components over the regulatory period of the repository, a combination of fresh fuel LCEs and burned fuel CRCs are necessary. The establishment of the MCNP code bias can be made using the LCEs and CRCs to provide Δk_c (discussed in Section 7.2) that is needed for the determination of the CL.

Sources and impacts of uncertainty involve the following:

- CRC calculations of k_{eff} are performed at elevated reactor temperatures. However, not all isotopes in the selected MCNP cross section library are available at elevated reactor temperatures, although uranium-235 is available at higher temperatures and so is uranium-

238 which dominates the SNF inventory and resonance absorption. This uncertainty is inherent in the computed code bias.

- An integral benchmark approach is used with regard to CRCs. The calculation of SNF isotopic material compositions produces uncertainty in the calculated SNF inventory that is used as input to MCNP. This uncertainty is accounted for by the isotopic model (BSC 2003b) and is assessed as an additional penalty on the critical limit.

- Additional uncertainty is caused by the water scattering kernel. A scattering kernel is used to adjust cross section data for the effects of molecular bonding, which is particularly important for the hydrogen that is the principal means of slowing down neutrons to thermal energies that can cause fission in SNF. Water at higher-temperatures (i.e., 587 K) will require benchmark cases (CRCs) to use a higher-temperature scattering kernel, while lower-temperature systems (i.e., waste package and LCEs) will use a lower-temperature kernel (i.e., 300 K). In a water-moderated thermal neutron system, higher-temperature scattering results in more energetic scattering reactions, thereby causing the system to have a slightly harder neutron spectrum. This will result in a slightly lower k_{eff} than if using the lower-temperature scattering kernel. Therefore, this uncertainty is accounted for by using the higher-temperature scattering kernel for computations of code bias from the CRCs, but using the lower-temperature kernel for applications in the waste package configurations.

6.4 DISCUSSION OF ALTERNATIVES

Alternative models and alternative code implementations of the Monte Carlo model were considered, as well as alternate nuclear data sets.

6.4.1 Model Alternatives

The Monte Carlo option is not the only means of solving the Neutron Transport Equation (Equation 1). Other solution methodologies include the Discrete Ordinates Method (Duderstadt and Hamilton 1976, pp. 117 to 120) and the Diffusion Theory Method (Duderstadt and Hamilton 1976, pp. 149 to 226). Both of these methodologies have been used successfully in reactor applications. The principal advantage of the Monte Carlo methodology over the Discrete Ordinates Method is that the Monte Carlo approach facilitates solutions in complex geometries like the waste package. Diffusion Theory codes do not work well in the presence of strong neutron absorbers, such as the boron contained in the steel of the waste package basket structure. Thus the Monte Carlo methodology provides the strongest alternative for repository criticality calculations.

6.4.2 Code Alternatives

The Monte Carlo simulation of the Neutron Transport Equation is implemented in a number of different computer codes. MCNP is one of the best known codes and is supported by Los Alamos National Laboratory. An alternative code supported by Oak Ridge National Laboratory is the KENO code, which is part of the SCALE system (CRWMS M&O 2000). KENO is often used by the U.S. Nuclear Regulatory Commission to check calculations for spent fuel casks, as is the British MONK code. The KENO code requires that its nuclear data libraries (typically derivatives of ENDF-B) be prepared explicitly for the type of fuel to be analyzed, because the neutron spectrum of

the fuel is used in the preparation of a compressed form of the nuclear data library. The variable neutron spectra of different fuel configurations under repository conditions would make it difficult to prepare an appropriate KENO library. MCNP and MONK do not require such nuclear data compression. MONK must be purchased via a commercial license, while MCNP is a Department of Energy-supported code. Thus MCNP is the preferred implementation of the Monte Carlo methodology.

6.4.3 Data Set Alternatives

The criticality analysis model that will be applied in evaluating waste package designs for commercial SNF uses a subset of the isotopes present in commercial SNF. The process for establishing the isotopes to be included is based on the nuclear, physical, and chemical properties and the presence of the commercial SNF isotopes in the nuclear data library. The nuclear properties considered are cross sections and half-lives of the isotopes; the physical properties are concentration (amount present in the SNF) and state (solid, liquid, or gas); and the chemical properties are the volatility and solubility of the isotopes. Time effects (during disposal) and relative importance of isotopes for criticality (combination of cross sections and concentrations) are considered in this selection process. None of the isotopes with significant positive reactivity effects (fissionable isotopes or isotopes that are significant moderators or reflectors) are removed from consideration, only non-fissile absorbers that are not significant moderators or reflectors. Thus, the selection process is conservative.

The selection process results in 14 actinides and 15 fission products (referred to as principal isotopes) as the SNF isotopes to be used for burnup credit applications. Table 4 lists these isotopes. The actinide uranium-233 from this table is not present in current generation commercial SNF. However, for long disposal time periods (tens of thousands of years), uranium-233 buildup is sufficient to be a potential criticality concern. Analyses supporting the selection of these isotopes are presented in *Principal Isotope Selection Report* (CRWMS M&O 1998d).

Table 4. Principal Isotopes for Commercial SNF Burnup Credit

^{95}Mo	^{145}Nd	^{151}Eu	^{236}U	^{241}Pu
^{99}Tc	^{147}Sm	^{153}Eu	^{238}U	^{242}Pu
^{101}Ru	^{149}Sm	^{155}Gd	^{237}Np	^{241}Am
^{103}Rh	^{150}Sm	^{233}U	^{238}Pu	^{242m}Am
^{109}Ag	^{151}Sm	^{234}U	^{239}Pu	^{243}Am
^{143}Nd	^{152}Sm	^{235}U	^{240}Pu	

CRCs are used to support the selection of the principal isotopes. This was accomplished by using SNF depleted isotopic inventories calculated using the SAS2H control module of the SCALE code package as discussed in *Summary Report of Commercial Reactor Critical Analyses Performed for the Disposal Criticality Analysis Methodology* (CRWMS M&O 1998c), using reactor operating history data from four different pressurized water reactors: Three Mile Island Unit 1, Crystal River Unit 3, Sequoyah Unit 2, and McGuire Unit 1. The reactor operating history information, pertinent details regarding assembly design schematics, and loading patterns were obtained from several technical reports (CRWMS M&O 1998e; CRWMS M&O 1998f; CRWMS M&O 1998g; CRWMS M&O 1998h). Four different sets of burned fuel isotopes, in addition to oxygen-16, were

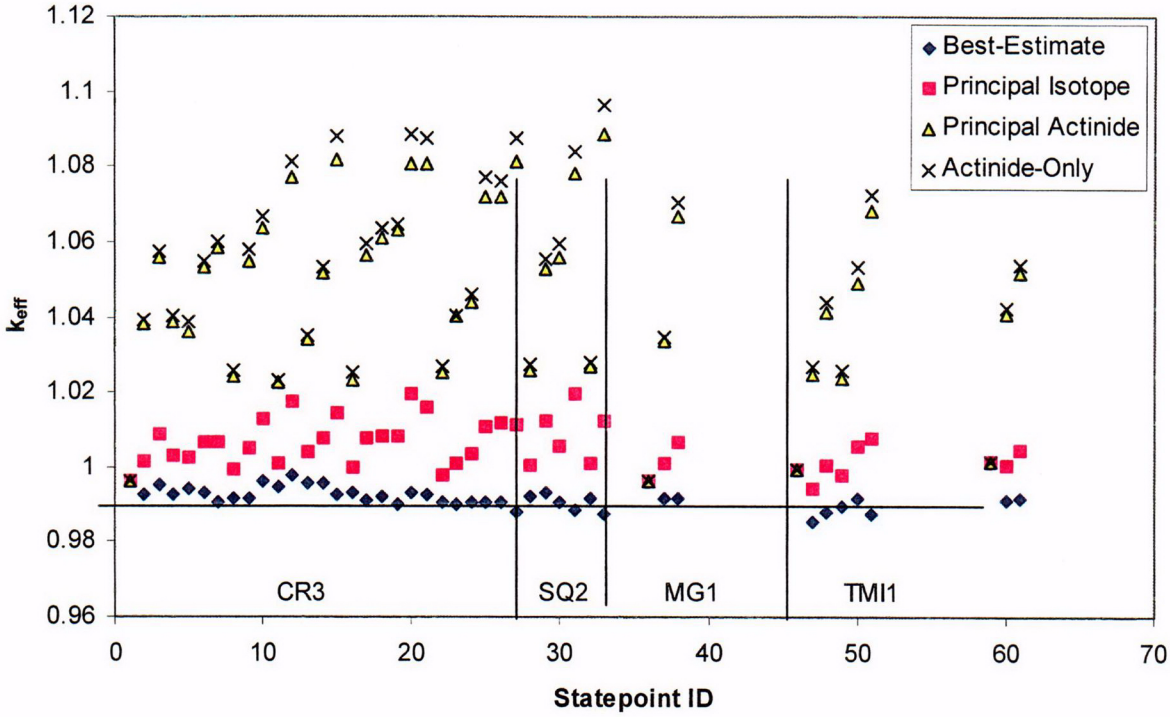
modeled for each of the CRC statepoints: best-estimate (consisting of up to 84 isotopes); principal isotopes (consisting of 29 "most important with respect to reactivity" fission products and actinides); principal actinides (consisting of 14 isotopes from uranium, plutonium, and americium); and actinide only (consisting of 10 major actinide elements found in spent fuel). The isotope sets used are presented in Table 5.

The CRC benchmark cases evaluated cover an initial enrichment range of 1.93 to 4.167 weight percent uranium-235 and an assembly average burnup range of 0 to 49 GWd/MTU. Core average burnups range from 0 GWd/MTU for the beginning of life CRC statepoints to 33 GWd/MTU. Figure 4 illustrates the k_{eff} values from the CRC benchmark results that were taken from *Summary Report of Commercial Reactor Critical Analyses Performed for the Disposal Criticality Analysis Methodology* (CRWMS M&O 1998c, pp. 40 to 43). The results indicate, as expected, that as the number of SNF isotopes modeled increases, the scatter in the k_{eff} data decreases.

Table 5. CRC Fuel Isotopes Set Description

Isotope	Set[a]	Isotope	Set[a]	Isotope	Set[a]	Isotope	Set[a]
H-3	BE	Pd-108	BE	Eu-153	BE, PI	Pu-238	BE, PI, PA, AO
He-4	BE	Ag-107	BE	Eu-154	BE	Pu-239	BE, PI, PA, AO
Li-6	BE	Ag-109	BE, PI	Eu-155	BE	Pu-240	BE, PI, PA, AO
Li-7	BE	Xe-131	BE	Gd-152	BE	Pu-241	BE, PI, PA, AO
Be-9	BE	Xe-134	BE	Gd-154	BE	Pu-242	BE, PI, PA, AO
O-16	BE, PI, PA, AO	Cs-135	BE	Gd-155	BE, PI	Am-241	BE, PI, PA, AO
As-75	BE	Ba-138	BE	Gd-156	BE	Am-242	BE, PI, PA
Kr-80	BE	Pr-141	BE	Gd-157	BE	Am-243	BE, PI, PA
Kr-82	BE	Nd-143	BE, PI	Gd-158	BE	Cm-242	BE
Kr-83	BE	Nd-145	BE, PI	Gd-160	BE	Cm-243	BE
Kr-84	BE	Nd-147	BE	Pa-233	BE	Cm-244	BE
Kr-86	BE	Nd-148	BE	U-233	BE, PI, PA	Cm-245	BE
Y-89	BE	Pm-147	BE	U-234	BE, PI, PA, AO	Cm-246	BE
Zr-93	BE	Pm-148	BE	U-235	BE, PI, PA, AO	Cm-247	BE
Nb-93	BE	Pm-149	BE	U-236	BE, PI, PA, AO	Cm-248	BE
Mo-95	BE, PI	Sm-147	BE, PI	U-237	BE	Xe-135	BE
Tc-99	BE, PI	Sm-149	BE, PI	U-238	BE, PI, PA, AO	Cs-133	BE
Ru-101	BE, PI	Sm-150	BE, PI	Np-235	BE	Ho-165	BE
Ru-103	BE	Sm-151	BE, PI	Np-236	BE	Th-232	BE
Rh-103	BE, PI	Sm-152	BE, PI	Np-237	BE, PI, PA		
Rh-105	BE	Eu-151	BE, PI	Np-238	BE		
Pd-105	BE	Eu-152	BE	Pu-237	BE		

NOTE: [a] BE = best-estimate; PI = principal isotope; PA = principal actinide; AO = actinide only



Source: CRWMS M&O 1998c, pp. 40-43

Figure 4. PWR CRC Eigenvalues

7. VALIDATION

A listing of corroborating/supporting data, models, or information used to complete the model validation activities, along with their sources is provided in Table 6.

Table 6. Supporting Information and Sources for Model Validation Activities

Description	Source
Guidance for validation of a calculational method	ANSI/ANS-8.1-1998
Criticality benchmark experiments	Durst et al. 1982; Miyoshi et al. 1997; Newman 1984; NEA 1998; ORNL 1995; Taylor 1965; Wittekind 1992; Bierman et al. 1984; Bierman et al. 1981; Bierman et al. 1977; Bierman and Clayton 1981; Bierman 1990; Baldwin et al. 1979; CRWMS M&O 1999a
Measured critical systems	CRWMS M&O 1998c
Trending parameters	CRWMS M&O 1999e
Material cross section libraries listed in Table 1	CRWMS M&O 1998d

Validation of the criticality model follows the methodology described in *Disposal Criticality Analysis Methodology Topical Report* (YMP 2003, Section 3.5.3.2), and the guidance given in ANSI/ANS-8.1-1998, *Nuclear Criticality Safety in Operations with Fissionable Material Outside Reactors*. Validation is the process of determining the applicability of a computational method and establishing the bias of the method by using benchmarks appropriate for the intended evaluation of operations. This section is organized as follows: (1) selected benchmark experiments and

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computational results; (2) bias and uncertainty calculation associated with the computer code used to calculate k_{eff} values, and establishment of CLs for given sets of experiments; and (3) criticality acceptance criteria.

Application of the criticality model is in the analyses of configuration classes selected from the Master Scenarios which are discussed in *Disposal Criticality Analysis Methodology Topical Report* (YMP 2003, Figures 3-2a and 3-2b). This report focuses on internal waste package configurations and parameters. The ROP of the waste package configurations chosen should be within the parameter range defined by the ROA of the experiments. If the ROA includes the ROP, the next step would be to establish lower bound tolerance limits, and other margins or penalties as necessary to establish an applicable CL. The term "penalty" is used in conjunction with extension of the ROA. The term "margin" is used to denote further reductions in the lower bound tolerance limits.

Criticality experiments were selected from a group of experiments that include LCEs and CRCs. The selected experiments are used to determine a bias and uncertainty associated with computer code analysis of the experiments. The bias is the deviation of the calculated k_{eff} values from unity. The range of certain physical characteristics of these experiments establish its ROA.

A configuration is defined by a set of parameters characterizing the quantity and physical arrangement of materials at a specific location that have a significant effect on criticality (e.g., fissile materials, neutron absorbing materials, reflecting materials, and moderators). A configuration class is a set of similar configurations whose composition and geometry are defined by specific parameters that distinguish one class from another. Within a class, the configuration parameters may vary over a given range. The configuration classes to be validated for are as follows:

Configuration class IP-1a: For this configuration class, the fissile material separates from the neutron absorber, which remains in place within the waste package. This configuration class can be reached from the standard scenario IP-1 presented in *Disposal Criticality Analysis Methodology Topical Report* (YMP 2003, Figure 3-2a) where the waste form degrades faster than the waste package internal structures. In this configuration class, the neutron absorber is not released from its carrier before the waste form degrades and the fissionable material degrades in place.

Configuration class IP-1b: For this configuration class, the fissile material separates from the neutron absorber, which remains in place within the waste package. This configuration class can be reached from the standard scenario IP-1 presented in *Disposal Criticality Analysis Methodology Topical Report* (YMP 2003, Figure 3-2a) where the waste form degrades faster than the waste package internal structures. In this configuration class, the neutron absorber is not released from its carrier before the waste form degrades and the degraded waste form is mobilized. The mobilized fissionable material accumulates at the bottom of the waste package. A mechanism to mobilize the degraded waste form is needed.

Configuration Class IP-2a: For this configuration class, both the waste package internal structures and the waste form degrade simultaneously. The corrosion product composition is a mixture of fissile material and degradation products from other internal structures. This configuration class can be reached from the standard scenario IP-2 presented in *Disposal Criticality Analysis Methodology Topical Report* (YMP 2003, Figure 3-2a) and will result in

the fissionable material accumulating at the bottom of the waste package. Since both fissionable waste form and waste package internal structures are fully degraded, with all the soluble degradation products removed, the only residual effect of a difference in degradation rates is the nature of any separation between the degradation products of the fissionable waste form and waste package internal structures. Intermediate configurations in which only the basket or the waste form is degraded first are covered by scenario IP-1 (configuration classes IP-1a and IP-1b above), or scenario IP-3 (configuration classes IP-3a, IP-3b, IP-3c, and IP-3d below).

Configuration Class IP-3a: For this configuration class, the waste package internal structures degrade but the waste form remains relatively intact. This configuration class can be reached from the standard scenario IP-3 presented in *Disposal Criticality Analysis Methodology Topical Report* (YMP 2003, Figure 3-2a), and results in an intact waste form at the bottom of the waste package surrounded by, and/or beneath, the degraded corrosion products.

Configuration Class IP-3b: For this configuration class, the waste package internal structures degrade but the waste form remains relatively intact. This configuration class can be reached from the standard scenario IP-3 presented in *Disposal Criticality Analysis Methodology Topical Report* (YMP 2003, Figure 3-2a). This configuration class has the waste package internal basket structure collapsing with the waste form and degradaded corrosion products stratified. Neutron absorbers are flushed from the waste package.

Configuration Class IP-3c: For this configuration class, the waste package internal structures degrade but the waste form remains relatively intact. This configuration class can be reached from the standard scenario IP-3 presented in *Disposal Criticality Analysis Methodology Topical Report* (YMP 2003, Figure 3-2a). This configuration class is characterized by the complete degradation of the basket structure support and neutron absorber plates. The soluble neutron absorber is flushed from the waste package. Two paths that lead to this configuration class apply to the waste package design in which either the basket structural support degrades prior to the neutron absorber plates or the neutron absorber plates degrade prior to the waste package internal structures.

Configuration Class IP-3d: For this configuration class, the waste package internal structures degrade but the waste form remains relatively intact. This configuration class can be reached from the standard scenario IP-3 presented in *Disposal Criticality Analysis Methodology Topical Report* (YMP 2003, Figure 3-2a). The neutron absorbing structure degrades significantly before structural collapse occurs. The absorber separates from the waste form and remains inside the waste package. The waste form and waste package internal structures maintain their integrity.

Configuration Class IP-4a: For this configuration class, the fissile material degrades faster than the waste package internal structures in a flow through geometry and moves away from the neutron absorber, which remains in the waste package. This configuration class can be reached from the standard scenario IP-4 presented in *Disposal Criticality Analysis Methodology Topical Report* (YMP 2003, Figure 3-2b). In this configuration class, the

waste form degrades prior to the neutron absorber being released from its carrier. The fissionable material remains in place to be locked in by its own hydration or by the hydration of waste package internal structures.

Configuration Class IP-4b: For this configuration class, the fissile material degrades faster than the waste package internal structures in a flow through geometry and moves away from the neutron absorber, which remains in the waste package. This configuration class can be reached from the standard scenario IP-4 presented in *Disposal Criticality Analysis Methodology Topical Report* (YMP 2003, Figure 3-2b). This configuration class considers the mobilization of the degraded waste form and its separation from the neutron absorber. The mobilized fissionable material hydrates and collects with other hydrated corrosion products and accumulates at the waste package bottom. A mechanism to mobilize the degraded waste form is needed.

Configuration Class IP-5a: For this configuration class, both the waste package internal structures and waste form have degraded at similar rates. This configuration class can be reached from the IP-5 standard scenario presented in *Disposal Criticality Analysis Methodology Topical Report* (YMP 2003, Figure 3-2b) (i.e., flow-through geometry occurring either prior to or after both waste form and basket degrade and hydrated products collect on the bottom of waste package). Flow-through flushing removes soluble neutron absorbers. This configuration class can also be obtained from degradation scenarios IP-1 or IP-3. IP-1 has the waste form degrading faster than basket and IP–3 has the basket degrading faster than waste form, but ultimately both waste form and other internal components degrade and accumulate on the bottom of the waste package.

Configuration Class IP-6a: For this configuration class, the waste package internal structures degrade faster than the waste form. This configuration class can be reached from the IP-6 standard scenario presented in *Disposal Criticality Analysis Methodology Topical Report* (YMP 2003, Figure 3-2b). The waste form is relatively intact and sitting at the bottom of the waste package surrounded by, and/or beneath, the degraded corrosion products. This configuration class is also obtained from degradation scenario IP-3 where the neutron absorber and waste package basket structure have significantly degraded before the waste package bottom failure.

7.1 CRITICALITY EXPERIMENT SELECTION

The calculation method used to establish the criticality potential for a waste package must be validated against measured data (criticality benchmark experiments). The criticality benchmark experiments must be applicable to the package under consideration. This section provides brief descriptions of the criticality benchmark experiments that have been selected to be utilized for validating the computational method. Since the criticality model is the process of establishing criticality potential for a given ROP of a configuration class established by the configuration generator model, the validation approach presented in this section is to calculate sets of CLs based on different groupings of experiments.

Two types of experimental data are used in the validation: LCEs and CRCs. Various parameters are trended with the k_{eff} values from the LCEs and the CRCs. These trends are used to establish biases and uncertainties of the criticality model.

Guidelines for experiment selection come from Lichtenwalter et al. (1997). Lichtenwalter et al. (1997) states, "There are three fundamental parameters that should be considered in the selection of suitable experiments for use in the evaluation of transportation and storage package designs. They are as follows: (1) geometry of construction; (2) materials of construction (including fissionable material); and (3) the inherent neutron energy spectrum affecting the fissionable material."

With these fundamental parameters in mind, CRCs fulfill each to a degree. The geometry of the waste package configuration and the CRC configuration are similar. Both approximate cylindrical systems and the fuel assembly geometric arrangement is identical when it comes down to lattice, pin pitch, structural materials, cladding, and guide tube positions. Differences arise in the assembly-to-assembly pitch, interstitial materials between assemblies, and moderator and fuel cross section temperature differences. Also, due to the size differences between a reactor pressure vessel and a waste package, a CRC has less neutron leakage than in a waste package.

The fuel assembly material compositions used in the CRC representations are sufficiently similar to the fuel assemblies used in the waste package representations. Both systems contain burned fuel isotopics. Since the waste package is designed to remain subcritical, the materials between assemblies (i.e., borated steel plates in waste package) are different between the waste package and the CRC. These materials cause a reduction in the neutron multiplication factor for the waste package environment.

The reflector and moderator materials are similar for both the CRC and the waste package. PWR CRCs contain borated moderator which is used for additional neutron population control. The moderator-to-fuel ratio is greater in the waste package due to the presence of full-density water. The temperature in the CRC environment is greater than in the waste package environment, which has an effect on Doppler broadening of the resonances and an increase in resonance absorption. Doppler broadening refers to a change in cross section resulting from thermal motion of nuclei in a target material. The end result of these minor differences in the moderator and reflector material compositions produces a small difference in the hydrogen-to-fissile atom (H/X) ratio between the two systems and causes a slight spectral shift.

The CRCs represent intact commercial SNF in known critical configurations. The k_{eff} values obtained from analysis of the CRCs do include any bias from SNF isotopic concentrations of the individual isotopes. Isotopic bias will be addressed as part of the isotopic model validation (BSC 2003b) and incorporated in the CL as described in Section 7.4.

LCEs benchmark the criticality model for a range of fissionable materials, enrichments of fissile isotopes, moderator materials, and absorber materials. The homogeneous LCEs are used to calculate bias and uncertainties for degraded waste forms and configurations where the CRCs are no longer applicable because the fuel assembly geometry has been lost.

7.1.1 CRC Experiments

The CRC k_{eff} values were calculated using the best-estimate isotope set corresponding to those listed in Table 5. Each of the CRC benchmark cases used water scattering kernels corresponding to a temperature of 500 K.

7.1.1.1 Crystal River Unit 3

The Crystal River Unit 3 plant operated by Progress Energy is a Babcock & Wilcox (B&W) PWR with 177 fuel assemblies. The fuel assemblies are the B&W 15x15 design type. A total of 33 CRC experiments have been evaluated for Crystal River Unit 3 where the core thermal power varied between 2452 MWt and 2544 MWt (CRWMS M&O 1998e, pp. 5 and 280-289).

Table 7 provides some general information about the Crystal River Unit 3 CRC experiments. The information includes the average burnup of the core in effective full power days (EFPD), the initial weight percent enrichments of the fuel batches in the core during the CRC experiment (fresh fuel is identified by "[]" around the enrichment values), the down time in days since the core was last at power before restarting, along with the calculated k_{eff} values, sigma (σ), and average energy of a neutron causing fission (AENCF). The pin pitch for the assemblies from this reactor was 1.44272 cm, which results in a moderator-to-fuel volume ratio of 1.7 (CRWMS M&O 1998e, p. 26).

Table 7. General CR3 CRC Statepoint Information

Case	Cycle length to statepoint (EFPD, Cycle)[a]	Initial Enrichments (wt% U-235)[a]	Core Average Burnup (GWd/MTU)[b]	Downtime (d)[a]	k_{eff}[a]	σ[a]	AENCF[c] (MeV)	CC[d]
CR1	0.0 (Cy 1A)	[1.93, 2.54, 2.83]	0.00	0.0	0.99601	0.00043	0.2344	3a, 3b, 3c, 3d
CR2	268.8 (Cy 1B)	1.93, 2.54, 2.83, 2.00	8.09	195.3	0.99285	0.0004	0.2504	
CR3	411.0 (Cy 1B)	1.93, 2.54, 2.83, 2.00	12.34	14.8	0.99502	0.00046	0.2518	
CR4	0.0 (Cy 2)	2.54, [2.64], 2.83	8.67	97.0	0.99282	0.00044	0.2498	
CR5	0.0 (Cy 3)	2.54, [2.62], 2.64, 2.83	7.50	164.0	0.99408	0.00045	0.2489	
CR6	168.5 (Cy 3)	2.54, 2.62, 2.64, 2.83	12.54	16.8	0.99304	0.00045	0.2536	
CR7	250.0 (Cy 3)	2.54, 2.62, 2.64, 2.83	14.98	12.3	0.99073	0.00045	0.2547	
CR8	0.0 (Cy 4)	2.62, [2.62], 2.64, [2.95]	6.92	73.0	0.99134	0.00047	0.2499	
CR9	228.1 (Cy 4)	2.62, 2.64, 2.95	14.00	15.2	0.99152	0.00046	0.2576	
CR10	253.0 (Cy 4)	2.62, 2.64, 2.95	14.77	24.0	0.99603	0.00047	0.2568	
CR11	0.0 (Cy 5)	2.62, 2.64, 2.95, [2.95, 3.29]	7.08	127.0	0.99479	0.00047	0.2475	
CR12	388.5 (Cy 5)	2.62, 2.64, 2.95, 3.29	19.12	5.0	0.99805	0.00045	0.2605	
CR13	0.0 (Cy 6)	2.62, 2.64, 2.95, 3.29, [3.49]	12.01	163.0	0.99561	0.00043	0.2513	
CR14	96.0 (Cy 6)	2.62, 2.64, 2.95, 3.29, 3.49	14.99	168.9	0.99579	0.00047	0.2557	
CR15	400.0 (Cy 6)	2.62, 2.64, 2.95, 3.29, 3.49	24.41	10.4	0.99273	0.00044	0.2612	
CR16	0.0 (Cy 7)	2.54, 2.62, 2.64, 3.29, 3.49, [3.84]	10.02	113.0	0.99324	0.00052	0.2504	
CR17	260.3 (Cy 7)	2.54, 2.62, 2.64, 3.29, 3.49, 3.84	18.09	18.9	0.99083	0.00045	0.2583	
CR18	291.0 (Cy 7)	2.54, 2.62, 2.64, 3.29, 3.49, 3.84	19.04	39.5	0.99222	0.00049	0.2598	
CR19	319.0 (Cy 7)	2.54, 2.62, 2.64, 3.29, 3.49, 3.84	19.91	109.5	0.98993	0.00047	0.2587	
CR20	462.3 (Cy 7)	2.54, 2.62, 2.64, 3.29, 3.49, 3.84	24.35	2.2	0.99321	0.00042	0.2582	
CR21	479.0 (Cy 7)	2.54, 2.62, 2.64, 3.29, 3.49, 3.84	24.87	7.2	0.99247	0.00046	0.2616	

Table 7. General CR3 CRC Statepoint Information (Continued)

Case	Cycle length to statepoint (EFPD, Cycle)[a]	Initial Enrichments (wt% U-235)[a]	Core Average Burnup (GWd/MTU)[b]	Downtime (d)[a]	k_{eff}[a]	σ[a]	AENCF[c] (MeV)	CC[d]
CR22	0.0 (Cy 8)	1.93, 2.62, 3.29, 3.49, 3.84, [3.94]	12.26	99.0	0.99039	0.00043	0.2532	3a, 3b, 3c, 3d
CR23	97.6 (Cy 8)	1.93, 2.62, 3.29, 3.49, 3.84, 3.94	15.27	15.5	0.99021	0.00046	0.2572	
CR24	139.8 (Cy 8)	1.93, 2.62, 3.29, 3.49, 3.84, 3.94	16.58	6.2	0.99063	0.00049	0.2582	
CR25	404.0 (Cy 8)	1.93, 2.62, 3.29, 3.49, 3.84, 3.94	24.74	44.4	0.99054	0.00042	0.2615	
CR26	409.6 (Cy 8)	1.93, 2.62, 3.29, 3.49, 3.84, 3.94	24.91	4.9	0.99067	0.00047	0.2610	
CR27	515.5 (Cy 8)	1.93, 2.62, 3.29, 3.49, 3.84, 3.94	28.19	7.6	0.98772	0.00044	0.2643	
CR28	0.0 (Cy 9)	1.93, 3.84, [3.90], 3.94	14.18	75.0	0.99208	0.00044	0.2546	
CR29	158.8 (Cy 9)	1.93, 3.84, 3.90, 3.94	19.10	2.1	0.99311	0.0005	0.2584	
CR30	219.0 (Cy 9)	1.93, 3.84, 3.90, 3.94	20.96	53.1	0.99078	0.00048	0.2597	
CR31	363.1 (Cy 9)	1.93, 3.84, 3.90, 3.94	25.42	1.6	0.98837	0.00048	0.2635	
CR32	0.0 (Cy 10)	3.84, 3.90, 3.94, [4.167]	15.24	55.0	0.99164	0.00052	0.2558	
CR33	573.7 (Cy 10)	3.84, 3.90, 3.94, 4.167	33.00	16.4	0.98725	0.00048	0.2660	

NOTES: [a] Values are from CRWMS M&O 1998c, pp. 40 and 41
[b] Simple average of statepoint assemblies nodal height weighted averages from CRWMS M&O 1998e, Sections 3 and 4
[c] Values are from CRWMS M&O 1999e, pp. 60, 61, and 64 through 66
[d] CC = configuration class applicability (IP-)

7.1.1.2 Three Mile Island Unit 1

The Three Mile Island Unit 1 plant operated by Exelon Nuclear Corporation is a B&W PWR with 177 fuel assemblies. The fuel assemblies are the B&W 15x15 design type. A total of three CRC experiments have been evaluated for Three Mile Island Unit 1 where the core thermal power was 2535 MWt (CRWMS M&O 1998h, pp. 5 and 65).

Table 8 provides some general information about the Three Mile Island Unit 1 CRC experiments. The information includes the average burnup of the core in EFPD, the initial weight percent enrichments of the fuel batches in the core during the CRC experiment (fresh fuel is identified by "[]" around the enrichment values), the down time in days since the core was last at power before restarting, along with the calculated k_{eff} values, sigma, and AENCF. The pin pitch for the assemblies from this reactor was 1.44272 cm, which results in a moderator-to-fuel volume ratio of 1.7 (CRWMS M&O 1998h, p. 5).

Table 8. General TMI1 CRC Statepoint Information

Case	Cycle length to statepoint (EFPD, Cycle)[a]	Initial Enrichments (wt% U-235)[a]	Core Average Burnup (GWd/MTU)[b]	Downtime (d)[a]	k_{eff}[a]	σ[a]	AENCF[c] (MeV)	CC[d]
TMI1	0.0 (Cy 1)	[2.06, 2.75, 3.05]	0.00	0.0	1.00141	0.00042	0.2353	3a, 3b, 3c, 3d
TMI2	0.0 (Cy 5)	2.64, 2.85, [2.85]	10.33	2,420.0	0.99088	0.00046	0.2476	
TMI3	114.4 (Cy 5)	2.64, 2.85	13.87	32.2	0.99162	0.00048	0.2498	

NOTES: [a] Values are from CRWMS M&O 1998c, p. 41.
[b] Simple average of statepoint assemblies nodal height weighted averages from CRWMS M&O 1998h, Sections 3 and 4.
[c] Values are from CRWMS M&O 1999e, pp. 60, 61, and 64 through 66.
[d] CC = configuration class applicability (IP-).

7.1.1.3 Sequoyah Unit 2

The Sequoyah Unit 2 plant operated by Tennessee Valley Authority Nuclear is a 1148 MWe Westinghouse PWR with 193 fuel assemblies. The fuel assemblies are the Westinghouse 17x17 design type. A total of three CRC experiments have been evaluated for Sequoyah Unit 2 (CRWMS M&O 1998c, p. 29).

Table 9 provides some general information about the Sequoyah Unit 2 CRC experiments. The information includes the average burnup of the core in EFPD, the initial weight percent enrichments of the fuel batches in the core during the CRC experiment (fresh fuel is identified by "[]" around the enrichment values), the down time in days since the core was last at power before restarting, along with the calculated k_{eff} values, sigma, and AENCF. The pin pitch for the assemblies from this reactor was 1.25984 cm, which results in a moderator-to-fuel volume ratio of 1.6 (CRWMS M&O 1998g, p. 7).

Table 9. General SQ2 CRC Statepoint Information

Case	Cycle length to statepoint (EFPD, Cycle)[a]	Initial Enrichments (wt% U-235)[a]	Core Average Burnup (GWd/MTU)[b]	Downtime (d)[a]	k_{eff}[a]	σ[a]	AENCF[c] (MeV)	CC[d]
SQ1	0.0 (Cy 1)	[2.10, 2.60, 3.10]	0.00	0.0	0.99631	0.00043	0.2374	3a, 3b, 3c, 3d
SQ2	0.0 (Cy 3)	2.60, 3.10, 3.50, [3.60, 3.80]	11.11	81.0	0.99158	0.00044	0.2518	
SQ3	210.9 (Cy 3)	2.60, 3.10, 3.50, 3.60, 3.80	19.20	995.7	0.9918	0.00050	0.2555	

NOTES: [a] Values are from CRWMS M&O 1998c, p. 41.
[b] Simple average of statepoint assemblies nodal height weighted averages from CRWMS M&O 1998g, Sections 3 and 4.
[c] Values are from CRWMS M&O 1999e, pp. 60, 61, and 64 through 66.
[d] CC = configuration class applicability (IP-).

7.1.1.4 McGuire Unit 1

The McGuire Unit 1 plant operated by Duke Power Company is a 1129 MWe Westinghouse PWR with 193 fuel assemblies. The fuel assemblies are the Westinghouse 17x17 design type. A total of six CRC experiments have been evaluated for McGuire Unit 1 (CRWMS M&O 1998c, p. 25).

Table 10 provides some general information about the McGuire Unit 1 CRC experiments. The information includes the average burnup of the core in EFPD, the initial weight percent enrichments of the fuel batches in the core during the CRC experiment (fresh fuel is identified by "[]" around the enrichment values), the down time in days since the core was last at power before restarting, along with the calculated k_{eff} values, sigma, and AENCF. The pin pitch for the assemblies from this reactor was 1.25984 cm, which results in a moderator-to-fuel volume ratio between 1.7 and 1.9 (CRWMS M&O 1998f, p. 7).

Table 10. General MG1 CRC Statepoint Information

Case	Cycle length to statepoint (EFPD, Cycle)[a]	Initial Enrichments (wt% U-235)[a]	Core Average Burnup (GWd/MTU)[b]	Downtime (d)[a]	k_{eff}[a]	σ[a]	AENCF[c] (MeV)	CC[d]
MG1	0.0 (Cy 1)	[2.108, 2.601, 3.106]	0.00	0.0	0.99946	0.00045	0.2390	3a, 3b, 3c, 3d
MG2	0.0 (Cy 6)	2.92, 3.204, 3.40, [3.60]	11.67	78.0	0.98541	0.00050	0.2351	
MG3	62.4 (Cy 6)	2.92, 3.204, 3.40, 3.60	14.34	62.7	0.98771	0.00049	0.2375	
MG4	0.0 (Cy 7)	2.92, 3.204, 3.40, 3.60, [3.75]	10.76	130.0	0.98954	0.00047	0.2362	
MG5	129.0 (Cy 7)	2.92, 3.204, 3.40, 3.60, 3.75	16.14	29.6	0.99175	0.00046	0.2388	
MG6	282.3 (Cy 7)	2.92, 3.204, 3.40, 3.60, 3.75	22.54	18.8	0.98723	0.00049	0.2426	

NOTES: [a] Values are from CRWMS M&O 1998c, p. 41.
[b] Simple average of statepoint assemblies nodal height weighted averages from CRWMS M&O 1998f, Sections 3 and 4.
[c] Values are from CRWMS M&O 1999e, pp. 60, 61, and 64 through 66.
[d] CC = configuration class applicability (IP-).

7.1.2 Lattice Laboratory Critical Experiments

The fresh fuel LCEs presented in this section represent moderated lattice configurations containing fissile oxide fuel. Each of the LCE configurations described in this section has been analyzed with the MCNP code system and used a water-scattering kernel corresponding to a temperature of 300 K. An experiment identifier for each benchmark configuration is provided for subsequent reference. The k_{eff}, σ, and AENCF values for each of the LCEs described in the following subsections were taken from Section 4 of *Summary Report of Laboratory Critical Experiment Analyses Performed for the Disposal Criticality Analysis Methodology* (CRWMS M&O 1999a).

In the subsequent tables the P/D term represents the pin pitch to pin outer diameter ratio, the W/F term represents the unit cell moderator-to-fuel volume ratio, and CC indicates configuration class applicability (IP-).

7.1.2.1 Critical Configurations of Subcritical Clusters of 2.35 Weight Percent Enriched UO_2 Rods in Water with Fixed Neutron Absorber Plates

Experiments with subcritical clusters of low-enrichment UO_2 fuel rods were performed at the Pacific Northwest Laboratory (PNL) and documented by Bierman et al. (1977). The four experiments modeled with MCNP consisted of three rectangular arrays of aluminum-clad fuel rods. The fuel rods comprising the arrays had a uniform enrichment of 2.35 weight percent uranium-235 with a 2.032 cm pitch and pellet and cladding outer diameters of 1.12 and 1.27 cm, respectively (Bierman et al. 1977, p. 7). The three arrays of fuel were arranged in a row and, in three of the experiments, sheets of neutron poison were interposed between adjacent arrays. The pertinent differences among these four experiments are shown in Table 11. These critical experiments help demonstrate the ability of MCNP to accurately predict the critical multiplication factor for configurations containing light-water reactor fuel separated by absorber plates.

Table 11. Clusters of 2.35 Weight Percent Uranium-235 Enriched UO_2 Fuel Rods with Different Absorber Plates

Exp ID	Interposed plate	P/D	k_{eff}	σ	AENCF (MeV)	CC
exp1	None	1.81	1.00084	0.00088	0.12095	2a, 3a, 3b, 3c, 3d, 4a
exp2	Boral™	1.81	0.99842	0.00088	0.12469	1a, 1b, 2a, 3a, 3b, 3c, 3d
exp3	Type 6061 Aluminum	1.81	0.99898	0.00089	0.12172	
exp4	Type 304 Stainless Steel	1.81	1.00104	0.00087	0.12003	

7.1.2.2 Water-Reflected Fuel Rod Clusters in Square Pitched Arrays

A series of critical experiments with clusters of aluminum clad UO_2 fuel rods in a large water-filled tank was performed over a period of several years at the Critical Mass Laboratory at PNL. Eight cases were analyzed under this category that correspond to water-reflected clusters at 2.032 cm square pitch with no absorber plates, reflecting walls, dissolved poison, or gadolinium impurity. Table 12 provides a brief description of the experiments which come from *International Handbook of Evaluated Criticality Safety Benchmark Experiments* (NEA 1998, Volume IV, LEU-COMP-THERM-001, p. 10). Each of the experiments used 2.35 weight percent uranium-235 enriched UO_2 fuel with an average loading of 17.08 g of uranium-235 per rod, with pellet and cladding outer diameters of 1.12 and 1.27 cm, respectively (NEA 1998, LEU-COMP-THERM-001, pp. 7 and 21).

Table 12. Water-Reflected Fuel Rod Cluster Critical Experiments

Exp ID	Description number of rods[a] (X x Y), number of clusters, cluster separation	P/D	k_{eff}	σ	AENCF (MeV)	CC
Case 1	20 x 18.08, 1 cluster	1.81	0.99436	0.00167	0.1229	1a, 2a, 3a, 3b, 3c, 3d, 4a
Case 2	20 x 17, 3 clusters, 11.92 ± 0.04 cm separation	1.81	0.99445	0.00158	0.1223	
Case 3[b]	20 x 16, 3 clusters, 8.41 ± 0.05 cm separation	1.81	0.99982	0.00159	0.1200	
Case 4	20 x 16 (center), 22 x 16 (two outer), 3 clusters, 10.05 ± 0.05 cm separation	1.81	0.99313	0.00161	0.1222	
Case 5	20 x 15, 3 clusters, 6.39 ± 0.05 cm separation	1.81	0.99310	0.00169	0.1204	
Case 6	20 x 15 (center), 24 x 15 (two outer), 3 clusters, 8.01 ± 0.06 cm separation	1.81	0.99831	0.00158	0.1221	
Case 7	20 x 14, 3 clusters, 4.46 ± 0.10 cm separation	1.81	0.99261	0.00138	0.1211	
Case 8[c]	19 x 6, 3 clusters, 7.57 ± 0.04 cm separation	1.81	0.99888	0.00151	0.1209	

NOTES: [a] For three-cluster configurations, the first dimension is along the direction of the cluster placement. The second dimension is the width of facing sides, as shown in Figure 5 of NEA 1998, Volume IV, p. 11 LEU-COMP-THERM-001.

[b] The cluster separation referenced was 8.41 cm, but footnote (d) in NEA 1998, Volume IV, LEU-COMP-THERM-001, p. 10, states that the cluster separation should be 0.762 cm less. Thus, 7.648 cm was represented in the MCNP case for the cluster separation.

[c] The cluster separation referenced was 7.57 cm, but footnote (d) in NEA 1998, Volume IV, LEU-COMP-THERM-001, p. 10, states that the cluster separation should be 0.762 cm less. Thus, 6.808 cm was represented in the MCNP case for the cluster separation.

7.1.2.3 Critical Configurations with Subcritical Clusters of 4.31 Weight Percent Enriched UO_2 Rods in Water with Reflecting Walls

Three experiments were performed at PNL and are documented in Bierman et al. (1981) and Bierman and Clayton (1981). In these experiments three similar fuel assemblies were laterally surrounded by reflectors of different compositions. The fuel lattices in each critical experiment contained 4.31 weight percent uranium-235 enriched UO_2 fuel rods on a square pitch of 1.892 cm. The distinguishing characteristics of each experiment are given in Table 13.

Table 13. Clusters of 4.31 Weight Percent Uranium-235 Enriched UO_2 Fuel Rods with Different Reflectors

Exp ID	Reflector	P/D	k_{eff}	σ	AENCF (MeV)	CC
exp5	uranium	1.50	1.00037	0.00107	0.27968	1a, 1b, 2a, 3a, 3b, 3c, 3d, 4a
exp6	lead	1.50	0.99675	0.00103	0.17662	
exp7	stainless steel	1.50	0.99724	0.00111	0.1784	

7.1.2.4 Critical Configurations with 4.31 Weight Percent Uranium-235 Enriched UO_2 Rods in Highly Borated Water Lattices

A set of four experiments was performed at PNL and documented by Durst et al. (1982). These experiments used 4.31 weight percent uranium-235 enriched UO_2 fuel rods arranged in square-pitch, water-moderated lattices of different size with various amounts of boric acid in the moderator. The characteristics of each of these experiments is provided in Table 14.

Table 14. Configurations with 4.31 Weight Percent Uranium-235 Enriched UO_2 Fuel Rods in Highly Borated Water Lattices

Exp ID	Description Pitch, # of Fuel Rods, Moderator	P/D	k_{eff}	σ	AENCF (MeV)	CC
exp8	1.89 cm, 357, non-borated water	1.50	1.00719	0.00110	0.17735	1a, 1b, 3a, 3b, 3c, 3d, 4a, 4b, 5a, 6a
exp9	1.89 cm, 1237, water with 2.55 g/l of boron	1.50	1.00827	0.00099	0.22171	
exp10	1.715 cm, 509, non-borated water	1.36	1.00660	0.00174	0.2239	
exp11	1.715 cm, 1192, water with 2.55 g/l of boron	1.36	1.00358	0.00157	0.26643	

7.1.2.5 Critical Configurations with Neutron Flux Traps

PNL performed experiments studying the effect of neutron flux traps on criticality. These experiments were documented by Bierman (1990) and served as the source for two configurations modeled with MCNP. These two critical experiments were each composed of four fuel rod arrays arranged in a square and separated by a neutron flux trap region. Each fuel lattice in a given configuration was nearly equal in size. The fuel rods were composed of aluminum-clad 4.31 weight percent uranium-235 enriched UO_2 fuel rods with a 1.891 cm pitch. The neutron flux traps were created by positioning two plates of Boral™ between interacting faces of each fuel lattice. The experimental configurations were moderated and closely reflected by full-density water. A brief description of these experiments is provided in Table 15.

Table 15. Configurations with Neutron Flux Traps

Exp ID	Configuration Description	P/D	k_{eff}	σ	AENCF (MeV)	CC
exp12	952 rods arranged in three 15x16 arrays, one 15x15 array, and a 15x15 array with a partial row of 7 rods	1.49	1.00546	0.00108	0.19461	1a, 2a, 3a, 3b, 3c, 3d, 4a, 4b, 5a, 6a
exp13	862 rods arranged in two 14x15 arrays, one 15x15 array, and a 14x15 array with a partial fifteenth row of 7 fuel rods	1.49	1.00371	0.00113	0.19421	

7.1.2.6 Electric Power Research Institute 2.35 Weight Percent Uranium-235 Enriched Light Water Reactor Fuel Critical Configurations

Criticality experiments were sponsored by Electric Power Research Institute (EPRI) for light water reactor fuel configurations. These were documented by EPRI and subsequently described by ORNL (1995, p. 52). Two critical experiment configurations composed of water-moderated lattices of 2.35 weight percent uranium-235 enriched UO_2 fuel rods were modeled with MCNP. The fuel rods were supported in a core structure composed of "eggcrate" type lattice plates with an upper lead shield. The configuration was closely reflected by full-density water laterally and below the fuel. These experiments are shown in Table 16.

Table 16. EPRI 2.35 Weight Percent Uranium-235 Enriched UO_2 Critical Configurations

Exp ID	Description Pitch, # of Fuel Rods	P/D	k_{eff}	σ	AENCF (MeV)	CC
exp14	1.562 cm, 708[a]	1.40	0.99593	0.00099	0.20945	1a, 2a, 3a, 3b, 3c, 3d, 4a
exp15	2.210 cm, 342	1.98	1.00074	0.00087	0.10984	

NOTE: [a] The MCNP representation used 709 rods due to symmetry used in the input specifications.

7.1.2.7 Water-Moderated, Lead-Reflected Uranium Dioxide Rod Array

This case is documented in *International Handbook of Evaluated Criticality Safety Benchmark Experiments* (NEA 1998, Volume IV, LEU-COMP-THERM-027, Sections 1, 2, and 3), and consisted of a 14 x 14 array of 4.74 weight percent uranium-235 enriched UO_2 fuel rods reflected on four sides by 30 cm-thick lead reflectors with no water gap between the array and the lead reflectors. This experiment was denoted as lct27-1 with relevant information listed in Table 17. The experiment was a subcritical approach extrapolated to critical; the neutron multiplication factor reached is within 0.1 percent of 1.000. The experiments were tests of the lead reflector effect.

Table 17. Lead-Reflected UO_2 Rod Array Critical Experiment

Exp ID	Pitch	P/D	k_{eff}	σ	AENCF (MeV)	CC
lct27-1	1.6 cm	2.03	1.0157	0.0005	0.1025	1a, 1b, 2a, 3a, 3b, 3c, 3d, 4a

7.1.2.8 Laboratory Critical Experiments from the Urania-Gadolinia: Nuclear Model Development and Critical Experiment Benchmark Report

A number of critical experiments were performed by B&W for urania fuel incorporating gadolinia as an integral burnable absorber. These experiments were documented in Newman (1984). The configurations modeled with MCNP included critical configurations containing arrangements of 2.46 weight percent uranium-235 enriched UO_2 fuel rods, 4.02 weight percent uranium-235 enriched UO_2 fuel rods, combination 4 weight percent Gd_2O_3 and 96 weight percent (1.944 weight percent uranium-235 enriched) UO_2 fuel rods, Ag-In-Cd absorber rods, and B_4C absorber rods. The central 45 x 45 array of rod lattice cells was separated into nine 15 x 15 arrays of rod lattice cells with a square pitch of 1.636 cm (0.644 in.[Newman 1984, p. 3-1]). The moderator-to-fuel volume ratio was between 2.7 and 3.2 depending on the fuel rod enrichment, which was calculated based on pitch and pellet dimensions from Newman (1984, pp. 3-6 and 3-7). These arrays were intended to simulate pressurized water reactor fuel assembly lattices.

Descriptions of the experimental configurations are provided in Table 18.

Table 18. Urania-Gadolinia Critical Experiments

Exp ID	Description[a]							Mod. Boron Conc. (ppm)	P/D	k_{eff}	σ	AENCF (MeV)	CC
	A	B	C	D	E	F	G						
ugd1	4808	0	0	0	0	0	153	1337.9	1.59	1.00033	0.00143	0.20132	
ugd2	4808	0	0	0	16	0	137	1250.0	1.59	0.99945	0.00145	0.19828	
ugd3	4788	0	20	0	0	0	153	1239.3	1.59	1.00054	0.00147	0.19948	
ugd4	4788	0	20	0	16	0	137	1171.7	1.59	1.00193	0.0015	0.19985	
ugd5	4780	0	28	0	0	0	153	1208.0	1.59	0.99955	0.00154	0.19752	
ugd6	4780	0	28	0	16	0	137	1155.8	1.59	0.99996	0.00152	0.19775	
ugd7	4780	0	28[b]	0	0	0	153	1208.8	1.59	1.0041	0.00148	0.19675	
ugd8	4772	0	36	0	0	0	153	1170.7	1.59	0.99929	0.00154	0.19756	
ugd9	4772	0	36	0	16	0	137	1130.5	1.59	1.00135	0.00156	0.19873	2a, 3a,
ugd10	4772	0	36	0	0	16	137	1177.1	1.59	0.9979	0.00144	0.2011	3b, 3c,
ugd12	3920	888	0	0	0	0	153	1899.3	1.56	0.9994	0.00161	0.20965	3d, 4a
ugd13	3920	888	0	16	0	0	137	1635.4	1.56	1.00049	0.00155	0.20841	
ugd14	3920	860	28	0	0	0	153	1653.8	1.56	1.00066	0.00156	0.20416	
ugd15	3920	860	28	16	0	0	137	1479.7	1.56	1.00158	0.00151	0.2056	
ugd16	3920	852	36	0	0	0	153	1579.4	1.56	1.00335	0.00151	0.20648	
ugd17	3920	852	36	16	0	0	137	1432.1	1.56	0.99912	0.00151	0.20341	
ugd18	3676	944	0	0	0	0	180	1776.8	1.56	0.99876	0.0015	0.20851	
ugd19	3676	928	16	0	0	0	180	1628.3	1.56	1.00133	0.00153	0.21011	
ugd20	3676	912	32	0	0	0	180	1499.0	1.56	1.00322	0.00153	0.20698	

NOTES: [a] Description column designations are as follows:
A - Number of 2.46 weight percent uranium-235 fuel rods
B - Number of 4.02 weight percent uranium-235 fuel rods
C - Number of Gd_2O_3 fuel rods
D - Number of B_4C rods
E - Number of Ag-In-Cd rods
F - Number of void rods
G - Number of water holes.
[b] Annular Gd_2O_3 fuel rods.

7.1.2.9 Saxton UO_2 and PuO_2-UO_2 Critical Configurations

Single- and multi-region uranium and plutonium oxide fueled cores, water moderated, clean, and borated, have been used in a series of critical experiments at the Westinghouse Reactor Evaluation Center in support of the Saxton Plutonium Program. In this series of experiments, criticality was achieved entirely by varying the water level inside the core tank. The fuel used in the experiments were UO_2 fuel with 5.74 weight percent uranium-235 enrichment and mixed oxide (MOX) fuel containing 6.6 weight percent PuO_2 and natural enriched UO_2 (Taylor 1965, p. A-1). This work was documented by Taylor (1965) and subsequently described by ORNL (1995, pp. 52 and 60). This section includes eight single-region configurations and six multi-region configurations. The fuel rod type, pitch, array size, moderator height, and boron concentration were adjusted in each LCE. Table 19 presents a description of the various single-region experiments, and Table 20 presents a description of the multi-region experiments.

Table 19. Saxton Single-Region Critical Configurations

Exp ID	Description	P/D	k_{eff}	σ	AENCF (MeV)	CC
ssr83	Fuel: UO_2; Pitch: 1.3208 cm; Configuration: 449 cylindrical; Critical water height: 95.25 cm	1.46	0.99299	0.00074	0.18197	1a, 2a, 3a, 3b, 3c, 3d, 4a
ssr48	Fuel: UO_2; Pitch: 1.4224 cm; Configuration: 19x19 square; Critical water height: 83.71 cm	1.57	0.9939	0.00071	0.15568	
ssr70	Fuel: MOX; Pitch: 1.3208 cm; Configuration: 22x23 square; Critical water height: 84.56 cm	1.54	0.99543	0.00072	0.2295	
ssr57	Fuel: MOX; Pitch: 1.4224 cm; Configuration: 19x19 square; Critical water height: 82.46 cm	1.66	0.99807	0.00075	0.1938	
ssr27	Fuel: MOX; Pitch: 1.4224 cm; Configuration: 21x21 square; Critical water height: 89.70 cm	1.66	0.99881	0.00082	0.2015	
ssr66	Fuel: MOX; Pitch: 1.8669 cm; Configuration: 13x13 square; Critical water height: 70.11 cm	2.18	1.00308	0.00073	0.1183	
ssr53	Fuel: MOX; Pitch: 2.0117 cm; Configuration: 12x12 square; Critical water height: 78.43 cm	2.35	1.00454	0.00066	0.1065	
ssr74	Fuel: MOX; Pitch: 2.6416 cm; Configuration: 11x11 square; Critical water height: 81.17 cm	3.08	1.00505	0.00068	0.079	

Table 20. Saxton Multi-Region Critical Configurations

Exp ID	Description	P/D	k_{eff}	σ	AENCF (MeV)	CC
smr1	Configuration: 19 x 19 square - 11 x 11 MOX center region, UO_2 outer region; Critical water height: 91.07 cm	1.60	0.99783	0.00073	0.1715	1a, 2a, 3a, 3b, 3c, 3d, 4a
smr9	Configuration: 19 x 19 square - 11 x 11 MOX center region, UO_2 outer region with Al plate at the fuel interface; Critical water height: 92.07 cm	1.60	0.99683	0.00078	0.1673	
smr5	Configuration: 27 x 27 square - 19 x 19 UO_2 center region, MOX outer region; Critical water height: 86.70 cm	1.61	0.99349	0.00073	0.1919	
smr11	Configuration: 27 x 27 square - 19 x 19 MOX center region, UO_2 outer region with water slot at the region boundary; Critical water height: 99.80 cm	1.61	0.99783	0.00078	0.0205	
smr12	Configuration: 27 x 27 square - 19 x 19 MOX center region, UO_2 outer region with Al slab at the interface; Critical water height: 106.35 cm	1.61	0.99992	0.0008	0.2049	
smr8	Configuration: 27 x 27 square - 19 x 19 MOX center region, UO_2 outer region with L shaped UO_2 insert in MOX region; Critical water height: 92.19 cm	1.61	0.99956	0.00068	0.2051	

7.1.2.10 Critical Configurations Simulating Light Water Reactor Fuel in Close Proximity Water Storage

B&W performed experiments simulating neutron multiplication in pool storage racks. These were documented in Baldwin et al. (1979). Nineteen such critical configurations, each containing a 3 x 3 array of 14 x 14 fuel rod assemblies with a square pin pitch of 1.636 cm (0.644 in. [Baldwin et al. 1979, p. 3-3]), were modeled with MCNP. The gaps between assemblies contained a number of B_4C rods and water, stainless steel sheets and water, borated aluminum sheets and water, or only water. The fuel rods were composed of 2.46 weight percent uranium-235 enriched UO_2 clad in Type 6061 aluminum with a diameter of 1.03 cm (Baldwin et al. 1979, p. 8-2). The B_4C rods were aluminum tubes filled with B_4C powder. Six sets of borated aluminum sheets were used in the critical experiments. The soluble boron concentration and moderator heights were adjusted to obtain a critical configuration. The key parameters which distinguish the twenty critical configurations are shown in Table 21.

Table 21. Close Proximity Critical Benchmarks

Exp ID	Description	P/D	k_{eff}	σ	AENCF (MeV)	CC
core2	Assembly spacing (pin pitch): 0; # B_4C rods: 0; Metal between unit assemblies: N/A	1.59	1.00058	0.00159	0.19988	1a, 2a, 3a, 3b, 3c, 3d, 4a
core3	Assembly spacing (pin pitch): 1; # B_4C rods: 0; Metal between unit assemblies: N/A	1.59	1.00019	0.00148	0.18078	
core4	Assembly spacing (pin pitch): 1; # B_4C rods: 84; Metal between unit assemblies: N/A	1.59	0.9948	0.0015	0.17908	
core5	Assembly spacing (pin pitch): 2; # B_4C rods: 64; Metal between unit assemblies: N/A	1.59	0.99445	0.00153	0.16919	
core6	Assembly spacing (pin pitch): 2; # B_4C rods: 64; Metal between unit assemblies: N/A	1.59	0.99556	0.00152	0.17216	
core7	Assembly spacing (pin pitch): 3; # B_4C rods: 34; Metal between unit assemblies: N/A	1.59	0.99463	0.00151	0.15963	
core8	Assembly spacing (pin pitch): 3; # B_4C rods: 34; Metal between unit assemblies: N/A	1.59	0.98895	0.00149	0.16496	
core9	Assembly spacing (pin pitch): 4; # B_4C rods: 0; Metal between unit assemblies: N/A	1.59	0.99298	0.00144	0.15528	
core10	Assembly spacing (pin pitch): 3; # B_4C rods: N/A; Metal between unit assemblies: None	1.59	0.99511	0.00148	0.16036	
core11	Assembly spacing (pin pitch): 1; # B_4C rods: N/A; Metal between unit assemblies: SS	1.59	0.99699	0.00148	0.17893	
core12	Assembly spacing (pin pitch): 2; # B_4C rods: N/A; Metal between unit assemblies: SS	1.59	0.99549	0.00151	0.16671	
core13	Assembly spacing (pin pitch): 1; # B_4C rods: N/A; Metal between unit assemblies: B/Al set 5	1.59	0.99933	0.00151	0.18075	
core15	Assembly spacing (pin pitch): 1; # B_4C rods: N/A; Metal between unit assemblies: B/Al set 3	1.59	0.99107	0.00157	0.18348	
core16	Assembly spacing (pin pitch): 2; # B_4C rods: N/A; Metal between unit assemblies: B/Al set 3	1.59	0.99041	0.0015	0.16952	
core17	Assembly spacing (pin pitch): 1; # B_4C rods: N/A; Metal between unit assemblies: B/Al set 2	1.59	0.99365	0.00151	0.18187	
core18	Assembly spacing (pin pitch): 2; # B_4C rods: N/A; Metal between unit assemblies: B/Al set 2	1.59	0.9947	0.0015	0.16855	
core19	Assembly spacing (pin pitch): 1; # B_4C rods: N/A; Metal between unit assemblies: B/Al set 1	1.59	0.99383	0.00153	0.18354	
core20	Assembly spacing (pin pitch): 2; # B_4C rods: N/A; Metal between unit assemblies: B/Al set 1	1.59	0.99392	0.00151	0.16933	
core21	Assembly spacing (pin pitch): 3; # B_4C rods: N/A; Metal between unit assemblies: B/Al set 1	1.59	0.9916	0.0014	0.16225	

7.1.2.11 Electric Power Research Institute Mixed Oxide Critical Configurations

Analysis of Fresh Fuel Critical Experiments Appropriate for Burnup Credit Validation (ORNL 1995, p. 60) describes criticality tests with MOX fuel performed for EPRI. Six critical experiment configurations composed of unborated and borated water moderated lattices of 2 weight percent PuO_2 (8 weight percent plutonium-240) and 98 weight percent natural UO_2 fuel rods were modeled with MCNP. Although the relative distribution of the plutonium isotopes differs from that found in burned light water reactor fuel, the ratio of plutonium/uranium-235 (2.79) bounds that calculated for such fuel (1.01) (ORNL 1995, p. 60). The fuel rods were 1.283 cm in diameter (ORNL 1995, p. 65), clad with aluminum, and supported in a core structure composed of "eggcrate" type lattice plates with an upper lead shield. The configurations were closely reflected with full-density water laterally and below the core. These experiments are denoted as "exp22" through "exp27" and brief descriptions of the variations are provided in Table 22.

Table 22. EPRI Mixed Oxide Critical Configurations

Exp ID	Description	P/D	k_{eff}	σ	AENCF (MeV)	CC
exp22	Pitch =1.778 cm, 469 fuel rods, unborated water moderator	1.39	0.99624	0.00174	0.25557	1a, 2a, 3a, 3b, 3c, 3d, 4a
exp23	Pitch =1.778 cm, 761 fuel rods, 680.9 ppm borated water moderator	1.39	1.0005	0.00169	0.27397	
exp24	Pitch =2.210 cm, 197 fuel rods, unborated water moderator	1.72	1.00302	0.00171	0.16128	
exp25	Pitch =2.210 cm, 761 fuel rods, 1090.4 ppm borated water moderator	1.72	1.00835	0.00161	0.18944	
exp26	Pitch =2.515 cm, 160 fuel rods, unborated water moderator	1.96	1.00709	0.0016	0.13192	
exp27	Pitch =2.515 cm, 689 fuel rods, 767.2 ppm borated water moderator	1.96	1.00752	0.00155	0.15372	

7.1.2.12 Critical Triangular Lattice of MOX & UO_2 Fuel Rods

Bierman et al. (1984) documented critical experiments performed at PNL incorporating both urania and MOX fuel rods in a triangular lattice. One such experiment, designated "exp34," contained a triangular lattice of uniformly distributed PuO_2-UO_2 and UO_2 fuel rods. The fuel rods were placed in a uniform distribution with a plutonium/uranium-235 ratio approximating that of a 20,000 MWd/MTU burnup. Each PuO_2-UO_2 fuel rod was surrounded by six UO_2 fuel rods with a triangular lattice pitch. The UO_2 rods were 4.31 weight percent uranium-235 enriched, and the MOX fuel was 2 weight percent PuO_2 and 98 weight percent natural UO_2. Information for this experiment is provided in Table 23.

Table 23. Critical Configuration of MOX and UO_2 Fuel Rods in a Triangular Lattice

Exp ID	Description	P/D[b]	k_{eff}	σ	AENCF (MeV)	CC
exp34	583 MOX fuel rods with 1174 UO_2 fuel rods with a 1.598 cm pitch[a]	1.26	0.9875	0.00168	0.37762	2a, 3a, 3b, 3c, 3d, 4a

NOTES: [a] Configuration evaluated corresponds to lattice 32 in Bierman et al. 1984, p. F.66
[b] Fuel pellet dimensions from Bierman et al. 1984, pp. 2.9 and 2.10

7.1.3 Homogeneous Solution Experiments

The LCEs presented in this section represent solutions containing uranium, plutonium, or both uranium and plutonium. Each of the LCE configurations described in this section have been analyzed with the MCNP code system. An experiment identifier for each configuration is provided for subsequent reference in this document. With a few exceptions that are noted in the text, the vast majority of the assessed benchmarks come from *International Handbook of Evaluated Criticality Safety Benchmark Experiments* (NEA 1998).

The following sections briefly describe the LCEs according to the grouping in which the results are presented.

7.1.3.1 Mixed Plutonium and Natural Uranium Nitrate Solutions

The experiments involving plutonium and uranium with naturally occurring isotopic ratios are from *International Handbook of Evaluated Criticality Safety Benchmark Experiments* (NEA 1998, Volume VI) and are listed in Table 24.

Table 24. Configurations Incorporating Mixed Plutonium and Natural Uranium Nitrate Solutions

Exp ID	Description	k_{eff}	σ	AENCF (MeV)	CC
Water Reflected Annular Cylindrical Tank with Central Bottle and Annular Inserts (NEA 1998, Volume VI, MIX-SOL-THERM-001, Sections 1, 2, and 3)					
PNL3187	102.19 g Pu/l, 365.20 g U/l, 2% B_4C Concrete Annulus, No Bottle, CH: 48.55 cm, H/Pu-239 (annular tank) = 234, 91.118 wt% Pu-239 in Pu	0.99821	0.00116	0.04158	1a, 1b, 2a, 4a, 4b, 5a, 6a
PNL3391	103.37 g Pu/l, 363.66 g U/l, 0% B_4C Concrete Annulus, Bottle 2, CH: 27.67 cm, H/Pu-239 (annular tank) = 231, H/Pu-239 (bottle) = 231, 91.118 wt% Pu-239 in Pu	0.99318	0.00112	0.04075	
PNL3492	103.37 g Pu/l, 363.66 g U/l, 1% B_4C Concrete Annulus, Bottle 2, CH: 37.19 cm, H/Pu-239 (annular tank) = 225, H/Pu-239 (bottle) = 231, 91.117 wt% Pu-239 in Pu	0.99619	0.00113	0.04386	
PNL3593	107.91 g Pu/l, 379.55 g U/l, 6% B_4C Concrete Annulus, Bottle 2, CH: 51.10 cm, H/Pu-239 (annular tank) = 220, H/Pu-239 (bottle) = 231, 91.117 wt% Pu-239 in Pu	0.99694	0.00121	0.04614	
PNL3694	108.27 g Pu/l, 380.41 g U/l, No Concrete Annulus, Bottle 2, CH: 32.86 cm, H/Pu-239 (annular tank) = 219, H/Pu-239 (bottle) = 231, 91.117 wt% Pu-239 in Pu	1.00275	0.00113	0.04483	
PNL3795	195.61 g Pu/l, 6.5 g U/l, 2% B_4C Concrete Annulus, Bottle 3, CH: 27.51 cm, H/Pu-239 (annular tank) = 125, H/Pu-239 (bottle) = 126, 91.572 wt% Pu-239 in Pu	1.00302	0.00117	0.03965	
PNL3896	110.13 g Pu/l, 3.8 g U/l, 2% B_4C Concrete Annulus, Bottle 3, CH: 25.69 cm, H/Pu-239 (annular tank) = 242, H/Pu-239 (bottle) = 126, 91.572 wt% Pu-239 in Pu	1.00263	0.0011	0.02357	

Table 24. Configurations Incorporating Mixed Plutonium and Natural Uranium Nitrate Solutions (Continued)

Exp ID	Description	k_{eff}	σ	AENCF (MeV)	CC
PNL3897	58.30 g Pu/l, 2.3 g U/l, 2% B_4C Concrete Annulus, Bottle 3, CH: 28.94 cm, H/Pu-239 (annular tank) = 477, H/Pu-239 (bottle) = 126, 91.572 wt% Pu-239 in Pu	1.00323	0.00125	0.01447	
PNL3898	72.74 g Pu/l, 247.33 g U/l, 2% B_4C Concrete Annulus, Bottle 2, CH: 39.58 cm, H/Pu-239 (annular tank) = 354, H/Pu-239 (bottle) = 231, 91.117 wt% Pu-239 in Pu	1.00297	0.00118	0.02973	
PNL3808	47.08 g Pu/l, 161.72 g U/l, 2% B_4C Concrete Annulus, Bottle 2, CH: 45.09 cm, H/Pu-239 (annular tank) = 569, H/Pu-239 (bottle) = 231, 91.117 wt% Pu-239 in Pu	1.00178	0.00095	0.02059	
PNL3999	73.64 g Pu/l, 250.30 g U/l, Polyethylene with Cd Cover Annulus, Bottle 2, CH: 79.18 cm, H/Pu-239 (annular tank) = 349, H/Pu-239 (bottle) = 349, 91.117 wt% Pu-239 in Pu	1.00707	0.00108	0.02933	
PNL5300	74.25 g Pu/l, 251.64 g U/l, Solid Polyethylene with Cd Cover Center, CH: 104.62 cm, H/Pu-239 (annular tank) = 346, 91.117 wt% Pu-239 in Pu	1.0067	0.00105	0.02917	
Water Reflected Cylindrical Tank With a 68.68 cm Inner Diameter (ID), 91.102 wt% Pu-239 in Pu (NEA 1998, Volume VI, MIX-SOL-THERM-002, Sections 1, 2, and 3)					
PNL1158	11.83 g Pu/l, 11.05 g U/l, CH: 76.80 cm, H/Pu-239 = 2,403	1.00686	0.00067	0.00393	1a, 1b, 2a, 4a, 4b, 5a, 6a
PNL1159	11.73 g Pu/l, 10.78 g U/l, CH: 83.14 cm, H/Pu-239 = 2,435	1.00558	0.00064	0.0038	
PNL1161	12.19 g Pu/l, 41.04 g U/l, CH: 81.72 cm, H/Pu-239 = 2,317	1.00751	0.00066	0.00597	
Water/Polyethylene Reflected Cylindrical Tank With Various Diameters, 93.95 wt% Pu-239 in Pu (NEA 1998, Volume VI, MIX-SOL-THERM-003, Sections 1, 2, and 3)					
awre1	101.3 g Pu/l, 228.5 g U/l, ID = 25.425 cm, CH: 56.31 cm, H/Pu-239 = 239	1.01511	0.0012	0.03133	1a, 1b, 2a, 4a, 4b, 5a, 6a
awre2	101.3 g Pu/l, 228.5 g U/l, ID = 30.62 cm, CH: 29.89 cm, H/Pu-239 = 239	1.01167	0.00117	0.03206	
awre3	101.3 g Pu/l, 228.5 g U/l, ID = 37.99 cm, CH: 21.17 cm, H/Pu-239 = 239	1.01028	0.00114	0.03183	
awre4	101.3 g Pu/l, 228.5 g U/l, ID = 50.72 cm, CH: 16.05 cm, H/Pu-239 = 239	1.00486	0.00111	0.03228	
awre5	31.58 g Pu/l, 71.3 g U/l, ID = 30.62 cm, CH: 46.18 cm, H/Pu-239 = 847	1.00875	0.00101	0.01062	
awre6	31.58 g Pu/l, 71.3 g U/l, ID = 37.99 cm, CH: 28.24 cm, H/Pu-239 = 847	1.01337	0.00108	0.01053	
awre7	31.58 g Pu/l, 71.3 g U/l, ID = 50.72 cm, CH: 20.39 cm, H/Pu-239 = 847	1.0064	0.00102	0.01089	
awre8	18.61 g Pu/l, 42.2 g U/l, ID = 37.99 cm, CH: 72.86 cm, H/Pu-239 = 1461	1.01255	0.00091	0.00684	
awre9	18.61 g Pu/l, 42.2 g U/l, ID = 50.72 cm, CH: 33.59 cm, H/Pu-239 = 1461	1.00977	0.00088	0.00684	
awre10	17.50 g Pu/l, 39.6 g U/l, ID = 50.72 cm, CH: 37.16 cm, H/Pu-239 = 1556	1.00839	0.00081	0.00648	

Table 24. Configurations Incorporating Mixed Plutonium and Natural Uranium Nitrate Solutions (Continued)

Exp ID	Description	k_{eff}	σ	AENCF (MeV)	CC
Cylindrical Tank With a 35.39 cm ID and either Water Reflector, Concrete Reflector, or No Reflector, 91.118 wt% Pu-239 in Pu (NEA 1998, Volume VI, MIX-SOL-THERM-004, Sections 1, 2, and 3)					
PNL1577	172.56 g Pu/l, 262.79 g U/l, No Reflector, CH: 57.97 cm, H/Pu-239 = 137	0.99645	0.00128	0.05956	1a, 1b, 2a, 4a, 4b, 5a, 6a
PNL1678	172.82 g Pu/l, 262.55 g U/l, Water Reflector, CH: 28.93 cm, H/Pu-239 = 136	0.99976	0.00115	0.05069	
PNL1783	173.22 g Pu/l, 262.88 g U/l, Concrete Reflector, CH: 30.60 cm, H/Pu-239 = 136	0.99976	0.00115	0.05386	
PNL1868	118.71 g Pu/l, 173.98 g U/l, Concrete Reflector, CH: 27.03 cm, H/Pu-239 = 214	1.00247	0.00119	0.03416	
PNL1969	119.04 g Pu/l, 174.67 g U/l, Water Reflector, CH: 25.26 cm, H/Pu-239 = 213	0.99967	0.00111	0.0336	
PNL2070	118.90 g Pu/l, 174.53 g U/l, No Reflector, CH: 41.08 cm, H/Pu-239 = 214	0.99925	0.00115	0.03743	
PNL2565	41.69 g Pu/l, 63.38 g U/l, No Reflector, CH: 44.46 cm, H/Pu-239 = 664	1.00363	0.00112	0.01295	
PNL2666	41.89 g Pu/l, 63.65 g U/l, Water Reflector, CH: 28.11 cm, H/Pu-239 = 660	1.00337	0.00105	0.0116	
PNL2767	41.83 g Pu/l, 63.55 g U/l, Concrete Reflector, CH: 29.36 cm, H/Pu-239 = 661	1.00629	0.00113	0.01197	

NOTE: CH = Critical Height

7.1.3.2 Plutonium Nitrate Solutions

The experiments involving plutonium are from *International Handbook of Evaluated Criticality Safety Benchmark Experiments* (NEA 1998, Volume I) and are listed in Table 25.

Table 25. Configurations Incorporating Plutonium Nitrate Solutions

Exp ID	Description	k_{eff}[a]	σ	AENCF (MeV)	CC
Water Reflected 11.5-Inch Diameter Spheres, 0.049-in. thick shell of Stainless Steel Type 304L, 4.57 wt% Pu-240 in Pu, 95.12 wt% Pu-239 in Pu (NEA 1998, Volume I, PU-SOL-THERM-001, Sections 1, 2, and 3)					
pust1t1	73.0 g Pu/liter, CM: 945 gm, H/Pu-239 = 371	1.00995	0.00102	0.01252	1a, 1b, 2a, 4a, 4b, 5a, 6a
pust1t2	96.0 g Pu/liter, CM: 1243 gm, H/Pu-239 = 272	1.01109	0.001	0.01702	
pust1t3	119.0 g Pu/liter, CM: 1541 gm, H/Pu-239 = 216	1.01396	0.00094	0.02159	
pust1t4	132.0 g Pu/liter, CM: 1709 gm, H/Pu-239 = 190	1.00643	0.00104	0.02397	
pust1t5	140.0 g Pu/liter, CM: 1813 gm, H/Pu-239 = 180	1.01014	0.00101	0.02479	
pust1t6	268.7 g Pu/liter, CM: 3480 gm, H/Pu-239 = 91	1.00831	0.00104	0.04809	

Table 25. Configurations Incorporating Plutonium Nitrate Solutions (Continued)

Exp ID	Description	k_{eff}	σ	AENCF (MeV)	CC
Water Reflected 13-Inch Diameter Spheres, 0.050-in. thick shell of Stainless Steel Type 347 Unless Otherwise Indicated (NEA 1998, Volume I, PU-SOL-THERM-003, Sections 1, 2, and 3)					
pu003-1	33.32 g Pu/liter, CM: 631 gm, H/Pu-239 = 788, 1.76 wt% Pu-240	1.00962	0.00091	0.00623	1a, 1b, 2a, 4a, 4b, 5a, 6a
pu003-2	34.32 g Pu/liter, CM: 650 gm, H/Pu-239 = 756, 1.76 wt% Pu-240	1.00885	0.00091	0.00651	
pu003-3	37.43 g Pu/liter, CM: 709 gm, H/Pu-239 = 699, 3.12 wt% Pu-240	1.01228	0.00092	0.00693	
pu003-4	38.12 g Pu/liter, CM: 722 gm, H/Pu-239 = 682, 3.12 wt% Pu-240	1.00965	0.00094	0.0072	
pu003-5	40.65 g Pu/liter, CM: 770 gm, H/Pu-239 = 627, 3.12 wt% Pu-240	1.01393	0.00092	0.00785	
pu003-6	44.09 g Pu/liter, CM: 835 gm, H/Pu-239 = 563, 3.12 wt% Pu-240	1.01214	0.00091	0.00845	
pu003-7	35.98 g Pu/liter, CM: 649 gm, H/Pu-239 = 738, 3.12 wt% Pu-240, 20 Gauge 2S Al Shell	1.01369	0.00093	0.00678	
pu003-8	36.81 g Pu/liter, CM: 664 gm, H/Pu-239 = 714, 3.12 wt% Pu-240, 20 Gauge 2S Al Shell	1.01175	0.00095	0.00703	
Water Reflected 14-Inch Diameter Spheres, 0.050-in. thick shell of Stainless Steel Type 347 (NEA 1998, Volume I, PU-SOL-THERM-004, Sections 1, 2, and 3)					
pu004-1	26.27 g Pu/liter, CM: 621 gm, H/Pu-239 = 987, 0.54 wt% Pu-240	1.01134	0.00088	0.00524	1a, 1b, 2a, 4a, 4b, 5a, 6a
pu004-2	26.31 g Pu/liter, CM: 622 gm, H/Pu-239 = 977, 0.54 wt% Pu-240	1.00448	0.00082	0.00541	
pu004-3	27.20 g Pu/liter, CM: 643 gm, H/Pu-239 = 935, 0.54 wt% Pu-240	1.00916	0.00087	0.00538	
pu004-4	28.09 g Pu/liter, CM: 664 gm, H/Pu-239 = 889, 0.54 wt% Pu-240	1.00712	0.00086	0.00561	
pu004-5	27.58 g Pu/liter, CM: 652 gm, H/Pu-239 = 942, 1.76 wt% Pu-240	1.00753	0.00091	0.00543	
pu004-6	28.60 g Pu/liter, CM: 676 gm, H/Pu-239 = 927, 3.12 wt% Pu-240	1.00862	0.00087	0.00564	
pu004-7	29.57 g Pu/liter, CM: 699 gm, H/Pu-239 = 892, 3.12 wt% Pu-240	1.01248	0.0009	0.0056	
pu004-8	29.95 g Pu/liter, CM: 708 gm, H/Pu-239 = 869, 3.12 wt% Pu-240	1.00778	0.00086	0.0062	
pu004-9	31.60 g Pu/liter, CM: 747 gm, H/Pu-239 = 805, 3.12 wt% Pu-240	1.00965	0.00089	0.00619	
pu04-10	35.36 g Pu/liter, CM: 836 gm, H/Pu-239 = 689, 3.12 wt% Pu-240	1.00987	0.00092	0.00715	
pu04-11	39.38 g Pu/liter, CM: 931 gm, H/Pu-239 = 592, 3.12 wt% Pu-240	1.0095	0.00092	0.00805	
pu04-12	29.44 g Pu/liter, CM: 696 gm, H/Pu-239 = 893, 3.12 wt% Pu-240	1.01108	0.00087	0.00594	
pu04-13	29.27 g Pu/liter, CM: 692 gm, H/Pu-239 = 903, 3.43 wt% Pu-240	1.00856	0.00091	0.00579	

Table 25. Configurations Incorporating Plutonium Nitrate Solutions (Continued)

Exp ID	Description	k_{eff}[a]	σ	AENCF (MeV)	CC
Water Reflected 14-Inch Diameter Spheres, 0.050-in. thick shell of Stainless Steel Type 347 (NEA 1998, Volume I, PU-SOL-THERM-005, Sections 1, 2, and 3)					
pu005-1	29.65 g Pu/liter, CM: 701 gm, H/Pu-239 = 903, 4.05 wt% Pu-240	1.0086	0.00088	0.00571	1a, 1b, 2a, 4a, 4b, 5a, 6a
pu005-2	30.54 g Pu/liter, CM: 722 gm, H/Pu-239 = 868, 4.05 wt% Pu-240	1.00908	0.00088	0.00589	
pu005-3	31.43 g Pu/liter, CM: 743 gm, H/Pu-239 = 834, 4.05 wt% Pu-240	1.01116	0.00091	0.0062	
pu005-4	33.54 g Pu/liter, CM: 793 gm, H/Pu-239 = 765, 4.05 wt% Pu-240	1.01197	0.00093	0.00664	
pu005-5	36.04 g Pu/liter, CM: 852 gm, H/Pu-239 = 694, 4.05 wt% Pu-240	1.01367	0.0009	0.00723	
pu005-6	38.49 g Pu/liter, CM: 910 gm, H/Pu-239 = 633, 4.05 wt% Pu-240	1.0102	0.00095	0.00766	
pu005-7	40.91 g Pu/liter, CM: 967 gm, H/Pu-239 = 581, 4.05 wt% Pu-240	1.01073	0.00094	0.00838	
pu005-8	30.58 g Pu/liter, CM: 723 gm, H/Pu-239 = 869, 4.40 wt% Pu-240	1.00799	0.00091	0.00593	
pu005-9	31.85 g Pu/liter, CM: 753 gm, H/Pu-239 = 825, 4.40 wt% Pu-240	1.01023	0.00089	0.00631	
Water Reflected Partly Filled 11.5-Inch Diameter Spheres, 0.049-in. thick shell of Stainless Steel Type 304L, 4.67 wt% Pu-240, 95.059 wt% Pu-239 in Pu (NEA 1998, Volume I, PU-SOL-THERM-007, Sections 1, 2, and 3)					
pu007-2	232 g Pu/liter, Critical Volume: 12.35 liters, Height Above Sphere Center: 10.8373 cm, H/Pu-239 = 110	1.01024	0.00102	0.04021	1a, 1b, 2a, 4a, 4b, 5a, 6a
pu007-3	221 g Pu/liter, Critical Volume: 12.35 liters, Height Above Sphere Center: 10.8373 cm, H/Pu-239 = 114	1.00591	0.00111	0.03928	
pu007-5	100.2 g Pu/liter, Critical Volume: 12.39 liters, Height Above Sphere Center: 10.9741 cm, H/Pu-239 = 268	1.01502	0.00106	0.01764	
pu007-6	101.5 g Pu/liter, Critical Volume: 12.30 liters, Height Above Sphere Center: 10.6720 cm, H/Pu-239 = 262	1.00873	0.00101	0.01799	
pu007-7	100.1 g Pu/liter, Critical Volume: 12.39 liters, Height Above Sphere Center: 10.9741 cm, H/Pu-239 = 266	1.01053	0.00103	0.01783	
pu007-8	101.6 g Pu/liter, Critical Volume: 12.37 liters, Height Above Sphere Center: 10.9051 cm, H/Pu-239 = 258	1.00254	0.00103	0.0181	
pu007-9	101.6 g Pu/liter, Critical Volume: 12.23 liters, Height Above Sphere Center: 10.4503 cm, H/Pu-239 = 260	1.00327	0.00106	0.01815	
pu07-10	93.5 g Pu/liter, Critical Volume: 12.35 liters, Height Above Sphere Center: 10.8373 cm, H/Pu-239 = 285	1.00706	0.00104	0.01653	

Table 25. Configurations Incorporating Plutonium Nitrate Solutions (Continued)

Exp ID	Description	k_{eff}	σ	AENCF (MeV)	CC
Unreflected 48-inch Diameter Sphere, 0.303-inch thick shell of Type 1100 Aluminum, 97.386 wt% Pu-239 and 2.521 wt% Pu-240 in Pu (NEA 1998, Volume I, PU-SOL-THERM-009, Sections 1, 2, and 3)					
pust9-1	10.02 g Pu/liter, Critical Volume: 656.6 liters, Height Above Sphere Center: 15.9558 cm, H/Pu-239 = 2648	1.01886	0.00088	0.00257	1a, 1b, 2a, 4a, 4b, 5a, 6a
pust9-2	9.539 g Pu/liter, Critical Volume: 906.5 liters, Height Above Sphere Center: 45.3705 cm, H/Pu-239 = 2779	1.0239	0.00089	0.00266	
pust9-3	9.457 g Pu/liter, Critical Volume: 949.1 liters, Full Sphere, H/Pu-239 = 2803	1.02176	0.00089	0.00246	
Water Reflected Cylinders, 0.062-inch thick shell of Stainless Steel Type 347, 2.9 wt% Pu-240 in Pu (NEA 1998, Volume I, PU-SOL-THERM-010, Sections 1, 2, and 3)					
pu10091	99.09 g Pu/liter, IR = 11.4264 cm, CH: 30.7086 cm, CM: 1249 g, H/Pu-239 = 267	1.02337	0.00101	0.01675	1a, 1b, 2a, 4a, 4b, 5a, 6a
pu10092	73.92 g Pu/liter, IR = 11.4264 cm, CH: 35.4076 cm, CM: 1073 g, H/Pu-239 = 357	1.02091	0.00097	0.01299	
pu10093	54.53 g Pu/liter, IR = 11.4264 cm, CH: 44.5770 cm, CM: 997 g, H/Pu-239 = 484	1.01316	0.00097	0.00994	
pu10111	54.53 g Pu/liter, IR = 13.9684 cm, CH: 25.6032 cm, CM: 856 g, H/Pu-239 = 485, Extra 0.065 inch layer of stainless steel placed around cylinder	1.01879	0.00099	0.01001	
pu10112	47.21 g Pu/liter, IR = 13.9684 cm, CH: 28.1686 cm, CM: 815 g, H/Pu-239 = 558, Extra 0.065 inch layer of stainless steel placed around cylinder	1.01543	0.00098	0.00873	
pu10113	47.21 g Pu/liter, IR = 13.9684 cm, CH: 27.0764 cm, CM: 784 g, H/Pu-239 = 558	1.01615	0.00092	0.00852	
pu10114	41.73 g Pu/liter, IR = 13.9684 cm, CH: 32.6390 cm, CM: 835 g, H/Pu-239 = 606	1.00903	0.00091	0.0079	
pu10115	36.90 g Pu/liter, IR = 13.9684 cm, CH: 43.0022 cm, CM: 973 g, H/Pu-239 = 665	1.01069	0.00093	0.00755	
pu10116	63.99 g Pu/liter, IR = 13.9684 cm, CH: 22.8092 cm, CM: 895 g, H/Pu-239 = 414	1.01992	0.00101	0.01114	
pu10117	48.98 g Pu/liter, IR = 13.9684 cm, CH: 25.9588 cm, CM: 780 g, H/Pu-239 = 535	1.01146	0.00092	0.00879	
pu10121	48.75 g Pu/liter, IR = 15.2390 cm, CH: 22.3520 cm, CM: 799 g, H/Pu-239 = 543	1.0156	0.00097	0.00896	
pu10122	42.29 g Pu/liter, IR = 15.2390 cm, CH: 25.2476 cm, CM: 779 g, H/Pu-239 = 618	1.01616	0.00095	0.00776	
pu10123	36.52 g Pu/liter, IR = 15.2390 cm, CH: 28.4734 cm, CM: 758 g, H/Pu-239 = 728	1.02352	0.00094	0.00691	
pu10124	31.14 g Pu/liter, IR = 15.2390 cm, CH: 33.4264 cm, CM: 759 g, H/Pu-239 = 850	1.01642	0.00087	0.0061	

Table 25. Configurations Incorporating Plutonium Nitrate Solutions (Continued)

Exp ID	Description	k_{eff}[a]	σ	AENCF (MeV)	CC
Unreflected 16- & 18-Inch Diameter Spheres, 0.050-in. thick shell of Stainless Steel Type 347, 0.020-in. thick Cd Cover on the 18-inch sphere, 4.2 wt% Pu-240 in Pu (NEA 1998, Volume I, PU-SOL-THERM-011, Sections 1, 2, and 3)					
pu11161	34.96 g Pu/liter, IR = 20.1206 cm, CM: 1194 g, H/Pu-239 = 765	1.01661	0.00103	0.00738	1a, 1b, 2a, 4a, 4b, 5a, 6a
pu11162	36.22 g Pu/liter, IR = 20.1206 cm, CM: 1237 g, H/Pu-239 = 736	1.02377	0.00101	0.00777	
pu11163	38.13 g Pu/liter, IR = 20.1206 cm, CM: 1302 g, H/Pu-239 = 691	1.02224	0.00101	0.00827	
pu11164	38.16 g Pu/liter, IR = 20.1206 cm, CM: 1303 g, H/Pu-239 = 682	1.01688	0.00105	0.00845	
pu11165	43.43 g Pu/liter, IR = 20.1206 cm, CM: 1483 g, H/Pu-239 = 575	1.01338	0.00104	0.00973	
pu11181	22.35 g Pu/liter, IR = 22.6974 cm, CM: 1095 g, H/Pu-239 = 1208	1.00169	0.00089	0.00505	
pu11182	23.27 g Pu/liter, IR = 22.6974 cm, CM: 1140 g, H/Pu-239 = 1151	1.0068	0.00088	0.00549	
pu11183	23.10 g Pu/liter, IR = 22.6974 cm, CM: 1132 g, H/Pu-239 = 1158	1.00336	0.00097	0.00514	
pu11184	23.82 g Pu/liter, IR = 22.6974 cm, CM: 1167 g, H/Pu-239 = 1100	1.00285	0.00088	0.00547	
pu11185	25.20 g Pu/liter, IR = 22.6974 cm, CM: 1235 g, H/Pu-239 = 1039	1.01131	0.00093	0.00593	
pu11186	27.49 g Pu/liter, IR = 22.6974 cm, CM: 1347 g, H/Pu-239 = 908	1.00796	0.00097	0.00633	
pu11187	23.94 g Pu/liter, IR = 22.6974 cm, CM: 1173 g, H/Pu-239 = 1103	1.00792	0.00088	0.00548	

NOTE: [a] Calculated k_{eff} values for the Pu solution experiments which significantly exceed a value of 1.01 are often found when using the ENDF/B-V libraries. The most likely reason is that the Pu cross sections have a tendency to over-predict k_{eff}, but since the calculated values are over-predictions of a critical system, this is considered conservative with respect to criticality safety applications.
CH = Critical Height; CM = Critical Mass; IR = Internal Radius

7.1.3.3 Low-Enrichment Uranium Solutions

The first set of experiments involving low-enrichment uranium is from *International Handbook of Evaluated Criticality Safety Benchmark Experiments* (NEA 1998, Volume IV); the second set (case prefix "LEUJ") is from work at the Japan Atomic Energy Research Institute (Miyoshi et al. 1997), and the third set (case prefix SPHU9) is cases that look at UO_3-H_2O critical solutions (Wittekind 1992). These experiments are listed in Table 26.

Table 26. Configurations Incorporating Low-Enrichment Uranium Solutions

Exp ID	Description	k_{eff}	σ	AENCF (MeV)	CC
174 Liter Spherical Tank of 4.9% Enriched UO2F2 Solutions, 34.399 cm Radius, 0.1588 cm thick 1100 Aluminum Shell (NEA 1998, Volume IV, LEU-SOL-THERM-002, Sections 1, 2, and 3)					
LEUST21	452.2 g U/liter, 22.11 g U-235/liter, Water Reflector, Critical Volume: 170.5 Liters Critical Mass = 3769.8 g U-235, H/U-235: 1098	0.99892	0.00053	0.02487	1a, 1b, 2a, 4a, 4b, 5a, 6a
LEUST22	491.7 g U/liter, 24.04 g U-235/liter, No Reflector, Critical Volume: 172 Liters, Critical Mass = 4134.9 g U-235, H/U-235: 1001	0.99469	0.00061	0.02832	
LEUST23	491.7 g U/liter, 24.04 g U-235/liter, Water Reflector, Critical Volume = 145.6 Liters, Critical Mass = 3500.2 g U-235, H/U-235: 1001	1.00078	0.00057	0.02665	
Cylindrical Tank With a 59.0 cm ID, 0.3 cm thick Stainless Steel SS 304, U-235 Enrichment of 9.97 wt% (Miyohsi et al. 1997)					
LEUJA01	310.1 g U/liter, 30.9 g U-235/liter, Water Reflector, Critical Height: 41.53 cm, Critical Mass = 3508.4 g U-235, H/U-235: 719.0, H/U: 72.5	1.00425	0.00085	0.01896	1a, 1b, 2a, 4a, 4b, 5a, 6a
LEUJA29	290.4 g U/liter, 29.0 g U-235/liter, Water Reflector, Critical Height: 46.70 cm, Critical Mass = 3702.6 g U-235, H/U-235: 771.3, H/U: 77.8	1.00377	0.00082	0.01806	
LEUJA33	270.0 g U/liter, 26.9 g U-235/liter, Water Reflector, Critical Height: 52.93 cm, Critical Mass = 3892.7 g U-235, H/U-235: 842.2, H/U: 84.9	0.99961	0.0009	0.01662	
LEUJA34	253.6 g U/liter, 25.3 g U-235/liter, Water Reflector, Critical Height: 64.85 cm, Critical Mass = 4485.6 g U-235, H/U-235: 895.8, H/U: 90.3	1.0029	0.00079	0.0159	
LEUJA46	241.9 g U/liter, 24.1 g U-235/liter, Water Reflector, Critical Height: 78.56 cm, Critical Mass = 5176.2 g U-235, H/U-235: 941.7, H/U: 95.0	1.00311	0.0008	0.01535	
LEUJA51	233.2 g U/liter, 23.3 g U-235/liter, Water Reflector, Critical Height: 95.50 cm, Critical Mass = 6083.5 g U-235, H/U-235: 982.5, H/U: 99.1	1.00279	0.0007	0.01479	
LEUJA54	225.3 g U/liter, 22.5 g U-235/liter, Water Reflector, Critical Height: 130.33 cm, Critical Mass = 8017.2 g U-235, H/U-235: 1017.5, H/U: 102.6	1.00246	0.00072	0.0144	
LEUJA14	313.0 g U/liter, 31.2 g U-235/liter, No Reflector, Critical Height: 46.83 cm, Critical Mass = 3994.6 g U-235, H/U-235: 709.2, H/U: 71.5	0.99755	0.00094	0.02001	
LEUJA30	290.7 g U/liter, 29.0 g U-235/liter, No Reflector, Critical Height: 54.20 cm, Critical Mass = 4297.3 g U-235, H/U-235: 770.0, H/U: 77.7	0.99885	0.00086	0.01881	
LEUJA32	270.0 g U/liter, 26.9 g U-235/liter, No Reflector, Critical Height: 63.55 cm, Critical Mass = 4673.7 g U-235, H/U-235: 842.2, H/U: 84.9	1.00143	0.00086	0.01757	
LEUJA36	253.9 g U/liter, 25.3 g U-235/liter, No Reflector, Critical Height: 83.55 cm, Critical Mass = 5779.1 g U-235, H/U-235: 896.0, H/U: 90.4	1.00185	0.00084	0.01665	
LEUJA49	241.9 g U/liter, 24.1 g U-235/liter, No Reflector, Critical Height: 112.27 cm, Critical Mass = 7397.3 g U-235, H/U-235: 942.2, H/U: 95.0	0.99875	0.00078	0.01593	

Table 26. Configurations Incorporating Low-Enrichment Uranium Solutions (Continued)

Exp ID	Description	k_{eff}	σ	AENCF (MeV)	CC
UO3-H2O Solution Experiments (Wittekind 1992, p. 43)					
SPHU9A	1.0059 wt% enriched U-235, H/U-235: 370.3, H/U: 3.772	0.9920[a] / 0.99004[b]	0.0060[c] / 0.00249[d]	0.2541	1a, 1b, 2a, 4a, 4b, 5a, 6a
SPHU9B	1.0059 wt% enriched U-235, H/U-235: 490.8, H/U: 4.999	0.9925 / 0.99269	0.0050 / 0.00249	0.2163	
SPHU9C	1.0059 wt% enriched U-235, H/U-235: 605.1, H/U: 6.164	0.9875 / 0.97871	0.0058 / 0.00256	0.1883	
SPHU9D	1.0059 wt% enriched U-235, H/U-235: 675.5, H/U: 6.881	0.9821 / 0.97914	0.0054 / 0.00242	0.1737	
SPHU9E	1.0059 wt% enriched U-235, H/U-235: 731.2, H/U: 7.449	0.9702 / 0.96607	0.0070 / 0.00163	0.1591	
SPHU9F	1.0704 wt% enriched U-235, H/U-235: 343.9, H/U: 3.728	1.0063 / 1.00952	0.0073 / 0.00261	0.2511	
SPHU9G	1.0704 wt% enriched U-235, H/U-235: 533.1, H/U: 5.778	1.0064 / 1.0136	0.0078 / 0.00246	0.1839	
SPHU9H	1.0704 wt% enriched U-235, H/U-235: 652.7, H/U: 7.075	0.9957 / 0.99713	0.0061 / 0.00198	0.1651	
SPHU9I	1.1586 wt% enriched U-235, H/U-235: 317.7, H/U: 3.728	1.0298 / 1.03372	0.0056 / 0.00274	0.2495	
SPHU9J	1.1586 wt% enriched U-235, H/U-235: 475.6, H/U: 5.926	1.0330 / 1.04207	0.0051 / 0.00224	0.1783	
SPHU9K	1.1586 wt% enriched U-235, H/U-235: 582.8, H/U: 6.838	1.0313 / 1.02951	0.0032 / 0.00216	0.1661	
SPHU9L	1.1586 wt% enriched U-235, H/U-235: 634.9, H/U: 7.449	1.0209 / 1.02281	0.0051 / 0.0021	0.1549	

NOTES: [a] For the UO_3-H_2O solution experiments the experimental determinations are the top numbers and were stated as k_∞ although the experiment was on a reflected sample (Wittekind 1992, p. 40).
[b] For the UO_3-H_2O solution experiments the calculated k_∞ value is the bottom number.
[c] For the UO_3-H_2O solution experiments the top number represents experimental uncertainty.
[d] For the UO_3-H_2O solution experiments the bottom number represents calculation uncertainty.

7.1.3.4 Low Enriched Uranyl Fluoride Solutions

This experiment involved an aqueous solution of about 5 weight percent enriched uranyl fluoride and is taken from *International Handbook of Evaluated Criticality Safety Benchmark Experiments* (NEA 1998, Volume IV, LEU-SOL-THERM-001, Sections 1, 2, and 3). This experiment used the Solution High Energy Burst Assembly-II, which is a critical assembly experiment that was operated at the Los Alamos Critical Experiments Facility. This experiment is listed in Table 27.

Table 27. Configurations Incorporating Uranyl Fluoride Solutions

Exp ID	Description	k_{eff}	σ	AENCF (MeV)	CC
lst1-1	Average solution density: 2.1092 g/cm3, Average uranium density: 0.9783 g/cm3, Average U-235 enrichment: 4.9977 atom percent, H/X: 453.9	1.01069	0.00085	0.0523	1a, 1b, 2a, 4a, 4b, 5a, 6a

7.2 CRITICAL LIMT COMPUTATION

An essential element of validating the criticality model used for calculating k_{eff} for a waste package is the determination of the CL. The CL is derived from the bias and uncertainties associated with the criticality code and modeling process. The CL for a configuration class is a limiting value of k_{eff} at which a configuration is considered potentially critical. The CL is characterized by statistical tolerance limits that account for biases and uncertainties associated with the criticality code trending process, and any uncertainties due to extrapolation outside the range of experimental data, or limitations in the geometrical or material representations used in the computational method.

7.2.1 Statistical Analyses

Evaluation of benchmark experiments that cover a wide range of parameters and configurations requires the determination of which groups of experiments can be statistically analyzed together and which should be analyzed separately. The benchmark experiments were grouped based on experimental similarity and are as follows:

- CRC Experiments
- Lattice LCEs (UO2 and MOX based fuel)
- Uranium Solution LCEs
- Plutonium Solution LCEs.

The Student t-distribution (Walpole et al. 1998, pp. 228 to 232) is used to test the benchmark group results to determine if they can be analyzed together or not.

With the Student t-test for two groups it can be determined, with 95 percent confidence, whether subsets have different mean values and thus should not be analyzed together. The equality test requires computing the statistic "*T*" in Equation 6.

$$T = \frac{\overline{Y}_1 - \overline{Y}_2}{\sqrt{\frac{(n-1)S_{y1}^2 + (m-1)S_{y2}^2}{n+m-2}}\sqrt{\frac{1}{n}+\frac{1}{m}}} \qquad \text{(Eq. 6)}$$

where

$\overline{Y}_1$ = the calculated multiplication factor averages for subset 1
$\overline{Y}_2$ = the calculated multiplication factor averages for subset 2
n = the number of observations for subset 1
m = the number of observations for subset 2
S_{y1}^2 = the variances for subset 1 (as shown in Equations 7)
S_{y2}^2 = the variances for subset 2 (as shown in Equations 8)

$$S_{y1}^2 = \frac{\sum_{i=1,n}(Y_i - \overline{Y}_1)^2}{n-1} \qquad \text{(Eq. 7)}$$

$$S_{y2}^2 = \frac{\sum_{i=1,m}(Y_i - \bar{Y}_2)^2}{m-1} \quad \text{(Eq. 8)}$$

The "T" statistic is compared to the Student t-distribution with 95 percent confidence and n+m-2 degrees of freedom. The null hypothesis "the two subsets of data can be statistically combined (the mean values are approximately equal)" would be accepted if $|T|<t_{\alpha/2,n+m-2}$ and rejected otherwise where α is defined below. Table 28 presents the test results.

Table 28. Equality Test Statistic Results

Subsets	UO_2 and MOX LCEs					
	Sample Size	Average k_{eff}	Variance	T statistic	$t_{\alpha/2,n+m-2}$[a]	Combine?
UO_2 LCEs	64	0.9985	2.282E-05	-1.2143	1.9897	Y
MOX LCEs	19	1.0000	2.777E-05			
	CRCs and LCEs					
CRCs	45	0.9922	1.029E-05	-8.3765	1.9790	N
LCEs	83	0.9988	2.237E-05			
	Uranium and Plutonium Solutions					
Uranium Solutions	28	1.0028	2.512E-04	-3.4257	1.9780	N
Plutonium Solutions	107	1.0094	3.942E-05			

NOTE: [a] α = 1-confidence level (i.e., 0.95).

7.2.2 Regression Analyses

The calculated multiplication factors for the benchmark experiments were trended against several parameters from each subset using a linear regression fit in order to determine whether a trend does exist and which parameters exhibit the strongest trends. A variation of the Student t-test along with the slope test was used to determine if a particular trend is considered statistically significant.

The linear regression fitted equation is in the form y(x) = a + bx. The slope test requires calculating the test statistic "*T*" as follows in Equation 9 along with the statistical parameters in Equations 10 and 11.

$$T = b\sqrt{\frac{(n-2)S_{xx}}{SS_R}} \quad \text{(Eq. 9)}$$

where b comes from the fitted linear regression equation

$$S_{xx} = \sum_{i=1,n}(x_i - \bar{x})^2 \quad \text{(Eq. 10)}$$

and

$$SS_R = \sum_{i=1,n}(y_i - a - bx_i)^2 \quad \text{(Eq. 11)}$$

The test statistic is compared to the Student t-distribution with 95 percent confidence and n-2 degrees of freedom. Given a null hypothesis of "no statistically significant trend exists (slope is zero)," the hypothesis would be accepted if $|T| < t_{\alpha/2,n-2}$ and rejected otherwise. Unless the data is

exceptional, the linear regression results will have a non-zero slope. By only accepting trends that the data supports with 95 percent confidence, trends due to the randomness of the data are eliminated.

7.2.2.1 Trending Evaluation

Trending against various parameters was performed in order to determine correlations between characteristics and the calculated multiplication factors for each subset. Depending on the type of benchmark, different trending parameters were evaluated in order to determine which exhibit the strongest trends. The regression statistics for the trend evaluations are presented in Tables 29 through 32 for each of the subsets and illustrated in Figures 5 through 18.

Table 29. CRC Trending Parameter Results

Trend Parameter	N	Slope	Intercept	S_{xx}	SS_R	r[a]	T	$t_{\alpha/2,n-2}$	Trend?
AENCF	45	-8.239E-02	1.013E+00	3.407E-03	4.298E-04	0.226	-1.521	2.02	No
Core Avg. BU	45	-2.403E-04	9.958E-01	2.567E+03	3.047E-04	0.572	-4.574	2.02	Yes
B ppm	45	1.301E-07	9.921E-01	1.078E+07	4.528E-04	0.020	0.132	2.02	No
ALF[b]	45	2.024E-02	9.177E-01	5.495E-02	4.304E-04	0.223	1.500	2.02	No

NOTES: [a] r represents the r-value correlation coefficient (positive square-root of squared correlation coefficient).
[b] ALF = average lethargy of a neutron causing fission.

Table 30. UO_2 and MOX LCE Trending Parameter Results

Trend Parameter	N	Slope	Intercept	S_{xx}	SS_R	r	T	$t_{\alpha/2,n-2}$	Trend?
AENCF	83	-6.336E-03	1.000E+00	1.941E-01	1.965E-03	0.063	-0.57	1.99	No
P/D	83	5.966E-03	9.890E-01	4.534E+00	1.811E-03	0.286	2.69	1.99	Yes
Pitch	83	6.723E-03	9.871E-01	5.687E+00	1.716E-03	0.361	3.48	1.99	Yes
W/F	83	1.156E-03	9.963E-01	1.238E+02	1.807E-03	0.290	2.72	1.99	Yes

Table 31. Uranium Solution Trending Parameter Results

Trend Parameter	N	Slope	Intercept	S_{xx}	SS_R	r	T	$t_{\alpha/2,n-2}$	Trend?
AENCF	28	2.184E-02	1.001E+00	2.247E-01	6.676E-03	0.126	0.65	2.06	No
H/X	28	-2.199E-05	1.019E+00	1.343E+06	6.134E-03	0.309	-1.66	2.06	No
ALF	28	-1.566E-03	1.011E+00	3.758E+01	6.691E-03	0.117	-0.60	2.06	No

Table 32. Plutonium Solution Trending Parameter Results

Trend Parameter	N	Slope	Intercept	S_{xx}	SS_R	r	T	$t_{\alpha/2,n-2}$	Trend?
AENCF	107	-2.545E-01	1.013E+00	1.976E-02	2.898E-03	0.554	-6.81	1.98	Yes
H/X	107	3.221E-06	1.007E+00	3.338E+07	3.832E-03	0.288	3.08	1.98	Yes
ALF	107	4.072E-03	9.817E-01	6.412E+01	3.115E-03	0.504	5.99	1.98	Yes

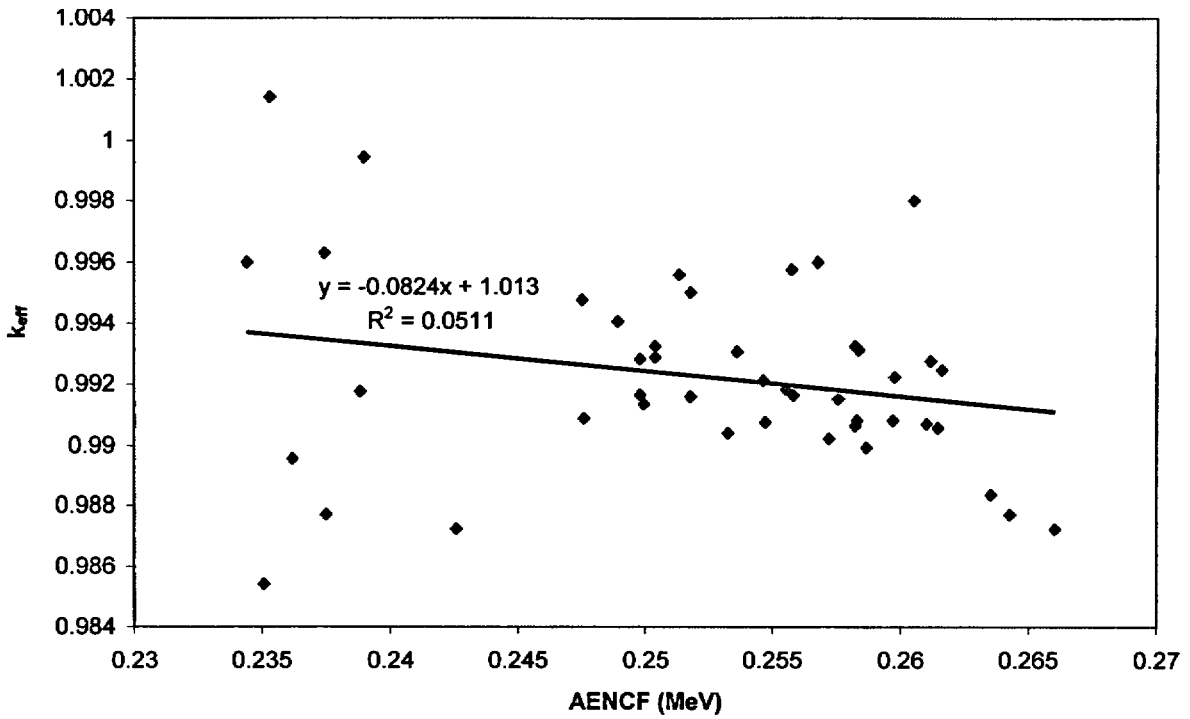

Figure 5. CRC Subset with AENCF as Trending Parameter

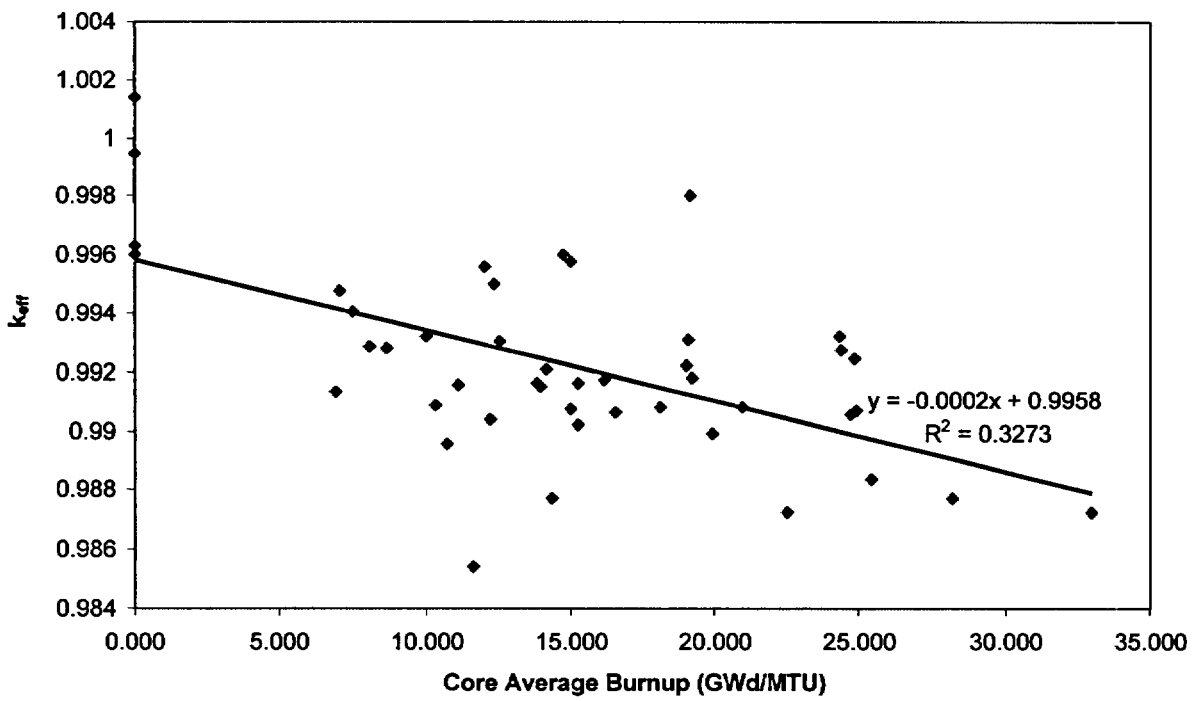

Figure 6. CRC Subset with Core Average Burnup as Trending Parameter

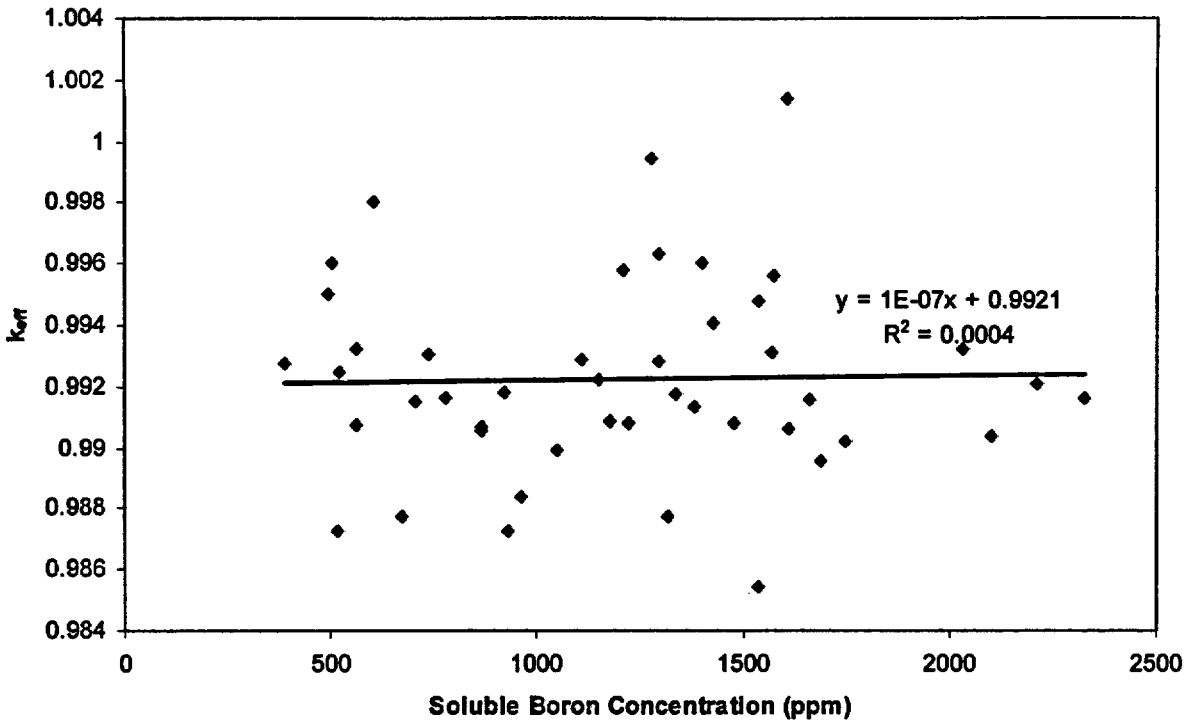

Figure 7. CRC Subset with Soluble Boron Concentration as Trending Parameter

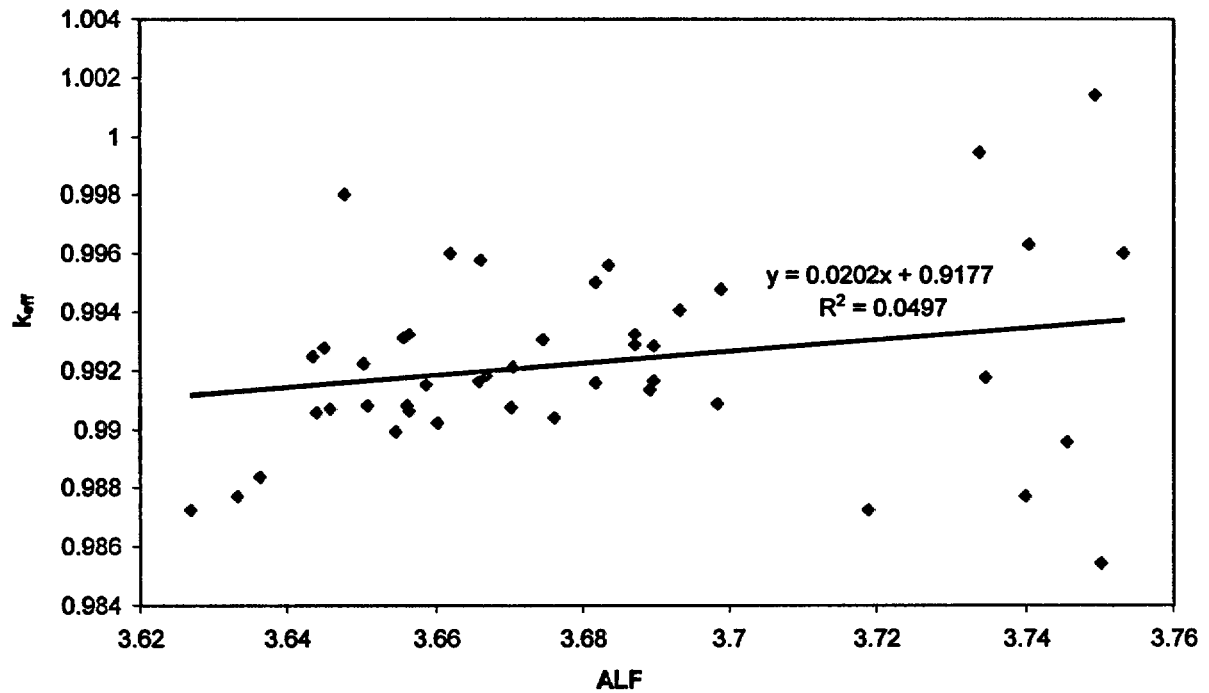

Figure 8. CRC Subset with ALF as Trending Parameter

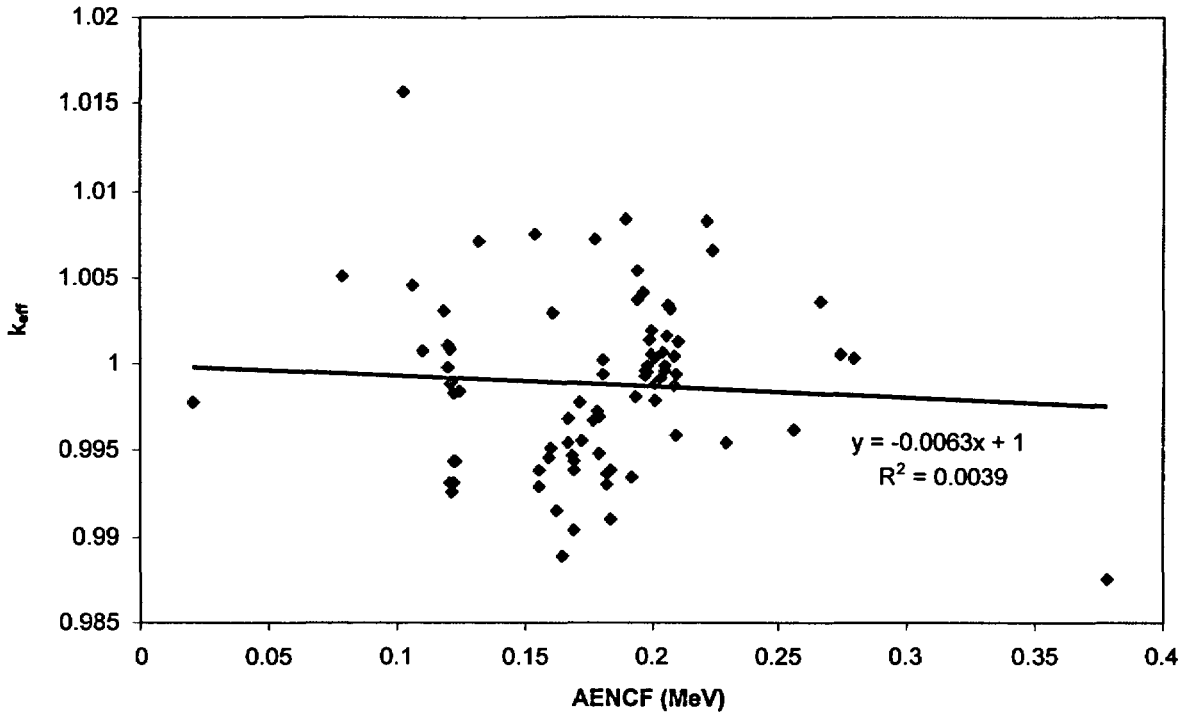

Figure 9. UO_2 and MOX LCE Subset with AENCF as Trending Parameter

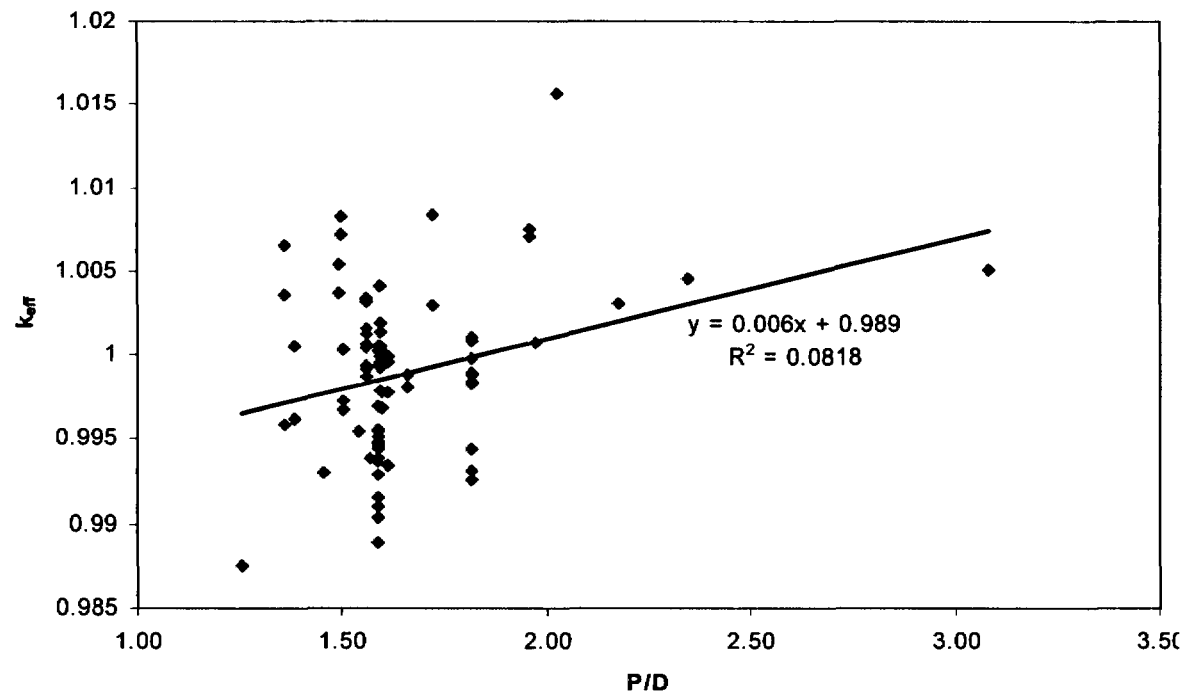

Figure 10. UO_2 and MOX LCE Subset with P/D as Trending Parameter

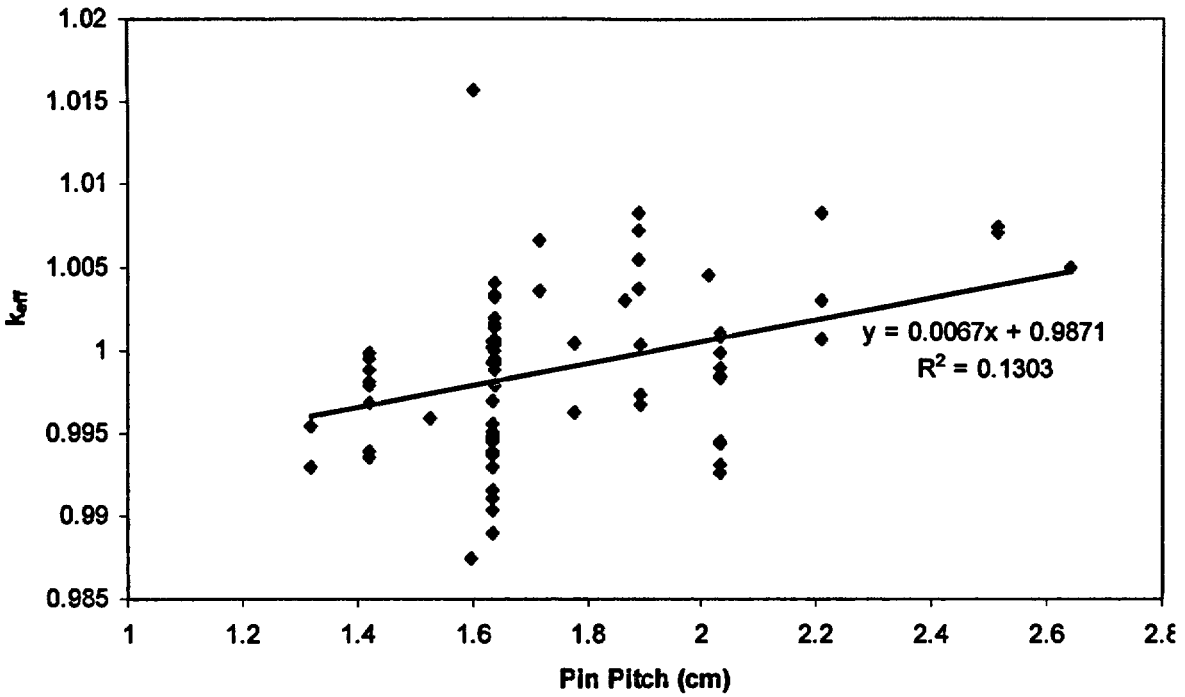

Figure 11. UO_2 and MOX LCE Subset with Pin Pitch as Trending Parameter

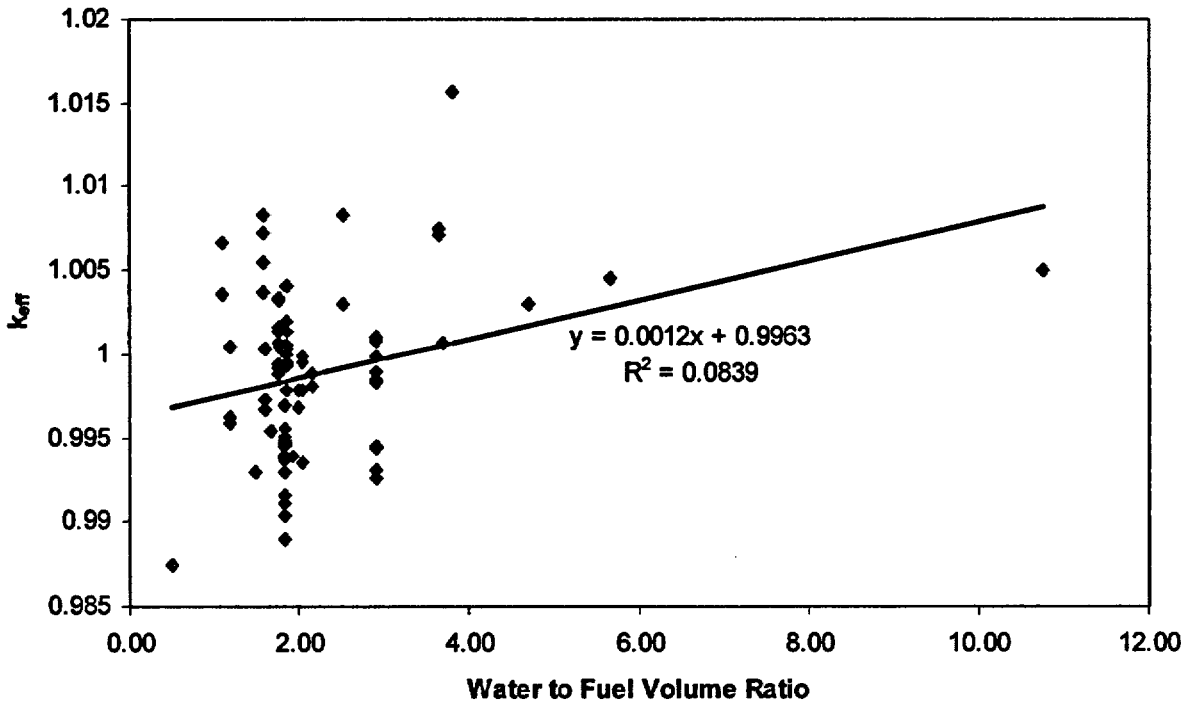

Figure 12. UO_2 and MOX LCE Subset with Moderator-to-Fuel Volume Ratio as Trending Parameter

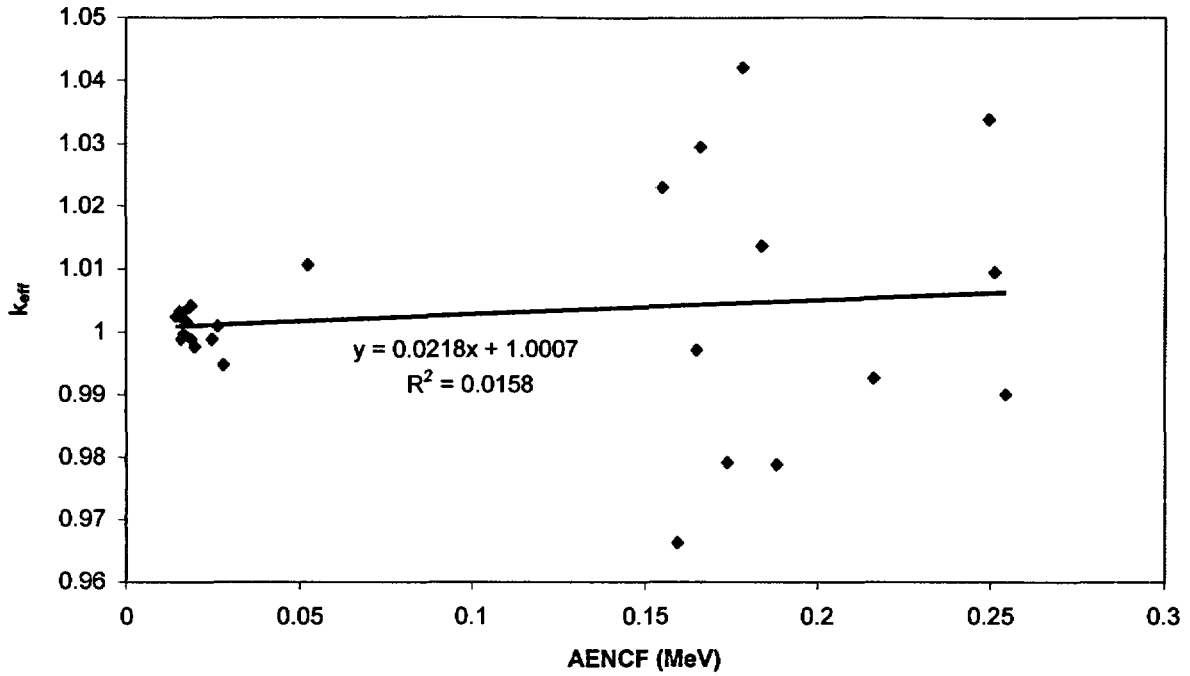

Figure 13. Uranium Solution Subset with AENCF as Trending Parameter

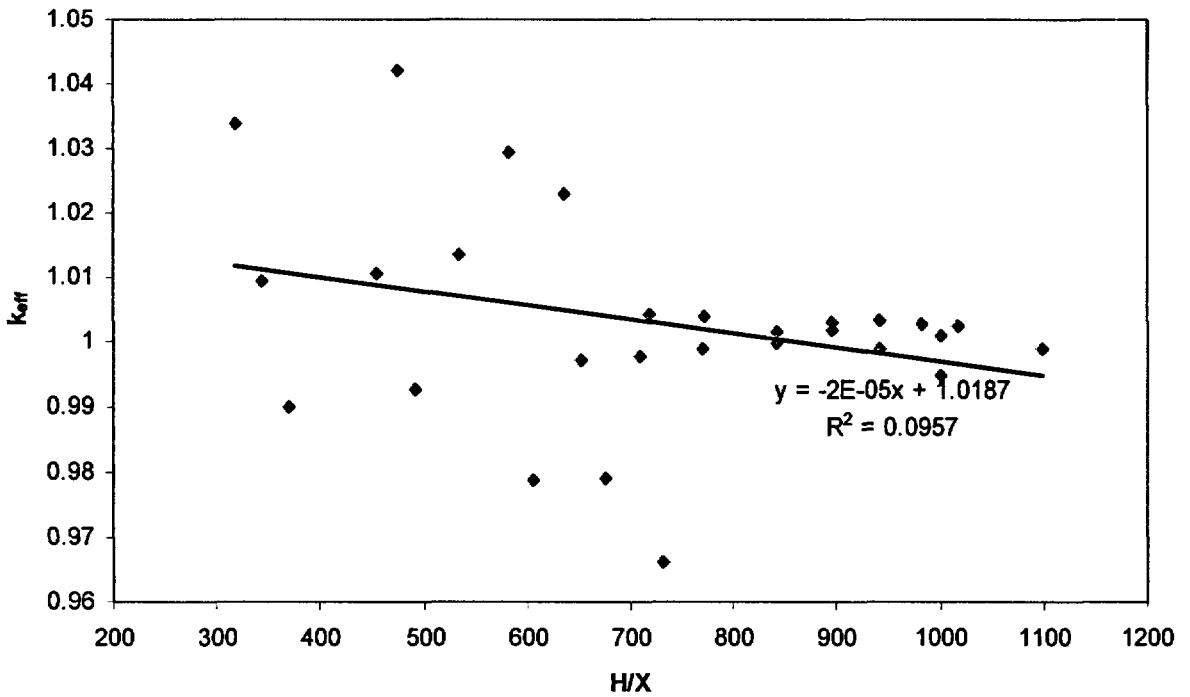

Figure 14. Uranium Solution Subset with H/X as Trending Parameter

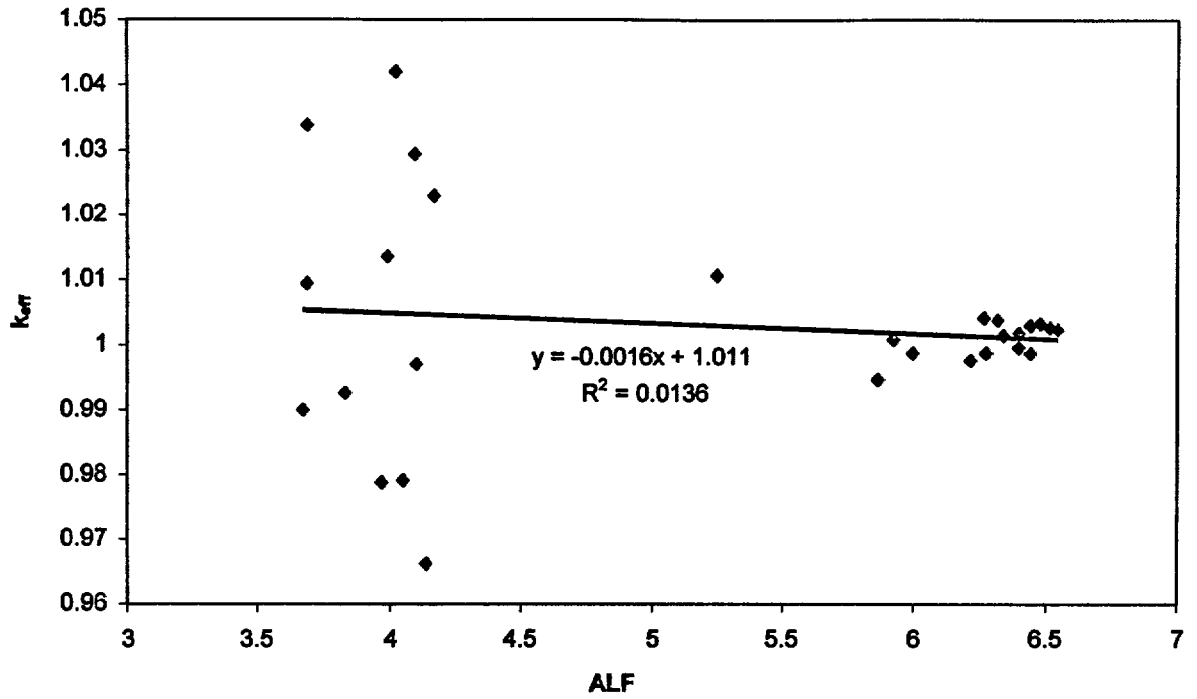

Figure 15. Uranium Solution Subset with ALF as Trending Parameter

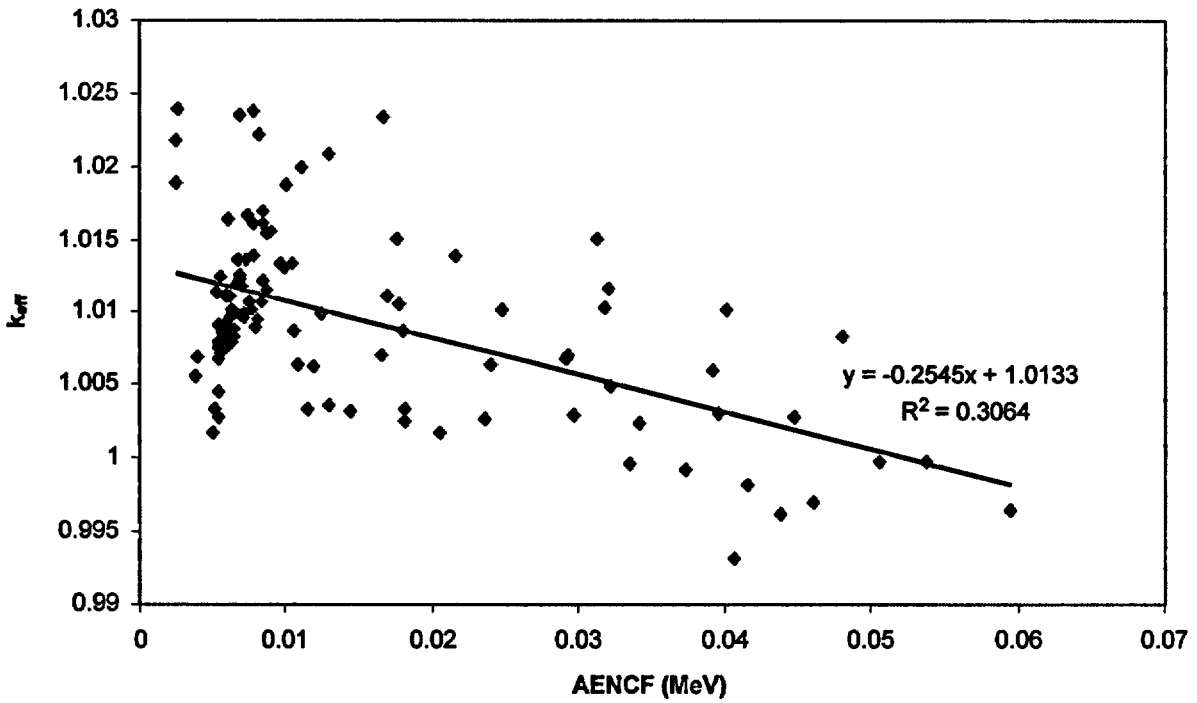

Figure 16. Plutonium Solution Subset with AENCF as Trending Parameter

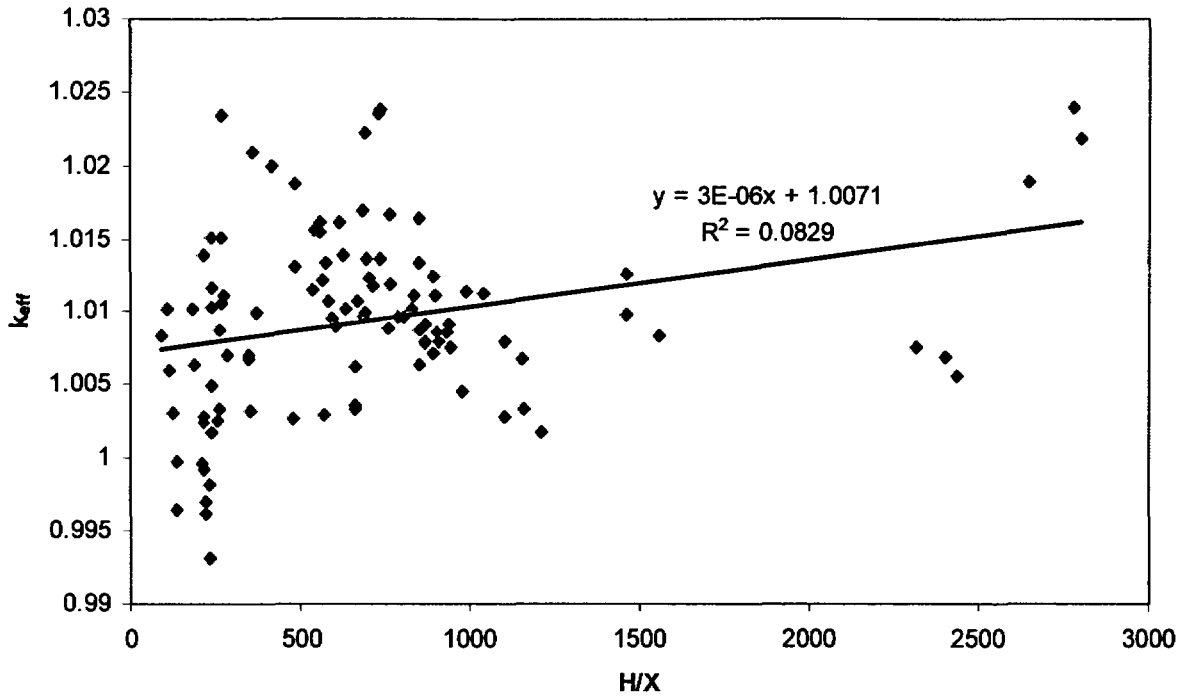

Figure 17. Plutonium Solution Subset with H/X as Trending Parameter

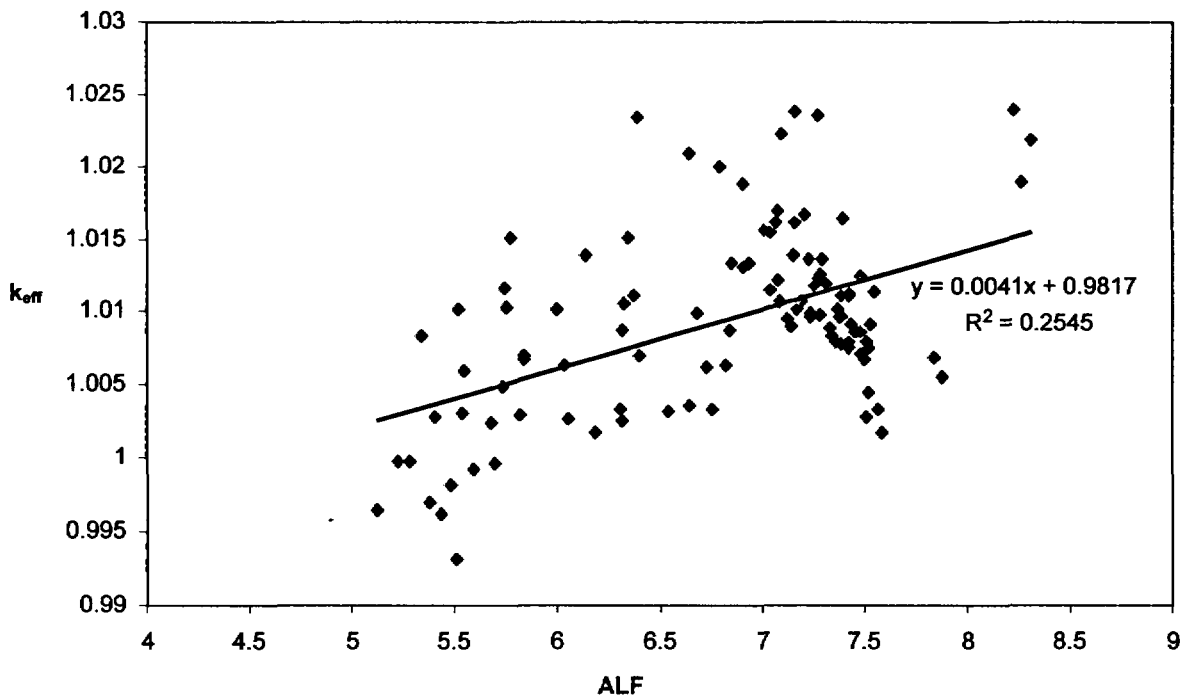

Figure 18. Plutonium Solution Subset with ALF as Trending Parameter

7.2.3 Lower Bound Tolerance Limit Determination

The lower bound tolerance limit is characterized by statistical tolerance limits that account for biases and uncertainties associated with the criticality code trending process. The lower bound tolerance

limit is calculated by CLREG only when a trending regression is identified as statistically significant. If no trend is identified, then the NDTL or the distribution-free tolerance limit method is used as previously discussed in Section 6.1.1.3.

CLREG is a computer program that calculates sets of lower bound tolerance limit functions based on benchmark experiment results. Each lower bound tolerance limit represents the value of k_{eff} at which a configuration is considered potentially critical. This method accounts for the criticality analysis method bias and uncertainty of the calculated critical k_{eff} values for a set of critical experiments that represent the waste package, as explained by linear regression trending. A complete discussion of the statistical methodology for CLREG is provided in the CLREG documentation (BSC 2001).

Lower bound tolerance limits were calculated for each subset of experiments for the parameter that had the most statistically significant trend. This is determined by which parameter has a correlation coefficient that is closest to one. The most conservative lower bound tolerance limit from experiments applicable to a particular configuration class is then selected for use in establishing the CL for that configuration.

The CLREG results, as a function of the most statistically significant trending parameters, are provided in Attachment I and illustrated in Figures 19 through 21, with the selected lower bound tolerance limit values presented in Table 33 for each of the subsets. The results presented in Table 33 were generated for a 95 percent confidence level covering 99.5 percent of the population. For the UO_2 solution experiments, Figures 22 and 23 show that the data set appears to be normally distributed therefore the NDTL method was used for calculating the lower bound tolerance limit.

Table 33. Lower Bound Tolerance Limits for Experiment Subsets

Subset	Trend Parameter	Lower Bound Tolerance Limt
CRCs	Core Average Burnup (BU)	f(BU) = -2.403E-4*BU + 0.9858
Lattice LCEs	Pin Pitch (P)	f(P) = 7.0175E-03*P + 0.9677 (1.32 cm ≤ P ≤ 1.89 cm); f(P) = 0.982 (1.89 cm < P ≤ 2.64 cm)[a]
UO_2 Solutions	None	f(x) = 0.952[b]
Plutonium Solutions	AENCF	f(AENCF) = 0.980 (2.46E-03 MeV ≤ AENCF ≤ 5.07E-02 MeV)

NOTES: [a] Upper limit set at 0.982 since no positive bias credit is taken.
[b] Calculated using the NDTL method with 95 percent confidence level covering 99.5 percent of the population.

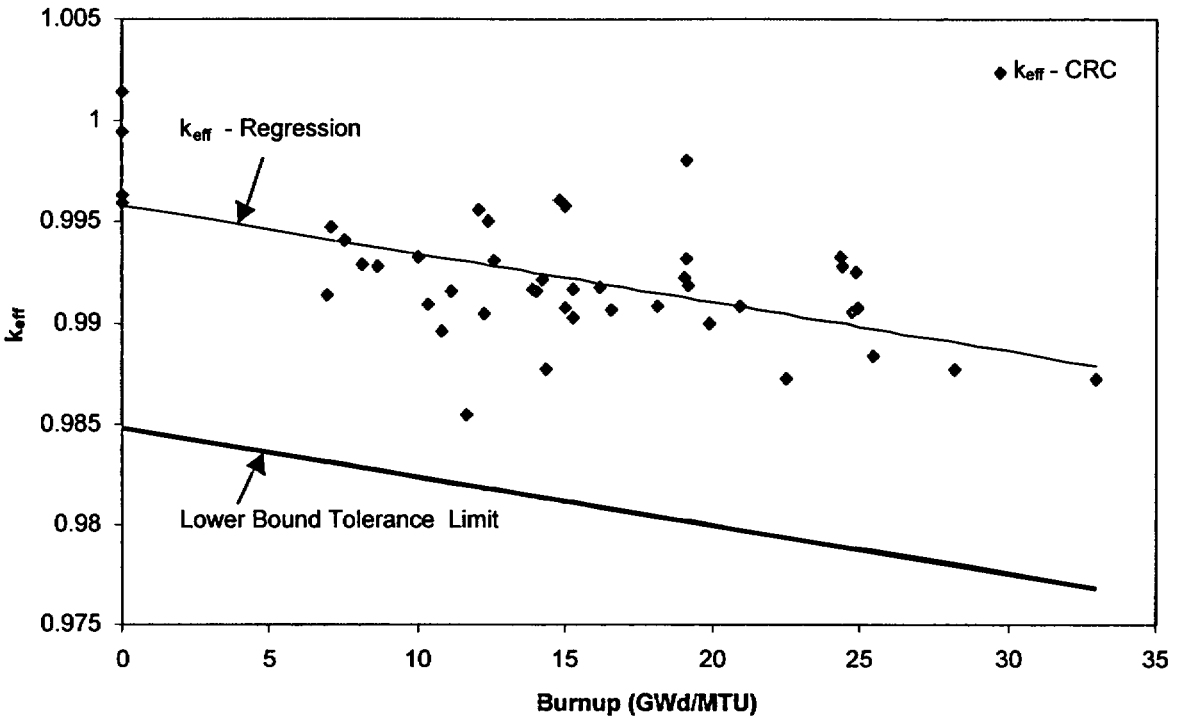

Figure 19. Critical Limit Plot for CRC Experiment Subset

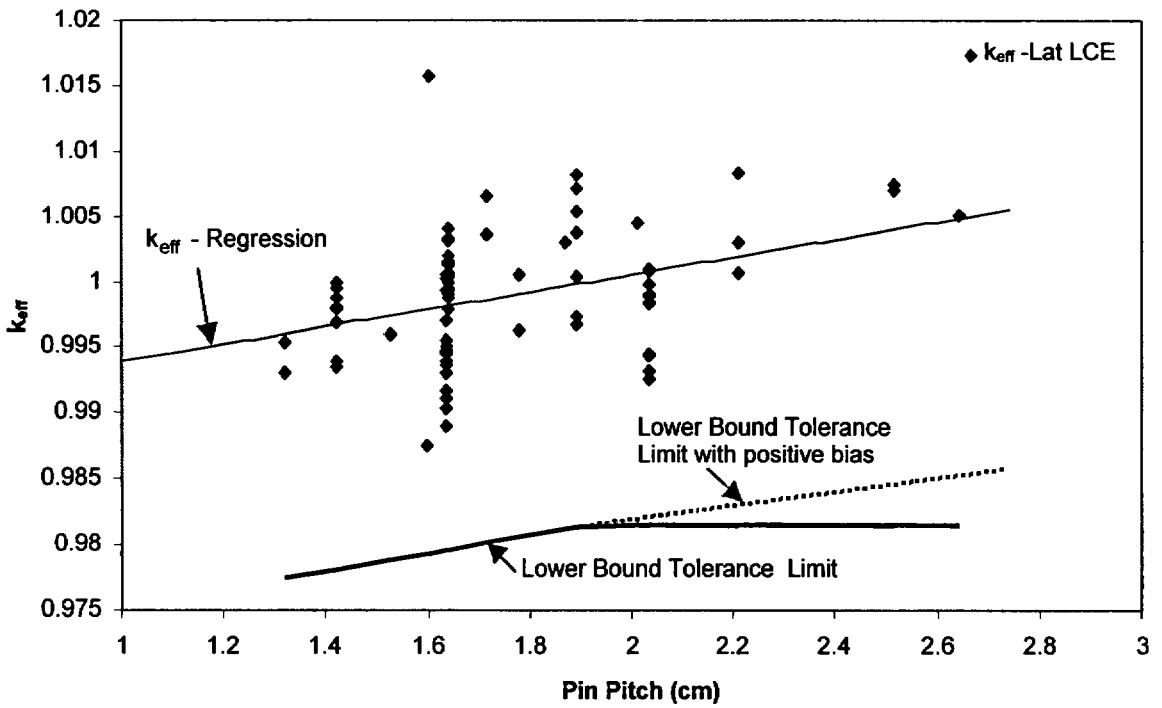

Figure 20. Critical Limit Plot for Lattice LCE Subset

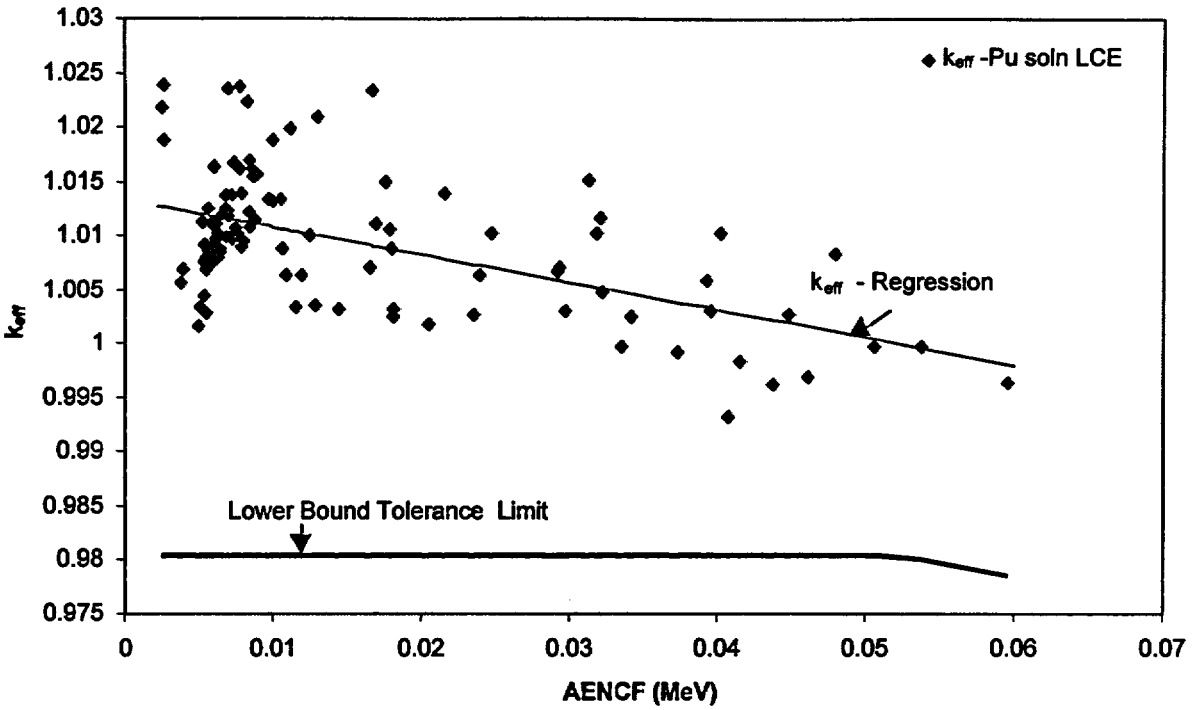

Figure 21. Critical Limit Plot for Plutonium Solution LCE Subset

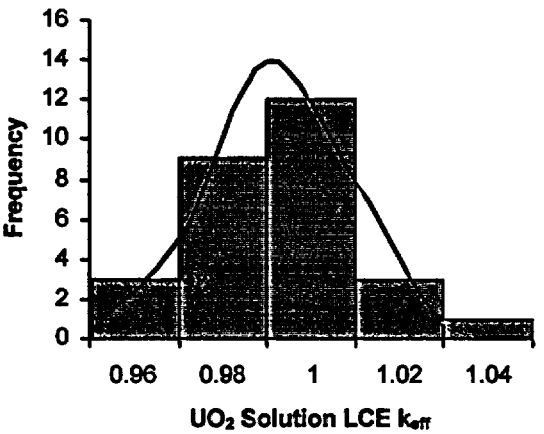

Figure 22. Histogram Plot for UO_2 Solution LCE k_{eff} Values

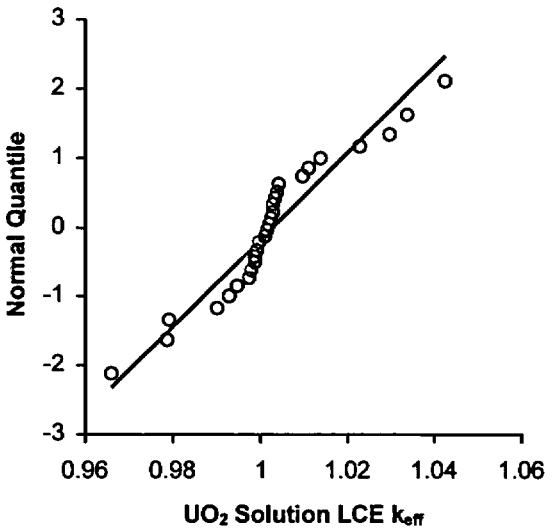

Figure 23. Normal Quantile Plot for UO_2 Solution LCE k_{eff} Values

7.2.4 Range of Applicability

When evaluating biases and uncertainties and choosing parameters (or areas) for which a bias would exhibit a trend, there are three fundamental areas (Lichtenwalter et al. 1997, p. 179) that should be considered:

1. Materials of the waste package and the waste form, especially the fissionable materials
2. The geometry of the waste package and waste forms
3. The inherent neutron energy spectrum affecting the fissionable materials.

In this case, the application is for four experiment subsets representative of a waste package in various forms of degradation as defined by the Master Scenarios (YMP 2003, Figures 3-2a and 3-2b).

Important areas for evaluating criticality are the geometry of the configuration, the concentration of important materials (reflecting materials, moderating materials, fissionable materials, and significant neutron absorbing materials), and the nuclear cross sections that characterize the nuclear reaction rates that will occur in a system containing fissionable and absorbing materials.

In a light-water moderated and reflected environment with fuel rods arranged in a lattice configuration, the neutronic behavior (spectra) is expected to be fairly constant in terms of relative distribution regardless of the surrounding environment. Differences in neutron spectra between the various configurations are expected to occur as a result of factors including H/X ratio, material differences, and moderator temperature differences.

Figure 24 illustrates the neutron flux spectral characteristics that were compared for a representative 21 PWR waste package (WP in Figure 24), a CRC statepoint, two MOX LCEs - SSR53 (12x12 PuO_2 lattice) and EXP22 (12x12 PuO_2 Lattice), and one fresh fuel LCE (SSR48 UO_2 lattice). The MCNP input and output files used to generate the spectral tallies are listed in Attachment III but contained in Attachment IV.

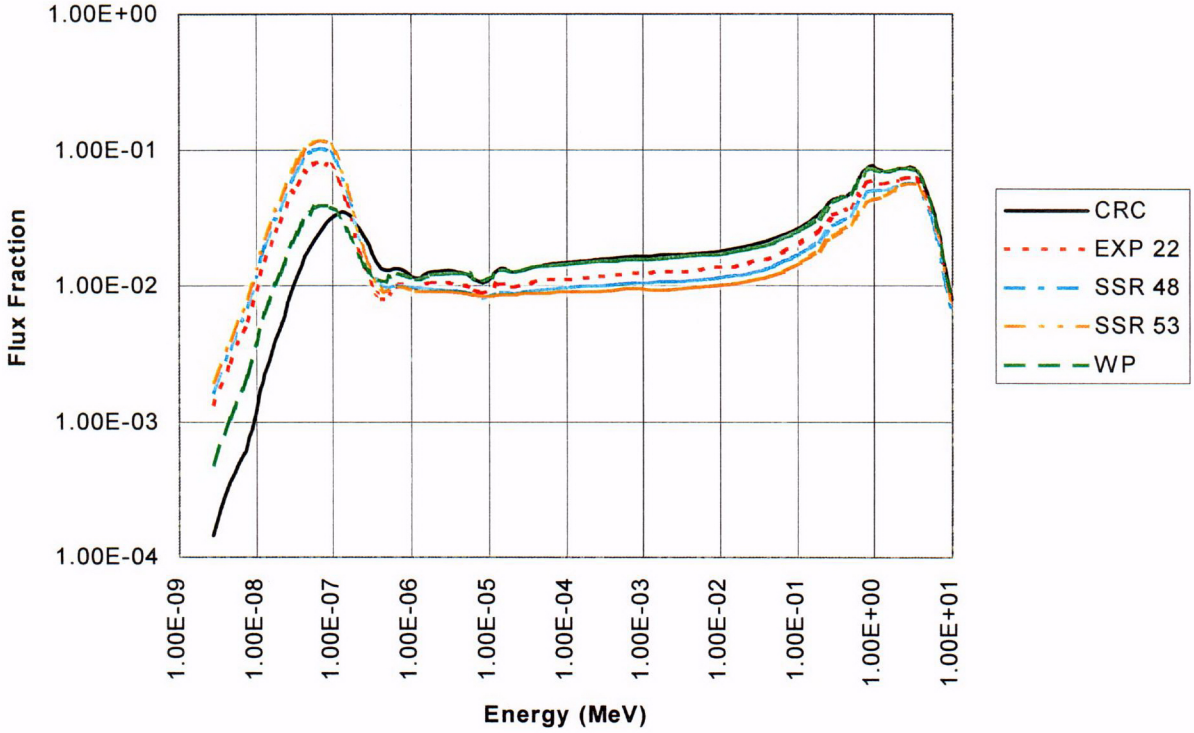

Figure 24. Neutron Energy Spectra of Waste Package and Critical Benchmarks

The commercial reactor used for the CRC data was the Crystal River Unit 3 PWR with statepoint data corresponding to a mid-cycle restart, performed 400 EFPD into Cycle 6. A fuel assembly arrangement in the CRC was modeled as shown in Figure 25. A 21-assembly area of the core was modeled in a fully flooded, intact waste package configuration as shown in Figure 25. The waste package representation was loaded with a grouping of 21 assemblies out of the CRC statepoint to remove material composition differences from the comparison. The burned fuel assemblies represented in the waste package varied in average assembly burnup from 16.4 through 34.4 GWd/MTU and initial enrichments of 2.64 through 3.49 weight percent uranium-235. Each of the fuel assemblies was modeled explicitly with 18 axial nodes in both the CRC and in the waste package and was depleted through each of their own unique operating history profiles.

C03

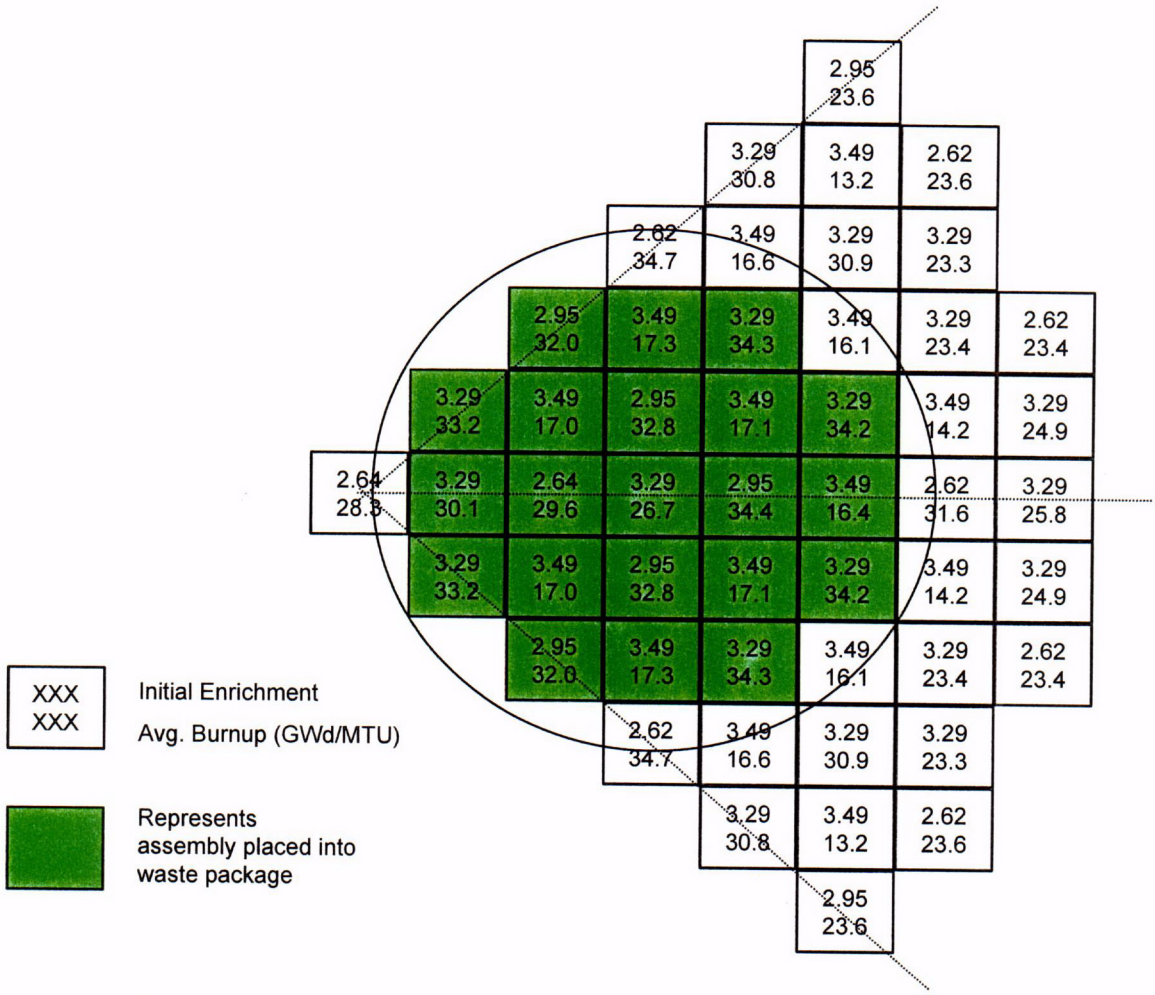

Figure 25. Radial Profile for CRC and Waste Package Spectral Comparison

A basic understanding of the effect of the spectral variations on reactivity can be achieved by evaluating the fission and absorption reaction rates between the systems. The energy dependent reaction rates are the product of the neutron flux spectrum and the energy dependent total macroscopic cross section. The probability of a fission reaction occurring in the fuel material when a neutron is absorbed in the fuel can be expressed in terms of cross sections. It is the ratio of the fission cross section to that of the total absorption cross section in the fuel material. A plot of reaction rate ratios for a fresh fuel waste package configuration is also provided for comparison against the LCEs in order to exhibit that the fuel material composition is what is governing the reaction rates. With the total macroscopic cross sections for the fuel region in the CRCs and waste package being composed of nearly the same isotopics, the fission probability in the fuel material for these two systems will be very nearly the same as shown in Figure 26. The magnitude of the fission to absorption ratio for the CRCs and waste package will vary based on burnup, but the shape and area under the curve are expected to remain similar between the two systems.

In the spectral characteristic comparisons, the average flux fraction versus energy was calculated across the system as well as the fission and reaction rates. Although spectral shifts of the type seen in the LCEs are the result of several effects (e.g., material, H/X ratio, etc.), when compared to the

waste package (WP in Figure 26), the results indicate that CRCs are just as adequate for benchmarks and more closely represents the reaction rates for burned fuel in a waste package configuration.

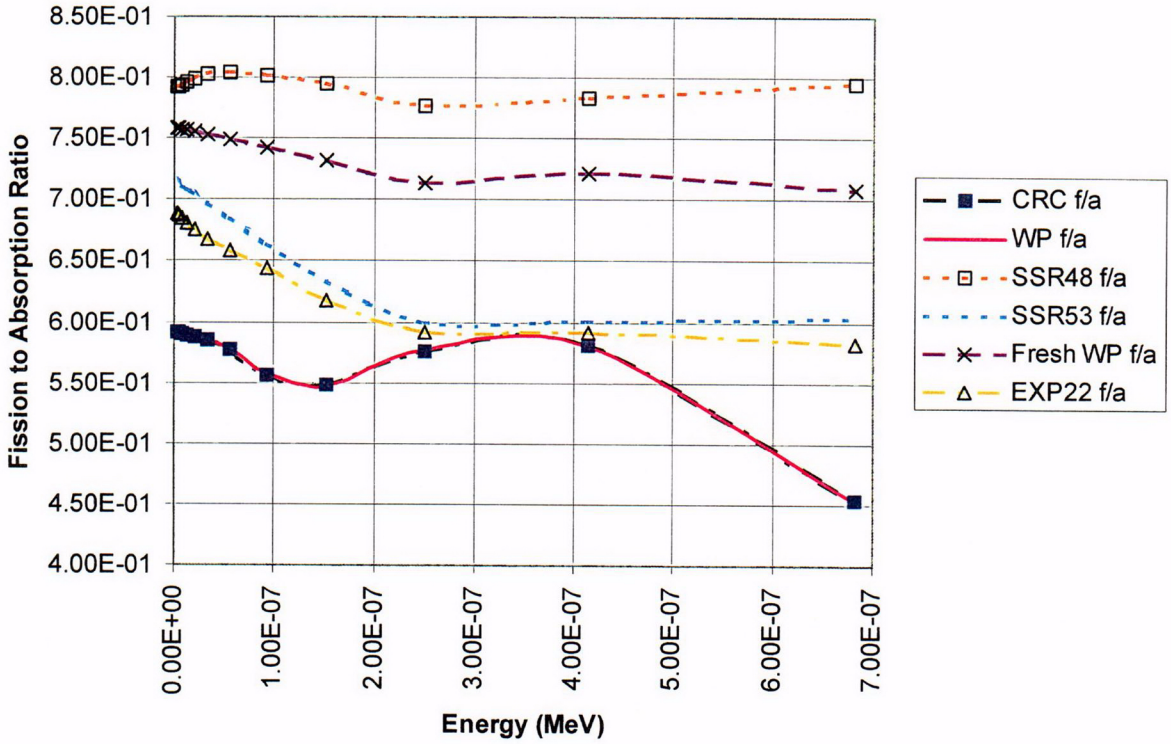

Figure 26. Thermal Region Reaction Ratio Comparison

The ROA covered by the current set of benchmark experiments are summarized in Table 34.

Table 34. Experiment Parameter Summary

Subset	Number of Experiments	Range of Applicability
CRCs	45	Initial enrichment (wt% ^{235}U): 1.93 through 4.17; System average burnup (GWd/MTU): 0.0 through 33; Applicable to intact lattice geometry; Pin pitch (cm): 1.26 through 1.44
Lattice LCEs	83	Initial enrichment (wt% ^{235}U): 2.35 through 5.74; mixture of uranium and MOX fuel; Pin Pitch (cm): 1.32 through 2.64 Applicable to intact lattice geometry
UO_2 Solutions	28	Initial enrichment (wt% ^{235}U): 1.01 through 9.97; H/X: 318 through 1098; Applicable to homogeneous mixtures
Plutonium Solutions	107	Initial enrichment (wt% ^{239}Pu): 91.1 through 99.5; H/X: 91 through 2803; AENCF (eV): 2.46E-03 through 5.07E-02; Applicable to homogeneous mixtures

7.2.5 Extension of the Range of Applicability

Since the validation approach is to calculate sets of CLs based on different groupings of benchmark experiments, the ROA and the ROP are the same, therefore, there is no need to extend the ROA. An example application extending the ROA where a trend is identified in the data is provided in Attachment II.

7.3 ACCEPTANCE CRITERIA

The acceptance criteria are determined by the final comparison of a configuration's k_{eff} with the applicable CL. In equation notation the acceptance criteria for a waste package system is as follows:

$$k_S + \Delta k_S < CL \qquad \text{(Eq. 12)}$$

where

k_s = calculated k_{eff} for the system

Δk_s = an allowance for

(a) statistical or convergence uncertainties, or both in the computation of k_s

(b) material and fabrication tolerances, and

(c) uncertainties due to the geometric or material representations used in the computational method

(Note: b and c above can be obviated through the use of bounding representations)

CL = the value of k_{eff} at which a configuration is considered potentially critical, accounting for the criticality analysis method bias and uncertainty, and any additional uncertainties (i.e., Δk_{EROA} and/or Δk_{ISO})

The applicability of the computational method is determined through the establishment of CLs based on standard statistical techniques applied to criticality benchmark experiments, and the determination of the ROA. The acceptance criteria for the four subsets of experiments that are applicable to different configuration classes are provided in Table 35. The lower bound tolerance limits (established in Section 7.2.3) are equivalent to the CL over the ROA for the experiment subsets provided in Table 34. If a ROP provided by the configuration generator model is beyond the ROA, then either additional benchmark experiments to encompass the ROP or applicable penalties (Δk_{EROA} and/or Δk_{ISO}) will need to be applied to the lower bound tolerance limit in establishing acceptance criteria.

Table 35. Acceptance Criteria for Experiment Subsets

Subset	Trend Parameter	Acceptance Criteria
CRCs	Core Average Burnup (BU)	$k_s + \Delta k_s < -2.403E\text{-}4*BU + 0.9858$
Lattice LCEs	Pin Pitch (P)	$k_s + \Delta k_s < 7.0175E\text{-}03*P + 0.9677$ (1.32 cm ≤ P ≤ 1.89 cm); $k_s + \Delta k_s < 0.982$ (1.89 cm < P ≤ 2.64 cm)
UO_2 Solutions	None	$k_s + \Delta k_s < 0.952$
Plutonium Solutions	AENCF	$k_s + \Delta k_s < 0.980$ (2.46E-03 MeV ≤ AENCF ≤ 5.07E-02 MeV)

8. CONCLUSIONS

This model report documents the criticality model and its validation. The validation uses current data for pressurized water reactor spent nuclear fuel and provides a validated model that may be updated as additional data becomes available. The criticality model process was discussed in

Section 6, and illustrates how criticality potential for configurations of fissionable materials is determined.

Based on the criticality benchmark experiment results presented throughout Section 7.1 in Tables 7 through 27, this report concludes that the criticality model is valid for evaluating the criticality potential of configurations of PWR fuel within the proposed repository at Yucca Mountain, Nevada. This model report recommends that the criticality model be implemented for PWR spent nuclear fuel. The MCNP code was selected to perform the Monte Carlo method along with ENDF/B cross section libraries as implemented by MCNP for representing neutron transport. A set of benchmark experiments was presented to cover the range of potential waste form configuration classes in Section 7.1. The major parameters covered by the benchmark experiments were burnup, initial enrichment, spectrum, and geometry. Criticality benchmark experiment trending parameter analyses were performed and the results presented in Tables 29 through 32. The selected benchmark experiments were separated into subset applicability from which CLs were statistically derived in Section 7.2, and a specified ROA was provided in Table 34. Acceptance criteria were established for the experiment subsets over the given ROA in Table 35.

The criticality model process documented in this report contributes to or meets the acceptance criteria stated in Section 4.2 through the development of criticality acceptance criteria for a given configuration class.

Three open items from Reamer (2000) were addressed in this model report. They were Open Items 13, 15, and 17, as listed in Section 4.2. Open Item 13 is addressed in Section 6.2 by accounting for uncertainties based on Δk_{EROA} and Δk_{ISO} in the CL calculation. The term Δk_m which represents an arbitrary margin to ensure subcriticality is not applicable for use in postclosure analyses since there is no requirement to maintain subcriticality during the postclosure time period. Open Item 15 is addressed in Section 6.2.1 by the use of the Δk_{ISO} term to the CL calculation. Open Item 17 is addressed in Section 6.2.1.2 because the methodology for extending the range of applicability follows the procedures defined in ANSI/ANS-8.1-1998, C4(a) and C4(b).

The criticality model is a process rather than a mathematical model, therefore data output is not developed. Application of the criticality model will be in analyses of the various configurations of fissionable materials anticipated over time in the proposed repository.

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9.2 CODES, STANDARDS, REGULATIONS, AND PROCEDURES

ANSI/ANS-8.1-1998. *Nuclear Criticality Safety in Operations with Fissionable Material Outside Reactors.* La Grange Park, Illinois: American Nuclear Society. TIC: 242363.

ANSI/ANS-8.17-1984. *Criticality Safety Criteria for the Handling, Storage, and Transportation of LWR Fuel Outside Reactors.* La Grange Park, Illinois: American Nuclear Society. TIC: 231625.

AP-2.22Q, Rev. 1, ICN 0. *Classification Analyses and Maintenance of the Q-List.* Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: DOC.20030807.0002.

9.3 SOFTWARE CODES

Software Code: CLREG. V1.0. PC - Windows 2000. 10528-1.0-01.

Software Code: MCNP. 4B2LV. HP. 30033 V4B2LV.

10. ATTACHMENTS

The description of the attachments is listed in Table 36.

Table 36. Attachment Listing

Attachment	Number of Pages	Description
I	6	CLREG Critical Limit function results
II	2	Results for example of the extension of the range of applicability
III	1	Listing of CLREG and MCNP spectral characteristic input and output files contained in Attachment IV
IV	N/A	Compact disc attachment containing CLREG and MCNP spectral characteristic input and output files

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ATTACHMENT I

This attachment lists the CLREG critical limit function results. The results for each of the subsets is provided in Tables I-1 through I-3. Descriptions for the meanings of the values in each column can be obtained from the CLREG documentation (BSC 2001).

Table I-1. CRCs with Core Average Burnup as Trend Parameter

Ind Var	K_{eff}(cc)	Pred K_{eff}	PreClos CL	LUTB CL	Bonf LTL
0.00E+00	0.996	0.996	0.991	0.985	0.984
0.00E+00	0.996	0.996	0.991	0.985	0.984
0.00E+00	0.999	0.996	0.991	0.985	0.984
0.00E+00	1.001	0.996	0.991	0.985	0.984
6.92E+00	0.991	0.994	0.989	0.983	0.983
7.08E+00	0.995	0.994	0.989	0.983	0.983
7.50E+00	0.994	0.994	0.989	0.983	0.983
8.09E+00	0.993	0.994	0.989	0.983	0.982
8.67E+00	0.993	0.994	0.989	0.983	0.982
1.00E+01	0.993	0.993	0.989	0.982	0.982
1.03E+01	0.991	0.993	0.988	0.982	0.982
1.08E+01	0.990	0.993	0.988	0.982	0.982
1.11E+01	0.992	0.993	0.988	0.982	0.982
1.17E+01	0.985	0.993	0.988	0.982	0.982
1.20E+01	0.996	0.993	0.988	0.982	0.981
1.23E+01	0.990	0.993	0.988	0.982	0.981
1.23E+01	0.995	0.993	0.988	0.982	0.981
1.25E+01	0.993	0.993	0.988	0.982	0.981
1.39E+01	0.992	0.992	0.988	0.981	0.981
1.40E+01	0.992	0.992	0.988	0.981	0.981
1.42E+01	0.992	0.992	0.988	0.981	0.981
1.43E+01	0.988	0.992	0.988	0.981	0.981
1.48E+01	0.996	0.992	0.987	0.981	0.981
1.50E+01	0.991	0.992	0.987	0.981	0.981
1.50E+01	0.996	0.992	0.987	0.981	0.981
1.52E+01	0.992	0.992	0.987	0.981	0.981
1.53E+01	0.990	0.992	0.987	0.981	0.981
1.61E+01	0.992	0.992	0.987	0.981	0.980
1.66E+01	0.991	0.992	0.987	0.981	0.980
1.81E+01	0.991	0.991	0.987	0.980	0.980
1.90E+01	0.992	0.991	0.986	0.980	0.980
1.91E+01	0.993	0.991	0.986	0.980	0.980
1.91E+01	0.998	0.991	0.986	0.980	0.980
1.92E+01	0.992	0.991	0.986	0.980	0.980
1.99E+01	0.990	0.991	0.986	0.980	0.980
2.10E+01	0.991	0.991	0.986	0.980	0.979
2.25E+01	0.987	0.990	0.986	0.979	0.979
2.44E+01	0.993	0.990	0.985	0.979	0.978
2.44E+01	0.993	0.990	0.985	0.979	0.978
2.47E+01	0.991	0.990	0.985	0.979	0.978
2.49E+01	0.992	0.990	0.985	0.979	0.978
2.49E+01	0.991	0.990	0.985	0.979	0.978
2.54E+01	0.988	0.990	0.985	0.979	0.978
2.82E+01	0.988	0.989	0.984	0.978	0.978
3.30E+01	0.987	0.988	0.983	0.977	0.976

Table I-2. Lattice LCEs with Pitch as Trend Parameter

Ind Var	K_{eff}(cc)	Pred K_{eff}	PreClos CL	LUTB CL	Bonf LTL
1.32E+00	0.993	0.996	0.987	0.977	0.977
1.32E+00	0.995	0.996	0.987	0.977	0.977
1.42E+00	0.994	0.997	0.988	0.978	0.977
1.42E+00	0.998	0.997	0.988	0.978	0.977
1.42E+00	0.998	0.997	0.988	0.978	0.977
1.42E+00	0.999	0.997	0.988	0.978	0.977
1.42E+00	1.000	0.997	0.988	0.978	0.977
1.42E+00	0.997	0.997	0.988	0.978	0.977
1.42E+00	0.993	0.997	0.988	0.978	0.977
1.42E+00	0.998	0.997	0.988	0.978	0.977
1.42E+00	1.000	0.997	0.988	0.978	0.977
1.53E+00	0.996	0.997	0.989	0.979	0.978
1.60E+00	0.988	0.998	0.989	0.979	0.978
1.60E+00	1.016	0.998	0.989	0.979	0.978
1.64E+00	0.995	0.998	0.990	0.980	0.979
1.64E+00	0.996	0.998	0.990	0.980	0.979
1.64E+00	0.994	0.998	0.990	0.980	0.979
1.64E+00	0.995	0.998	0.990	0.980	0.979
1.64E+00	1.000	0.998	0.990	0.980	0.979
1.64E+00	1.001	0.998	0.990	0.980	0.979
1.64E+00	0.989	0.998	0.990	0.980	0.979
1.64E+00	0.993	0.998	0.990	0.980	0.979
1.64E+00	0.995	0.998	0.990	0.980	0.979
1.64E+00	0.997	0.998	0.990	0.980	0.979
1.64E+00	0.995	0.998	0.990	0.980	0.979
1.64E+00	0.999	0.998	0.990	0.980	0.979
1.64E+00	0.991	0.998	0.990	0.980	0.979
1.64E+00	0.990	0.998	0.990	0.980	0.979
1.64E+00	0.994	0.998	0.990	0.980	0.979
1.64E+00	0.995	0.998	0.990	0.980	0.979
1.64E+00	0.994	0.998	0.990	0.980	0.979
1.64E+00	0.994	0.998	0.990	0.980	0.979
1.64E+00	0.992	0.998	0.990	0.980	0.979
1.64E+00	0.998	0.998	0.990	0.980	0.979
1.64E+00	0.999	0.998	0.990	0.980	0.979
1.64E+00	1.000	0.998	0.990	0.980	0.979
1.64E+00	1.001	0.998	0.990	0.980	0.979
1.64E+00	1.002	0.998	0.990	0.980	0.979
1.64E+00	1.003	0.998	0.990	0.980	0.979
1.64E+00	0.999	0.998	0.990	0.980	0.979
1.64E+00	0.999	0.998	0.990	0.980	0.979
1.64E+00	1.001	0.998	0.990	0.980	0.979
1.64E+00	1.003	0.998	0.990	0.980	0.979
1.64E+00	1.001	0.998	0.990	0.980	0.979
1.64E+00	0.999	0.998	0.990	0.980	0.979
1.64E+00	1.004	0.998	0.990	0.980	0.979
1.64E+00	1.000	0.998	0.990	0.980	0.979
1.64E+00	1.000	0.998	0.990	0.980	0.979
1.64E+00	1.000	0.998	0.990	0.980	0.979
1.64E+00	1.002	0.998	0.990	0.980	0.979
1.64E+00	1.001	0.998	0.990	0.980	0.979
1.64E+00	0.999	0.998	0.990	0.980	0.979
1.72E+00	1.007	0.999	0.990	0.980	0.979
1.72E+00	1.004	0.999	0.990	0.980	0.979
1.78E+00	1.001	0.999	0.990	0.981	0.980
1.78E+00	0.996	0.999	0.990	0.981	0.980

Table I-2. Lattice LCEs with Pitch as Trend Parameter (Continued)

Ind Var	K_{eff}(cc)	Pred K_{eff}	PreClos CL	LUTB CL	Bonf LTL
1.87E+00	1.003	1.000	0.991	0.981	0.980
1.89E+00	1.008	1.000	0.991	0.981	0.980
1.89E+00	1.007	1.000	0.991	0.981	0.980
1.89E+00	1.005	1.000	0.991	0.981	0.980
1.89E+00	1.004	1.000	0.991	0.981	0.980
1.89E+00	0.997	1.000	0.991	0.981	0.980
1.89E+00	0.997	1.000	0.991	0.981	0.980
1.89E+00	1.000	1.000	0.991	0.981	0.980
2.01E+00	1.005	1.001	0.991	0.982	0.981
2.03E+00	0.998	1.001	0.991	0.982	0.981
2.03E+00	0.993	1.001	0.991	0.982	0.981
2.03E+00	1.001	1.001	0.991	0.982	0.981
2.03E+00	0.993	1.001	0.991	0.982	0.981
2.03E+00	0.993	1.001	0.991	0.982	0.981
2.03E+00	1.000	1.001	0.991	0.982	0.981
2.03E+00	0.994	1.001	0.991	0.982	0.981
2.03E+00	0.994	1.001	0.991	0.982	0.981
2.03E+00	1.001	1.001	0.991	0.982	0.981
2.03E+00	0.999	1.001	0.991	0.982	0.981
2.03E+00	0.998	1.001	0.991	0.982	0.981
2.03E+00	0.999	1.001	0.991	0.982	0.981
2.21E+00	1.001	1.002	0.991	0.982	0.981
2.21E+00	1.003	1.002	0.991	0.982	0.981
2.21E+00	1.008	1.002	0.991	0.982	0.981
2.52E+00	1.007	1.004	0.991	0.982	0.981
2.52E+00	1.008	1.004	0.991	0.982	0.981
2.64E+00	1.005	1.005	0.991	0.982	0.981

Table I-3. Plutonium Solution Experiments with AENCF as Trend Parameter

Ind Var	K_{eff}(cc)	Pred K_{eff}	PreClos CL	LUTB CL	Bonf LTL
2.46E-03	1.022	1.013	0.991	0.980	0.980
2.57E-03	1.019	1.013	0.991	0.980	0.980
2.66E-03	1.024	1.013	0.991	0.980	0.980
3.80E-03	1.006	1.012	0.991	0.980	0.980
3.93E-03	1.007	1.012	0.991	0.980	0.980
5.05E-03	1.002	1.012	0.991	0.980	0.980
5.14E-03	1.003	1.012	0.991	0.980	0.980
5.24E-03	1.011	1.012	0.991	0.980	0.980
5.38E-03	1.009	1.012	0.991	0.980	0.980
5.41E-03	1.004	1.012	0.991	0.980	0.980
5.43E-03	1.008	1.012	0.991	0.980	0.980
5.47E-03	1.003	1.012	0.991	0.980	0.980
5.48E-03	1.008	1.012	0.991	0.980	0.980
5.49E-03	1.007	1.012	0.991	0.980	0.980
5.60E-03	1.012	1.012	0.991	0.980	0.980
5.61E-03	1.007	1.012	0.991	0.980	0.980
5.64E-03	1.009	1.012	0.991	0.980	0.980
5.71E-03	1.009	1.012	0.991	0.980	0.980
5.79E-03	1.009	1.012	0.991	0.980	0.980
5.89E-03	1.009	1.012	0.991	0.980	0.980
5.93E-03	1.011	1.012	0.991	0.980	0.980
5.93E-03	1.008	1.012	0.991	0.980	0.980
5.94E-03	1.011	1.012	0.991	0.980	0.980
5.97E-03	1.008	1.012	0.991	0.980	0.980
6.10E-03	1.016	1.012	0.991	0.980	0.980
6.19E-03	1.010	1.012	0.991	0.980	0.980
6.20E-03	1.011	1.012	0.991	0.980	0.980
6.20E-03	1.008	1.012	0.991	0.980	0.980
6.23E-03	1.010	1.012	0.991	0.980	0.980
6.31E-03	1.010	1.012	0.991	0.980	0.980
6.33E-03	1.008	1.012	0.991	0.980	0.980
6.48E-03	1.008	1.012	0.991	0.980	0.980
6.51E-03	1.009	1.012	0.991	0.980	0.980
6.64E-03	1.012	1.012	0.991	0.980	0.980
6.78E-03	1.014	1.012	0.991	0.980	0.980
6.84E-03	1.010	1.012	0.991	0.980	0.980
6.84E-03	1.013	1.012	0.991	0.980	0.980
6.91E-03	1.024	1.012	0.991	0.980	0.980
6.93E-03	1.012	1.012	0.991	0.980	0.980
7.03E-03	1.012	1.012	0.991	0.980	0.980
7.15E-03	1.010	1.011	0.991	0.980	0.980
7.20E-03	1.010	1.011	0.991	0.980	0.980
7.23E-03	1.014	1.011	0.991	0.980	0.980
7.38E-03	1.017	1.011	0.991	0.980	0.980
7.55E-03	1.011	1.011	0.991	0.980	0.980
7.66E-03	1.010	1.011	0.991	0.980	0.980
7.76E-03	1.016	1.011	0.991	0.980	0.980
7.77E-03	1.024	1.011	0.991	0.980	0.980
7.85E-03	1.014	1.011	0.991	0.980	0.980
7.90E-03	1.009	1.011	0.991	0.980	0.980
8.05E-03	1.010	1.011	0.991	0.980	0.980
8.27E-03	1.022	1.011	0.991	0.980	0.980
8.38E-03	1.011	1.011	0.991	0.980	0.980
8.45E-03	1.017	1.011	0.991	0.980	0.980
8.45E-03	1.012	1.011	0.991	0.980	0.980
8.52E-03	1.016	1.011	0.991	0.980	0.980

Table I-3. Plutonium Solution Experiments with AENCF as Trend Parameter (Continued)

Ind Var	K_{eff}(cc)	Pred K_{eff}	PreClos CL	LUTB CL	Bonf LTL
8.73E-03	1.015	1.011	0.991	0.980	0.980
8.79E-03	1.011	1.011	0.991	0.980	0.980
8.96E-03	1.016	1.011	0.991	0.980	0.980
9.73E-03	1.013	1.011	0.991	0.980	0.980
9.94E-03	1.013	1.011	0.991	0.980	0.980
1.00E-02	1.019	1.011	0.991	0.980	0.980
1.05E-02	1.013	1.011	0.991	0.980	0.980
1.06E-02	1.009	1.011	0.991	0.980	0.980
1.09E-02	1.006	1.011	0.991	0.980	0.980
1.11E-02	1.020	1.010	0.991	0.980	0.980
1.16E-02	1.003	1.010	0.991	0.980	0.980
1.20E-02	1.006	1.010	0.991	0.980	0.980
1.25E-02	1.010	1.010	0.991	0.980	0.980
1.30E-02	1.004	1.010	0.991	0.980	0.980
1.30E-02	1.021	1.010	0.991	0.980	0.980
1.45E-02	1.003	1.010	0.991	0.980	0.980
1.65E-02	1.007	1.009	0.991	0.980	0.980
1.68E-02	1.023	1.009	0.991	0.980	0.980
1.70E-02	1.011	1.009	0.991	0.980	0.980
1.76E-02	1.015	1.009	0.991	0.980	0.980
1.78E-02	1.011	1.009	0.991	0.980	0.980
1.80E-02	1.009	1.009	0.991	0.980	0.980
1.81E-02	1.003	1.009	0.991	0.980	0.980
1.82E-02	1.003	1.009	0.991	0.980	0.980
2.06E-02	1.002	1.008	0.991	0.980	0.980
2.16E-02	1.014	1.008	0.991	0.980	0.980
2.36E-02	1.003	1.007	0.991	0.980	0.980
2.40E-02	1.006	1.007	0.991	0.980	0.980
2.48E-02	1.010	1.007	0.991	0.980	0.980
2.92E-02	1.007	1.006	0.991	0.980	0.980
2.93E-02	1.007	1.006	0.991	0.980	0.980
2.97E-02	1.003	1.006	0.991	0.980	0.980
3.13E-02	1.015	1.005	0.991	0.980	0.980
3.18E-02	1.010	1.005	0.991	0.980	0.980
3.21E-02	1.012	1.005	0.991	0.980	0.980
3.23E-02	1.005	1.005	0.991	0.980	0.980
3.36E-02	1.000	1.005	0.991	0.980	0.980
3.42E-02	1.002	1.005	0.991	0.980	0.980
3.74E-02	0.999	1.004	0.991	0.980	0.980
3.93E-02	1.006	1.003	0.991	0.980	0.980
3.97E-02	1.003	1.003	0.991	0.980	0.980
4.02E-02	1.010	1.003	0.991	0.980	0.980
4.08E-02	0.993	1.003	0.991	0.980	0.980
4.16E-02	0.998	1.003	0.991	0.980	0.980
4.39E-02	0.996	1.002	0.991	0.980	0.980
4.48E-02	1.003	1.002	0.991	0.980	0.980
4.61E-02	0.997	1.002	0.991	0.980	0.980
4.81E-02	1.008	1.001	0.991	0.980	0.980
5.07E-02	1.000	1.000	0.991	0.980	0.980
5.39E-02	1.000	1.000	0.990	0.980	0.979
5.96E-02	0.996	0.998	0.989	0.979	0.978

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ATTACHMENT II

This attachment provides the results for an example of the extension of the ROA and associated Δk_{eff} penalty. Descriptions for the meanings of the values in each column can be obtained from the CLREG documentation (BSC 2001).

It is expected that the most limiting configuration class will be configuration class 1. This is where the waste package internal components degrade faster than the waste form. This will cause the system to lose boron from the basket materials and bring the intact lattice fuel assemblies into a more optimum spacing with regards to criticality. The current ROA for this configuration class covers lattice assemblies, varying in enrichment from 1.93 through 4.17 weight percent uranium-235, and a system average burnup range of 0.0 through 33.0 GWd/MTU. Many assembly burnups will be beyond this value, which may cause the system average to be greater than 33.0, therefore, an extension of the ROA is necessary to determine what the critical limit should be for a system average burnup greater than 33.0. The process of calculating the CL for the extension of ROA is performed by CLREG. An example of extending the burnup for the CRC benchmark experiments from the CLREG output is tabulated in Table II-1 and illustrated in Figure II-1.

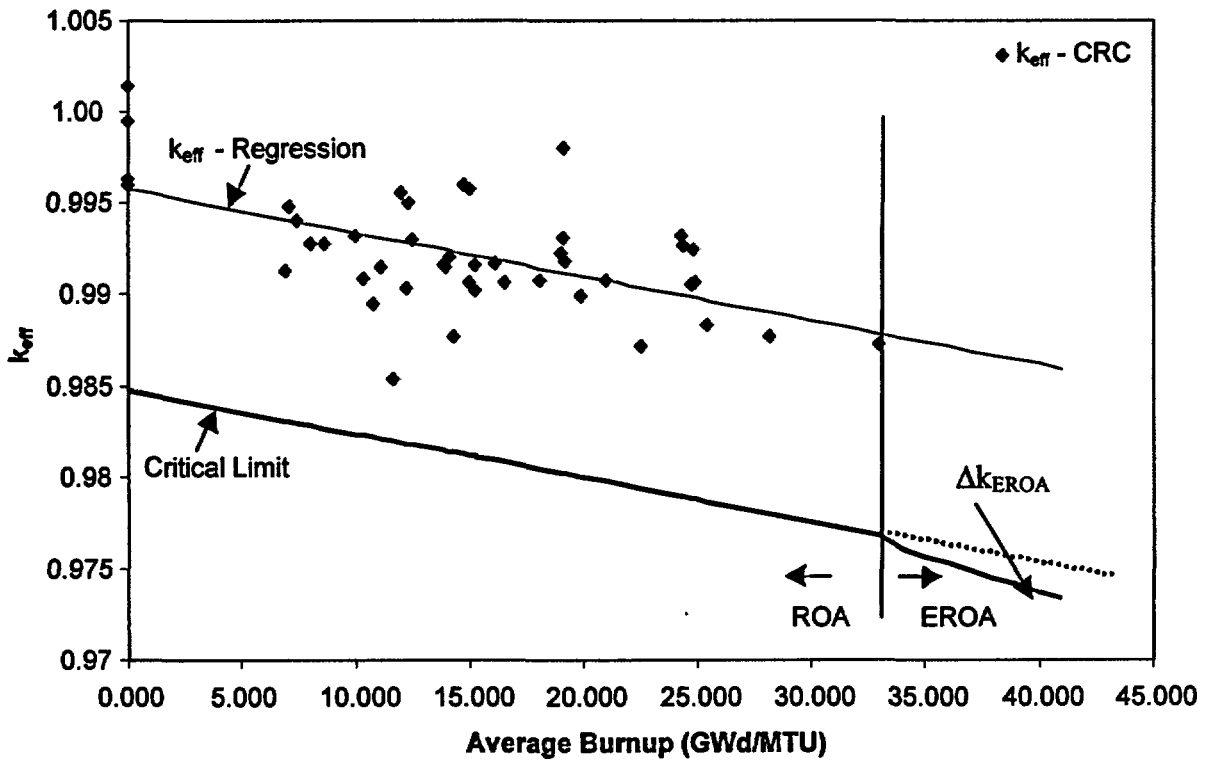

Figure II-1. Example of EROA

Table II-1. CRC EROA Results with Core Average Burnup as Trend Parameter

Ind Var	K_{eff}(cc)	Pred K_{eff}	PreClos CL	LUTB CL	Bonf LTL
0.00E+00	0.996	0.996	0.991	0.985	0.984
0.00E+00	0.996	0.996	0.991	0.985	0.984
0.00E+00	0.999	0.996	0.991	0.985	0.984
0.00E+00	1.001	0.996	0.991	0.985	0.984
6.92E+00	0.991	0.994	0.989	0.983	0.983
7.08E+00	0.995	0.994	0.989	0.983	0.983
7.50E+00	0.994	0.994	0.989	0.983	0.983
8.09E+00	0.993	0.994	0.989	0.983	0.982
8.67E+00	0.993	0.994	0.989	0.983	0.982
1.00E+01	0.993	0.993	0.989	0.982	0.982
1.03E+01	0.991	0.993	0.988	0.982	0.982
1.08E+01	0.990	0.993	0.988	0.982	0.982
1.11E+01	0.992	0.993	0.988	0.982	0.982
1.17E+01	0.985	0.993	0.988	0.982	0.982
1.20E+01	0.996	0.993	0.988	0.982	0.981
1.23E+01	0.990	0.993	0.988	0.982	0.981
1.23E+01	0.995	0.993	0.988	0.982	0.981
1.25E+01	0.993	0.993	0.988	0.982	0.981
1.39E+01	0.992	0.992	0.988	0.981	0.981
1.40E+01	0.992	0.992	0.988	0.981	0.981
1.42E+01	0.992	0.992	0.988	0.981	0.981
1.43E+01	0.988	0.992	0.988	0.981	0.981
1.48E+01	0.996	0.992	0.987	0.981	0.981
1.50E+01	0.991	0.992	0.987	0.981	0.981
1.50E+01	0.996	0.992	0.987	0.981	0.981
1.52E+01	0.992	0.992	0.987	0.981	0.981
1.53E+01	0.990	0.992	0.987	0.981	0.981
1.61E+01	0.992	0.992	0.987	0.981	0.980
1.66E+01	0.991	0.992	0.987	0.981	0.980
1.81E+01	0.991	0.991	0.987	0.980	0.980
1.90E+01	0.992	0.991	0.986	0.980	0.980
1.91E+01	0.993	0.991	0.986	0.980	0.980
1.91E+01	0.998	0.991	0.986	0.980	0.980
1.92E+01	0.992	0.991	0.986	0.980	0.980
1.99E+01	0.990	0.991	0.986	0.980	0.980
2.10E+01	0.991	0.991	0.986	0.980	0.979
2.25E+01	0.987	0.990	0.986	0.979	0.979
2.44E+01	0.993	0.990	0.985	0.979	0.978
2.44E+01	0.993	0.990	0.985	0.979	0.978
2.47E+01	0.991	0.990	0.985	0.979	0.978
2.49E+01	0.992	0.990	0.985	0.979	0.978
2.49E+01	0.991	0.990	0.985	0.979	0.978
2.54E+01	0.988	0.990	0.985	0.979	0.978
2.82E+01	0.988	0.989	0.984	0.978	0.978
3.30E+01	0.987	0.988	0.983	0.977	0.976
EROA Calculations					
3.40E+01	0.988	0.988	0.976	0.976	0.976
3.50E+01	0.987	0.987	0.976	0.976	0.976
3.60E+01	0.987	0.987	0.975	0.975	0.975
3.70E+01	0.987	0.987	0.975	0.975	0.975
3.80E+01	0.987	0.987	0.975	0.975	0.975
3.90E+01	0.986	0.986	0.974	0.974	0.974
4.00E+01	0.986	0.986	0.974	0.974	0.974
4.10E+01	0.986	0.986	0.973	0.973	0.973

ATTACHMENT III

This attachment contains a listing of the CLREG and MCNP files that are contained on the compact disc attachment (Attachment IV).

Filename	File Type	File Size (bytes)	File Date	File Time	Description
crcbu01.csv	Excel	1,045	9/09/2002	08:10a	Input file for CRC subset using burnup as the trend parameter
crcbu01out.csv	Excel	3,861	9/09/2002	08:12a	Output file for CRC subset using burnup as the trend parameter
crcbu01util	ASCII	3,186	9/09/2002	08:12a	CLREG generated utility file for CRC subset using burnup as the trend parameter
latlcepitch.csv	Excel	1,875	8/13/2002	04:52p	Input file for lattice LCE subset using pitch as the trend parameter
latlcepitchout.csv	Excel	7,053	8/13/2002	05:04p	Output file for lattice LCE subset using pitch as the trend parameter
latlcepitchutil	ASCII	4,900	8/13/2002	05:04p	CLREG generated utility file for lattice LCE subset using pitch as the trend parameter
pusolaencf.csv	Excel	2,651	8/13/2002	04:54p	Input file for Pu solution subset using AENCF as trend parameter
pusolaencfout.csv	Excel	9,069	8/13/2002	05:07p	Output file for Pu solution subset using AENCF as trend parameter
pusolaencfutil	ASCII	5,979	8/13/2002	05:07p	CLREG generated utility file for Pu solution subset using AENCF as trend parameter
crceroaout.csv	Excel	4,553	9/09/2002	08:20a	Output file for extension of the range of applicability example
crceroa.csv	Excel	1,125	9/09/2002	08:19a	Input file for extension of the range of applicability example
crceroautil	ASCII	3,546	9/09/2002	08:20a	CLREG generated utility file for extension of the range of applicability example
crc2O	ASCII	16,017,660	4/28/2003	08:28a	MCNP output file for flux tallies of fuel in reactor
crc2	ASCII	1,877,920	4/28/2003	08:28a	MCNP input file for flux tallies of fuel in reactor
crct4	ASCII	1,880,664	4/28/2003	08:27a	MCNP input file for reactor fission and absorption rates
crct4O	ASCII	16,636,263	4/28/2003	08:27a	MCNP output file for reactor fission and absorption rates
exp22e5	ASCII	6,709	4/28/2003	08:26a	LCE MCNP input file for spectral characteristics
exp22e5O	ASCII	641,684	4/28/2003	08:26a	LCE MCNP output file for spectral characteristics
freshwp	ASCII	29,567	4/28/2003	08:29a	MCNP input for fresh fuel waste package spectral characteristics
freshwpO	ASCII	930,880	4/28/2003	08:29a	MCNP output for fresh fuel waste package spectral characteristics
ssr48.i	ASCII	13,728	4/28/2003	08:28a	LCE MCNP input file for spectral characteristics
ssr48.O	ASCII	405,369	4/28/2003	08:28a	LCE MCNP output file for spectral characteristics
ssr53.i	ASCII	13,577	4/28/2003	08:28a	LCE MCNP input file for spectral characteristics
ssr53.O	ASCII	213,140	4/28/2003	08:28a	LCE MCNP output file for spectral characteristics
wp2	ASCII	694,945	4/28/2003	08:28a	MCNP input file for flux tallies of fuel in waste package
wp2O	ASCII	5,753,624	4/28/2003	08:28a	MCNP output file for flux tallies of fuel in waste package
WPt4	ASCII	705,142	4/28/2003	08:27a	MCNP input file for waste package fission and absorption rates
WPt4O	ASCII	6,419,716	4/28/2003	08:27a	MCNP output file for waste package fission and absorption rates