MODEL COVER SHEET

Complete Only Applicable Items

DOC.20030319.0001

2. Type of Mathematical Model

Process Model

Abstraction Model

System Model

Describe Intended Use of Model:

Quantify computational bias and uncertainty for criticality safety applications

Technical Contact/Department:

John M. Scaglione/ Risk & Criticality

3. Title:

Criticality Model Report

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

MDL-EBS-NU-000003 REV 00 ICN 01

5. Total Attachments:

4

6. Attachment Numbers – No. of Pages in Each:

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MODEL REVISION RECORD

1. Page: 2 of 84

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CONTENTS

	Page
ACRONYMS	9
1. PURPOSE	11
2. QUALITY ASSURANCE	13
3. USE OF COMPUTER SOFTWARE	15
3.1 MCNP	15
3.2 CLREG	15
4. INPUTS	17
4.1 DATA AND PARAMETERS	17
4.1.1 Material Cross Sections	17
4.1.2 Criticality Benchmark Experiments	19
4.2 CRITERIA	19
4.3 CODES AND STANDARDS	20
5. ASSUMPTIONS	21
6. MODEL DISCUSSION	23
6.1 DISCUSSION OF UNCERTAINTIES	24
6.2 DISCUSSION OF ALTERNATIVES	24
6.2.1 Code Alternatives	24
6.2.2 Data Set Alternatives	25
7. VALIDATION	29
7.1 CRITICALITY EXPERIMENT SELECTION	30
7.1.1 CRC Experiments	32
7.1.2 Lattice Laboratory Critical Experiments	35
7.1.3 Homogeneous Solution Experiments	43
7.2 BIAS AND UNCERTAINTY	53
7.2.1 Statistical Analyses	57
7.2.2 Regression Analyses	58
7.2.3 Critical Limit Determination	67
7.3 RANGE OF APPLICABILITY	70
7.4 ACCEPTANCE CRITERIA	74
7.5 FUTURE ACTIVITIES	76
8. CONCLUSIONS	77
9. INPUTS AND REFERENCES	79
10. ATTACHMENTS	83
ATTACHMENT I	I-1
ATTACHMENT II	II-1
ATTACHMENT III	III-1

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FIGURES

	Page
6-1. PWR CRC Eigenvalues	27
7-1. Process for Calculating Critical Limits.....	55
7-2. CRC Subset with AENCF as Trending Parameter	60
7-3. CRC Subset with Core Average Burnup as Trending Parameter	61
7-4. CRC Subset with Soluble Boron Concentration as Trending Parameter.....	61
7-5. CRC Subset with ALF as Trending Parameter	62
7-6. UO ₂ and MOX LCE Subset with AENCF as Trending Parameter.....	62
7-7. UO ₂ and MOX LCE Subset with P/D as Trending Parameter.....	63
7-8. UO ₂ and MOX LCE Subset with Pin Pitch as Trending Parameter	63
7-9. UO ₂ and MOX LCE Subset with Water to Fuel Volume Ratio as Trending Parameter	64
7-10. Uranium Solution Subset with AENCF as Trending Parameter.....	64
7-11. Uranium Solution Subset with H/X as Trending Parameter	65
7-12. Uranium Solution Subset with ALF as Trending Parameter	65
7-13. Plutonium Solution Subset with AENCF as Trending Parameter	66
7-14. Plutonium Solution Subset with H/X as Trending Parameter	66
7-15. Plutonium Solution Subset with ALF as Trending Parameter	67
7-16. Critical Limit Plot for CRC Experiment Subset	68
7-17. Critical Limit Plot for Lattice LCE Subset	69
7-18. Critical Limit Plot for Pu Solution LCE Subset.....	69
7-19. Neutron Energy Spectra of Waste Package and Critical Benchmarks	71
7-20. Radial Profile for CRC and Waste Package Spectral Comparison.....	72
7-21. Thermal Region Reaction Ratio Comparison	73
7-22. Process for Establishing Criticality Acceptance Criteria	75
II-1. Example of EROA	II-2

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TABLES

	Page
4-1. Selected MCNP ZAIIDs for Various Elements and Isotopes	17
6-1. Principal Isotopes for Commercial SNF Burnup Credit	25
6-2. CRC Fuel Isotopes Set Description	26
7-1. General CR3 CRC Statepoint Information	32
7-2. General TMI1 CRC Statepoint Information	34
7-3. General SQ2 CRC Statepoint Information	34
7-4. General MG1 CRC Statepoint Information	35
7-5. Clusters of 2.35 wt% UO ₂ Fuel Rods with Different Absorber Plates	36
7-6. Water-Reflected Fuel Rod Cluster Critical Experiments	36
7-7. Clusters of 4.31 wt% UO ₂ Fuel Rods with Different Reflectors	37
7-8. Configurations with 4.31 wt% UO ₂ Fuel Rods in Highly Borated Water Lattices.....	37
7-9. Configurations with Neutron Flux Traps	38
7-10. EPRI 2.35 wt% UO ₂ Critical Configurations.....	38
7-11. Lead-Reflected UO ₂ Rod Array Critical Experiment	38
7-12. Urania-Gadolinia Critical Experiments	39
7-13. Saxton Single-Region Critical Configurations	40
7-14. Saxton Multi-Region Critical Configurations.....	40
7-15. Close Proximity Critical Benchmarks.....	41
7-16. EPRI Mixed Oxide Critical Configurations.....	42
7-17. Critical Configuration of MOX and UO ₂ Fuel Rods in a Triangular Lattice.....	43
7-18. Configurations Incorporating Mixed Plutonium and Natural Uranium Nitrate Solutions	44
7-19. Configurations Incorporating Plutonium Nitrate Solutions	46
7-20. Configurations Incorporating Low-Enrichment Uranium Solutions	51
7-21. Configurations Incorporating Uranyl Fluoride Solutions	52
7-22. Equality Test Statistic Results	58
7-23. CRC Trending Parameter Results	59
7-24. UO ₂ and MOX LCE Trending Parameter Results	60
7-25. Uranium Solution Trending Parameter Results	60
7-26. Pu Solution Trending Parameter Results	60
7-27. Critical Limits for Experiment Subsets.....	68
7-28. Experiment Parameter Summary	73
10-1. Attachment Listing	83
I-1. CRCs with Core Average Burnup as Trend Parameter	I-1
I-2. Lattice LCEs with Pitch as Trend Parameter	I-2
I-3. Pu Solution Experiments with AENCF as Trend Parameter	I-3
II-1. CRC EROA Results with Core Average Burnup as Trend Parameter	II-1

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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
BSC	Bechtel SAIC Company, LLC
B&W	Babcock & Wilcox
CL	critical limit
CPU	central processing unit
CR3	Crystal River Unit 3
CRC	commercial reactor critical
CRWMS	Civilian Radioactive Waste Management System
DFTL	distribution free tolerance limit
DOE	U.S. Department of Energy
EFPD	Effective Full Power Days
EPRI	Electric Power Research Institute
EROA	extension of the range of applicability
FWF	fissionable waste form
LCE	laboratory critical experiment
LUTB	lower uniform tolerance band
M&O	Management & Operations
MG1	McGuire Unit 1
MOX	mixed oxide
NDTL	normal distribution tolerance limit
NRC	U.S. Nuclear Regulatory Commission
OCRWM	Office of Civilian Radioactive Waste Management
OIC	other internal components
PNL	Pacific Northwest Laboratory
PWR	pressurized water reactor
QARD	Quality Assurance Requirements and Description
ROA	range of applicability
ROP	range of parameters
SQ2	Sequoyah Unit 2
SNF	spent nuclear fuel
STN	Software Tracking Number
TMI1	Three Mile Island Unit 1

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1. PURPOSE

The purpose of the *Criticality Model Report* is to validate the MCNP (CRWMS M&O 1998h) code's ability to accurately predict the effective neutron multiplication factor (k_{eff}) for a range of conditions spanned by various critical configurations representative of the potential configurations commercial reactor assemblies stored in a waste package may take. Results of this work are an indication of the accuracy of MCNP for calculating eigenvalues, which will be used as input for criticality analyses for spent nuclear fuel (SNF) storage at the proposed Monitored Geologic Repository.

The scope of this report is to document the development and validation of the criticality model. The scope of the criticality model is only applicable to commercial pressurized water reactor fuel. Valid ranges are established as part of the validation of the criticality model. This model activity follows the description in BSC (2002a).

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2. QUALITY ASSURANCE

The activities associated with the development of this report have been performed in accordance with the U.S. Department of Energy Office of Civilian Radioactive Waste Management (OCRWM) *Quality Assurance Requirements and Description* (QARD) (DOE 2002) controls. The information provided in this report will be used in the methodology for evaluation of the proposed Monitored Geologic Repository engineered barrier system. A number of classification analyses (e.g., CRWMS M&O [1999a, Section 7]) have identified components of the engineered barrier system as items important to radiological safety and waste isolation. CRWMS M&O (1999a, Section 7) classifies the uncanistered fuel disposal container system, which is a part of the engineered barrier system, a quality level 1 item.

Electronic management of data was accomplished in accordance with the controls specified in the Technical Work Plan (BSC 2002a).

The work that is to be performed to support the License Application using this information will be performed in accordance with the then current versions of the QARD and Nuclear Regulatory Commission (NRC) regulations.

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3. USE OF COMPUTER SOFTWARE

The referenced results reported in this document were drawn from various documents that used software subject to the requirements of the QARD. 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. In addition, the following approved software was used.

3.1 MCNP

The baselined MCNP code (CRWMS M&O 1998h) was not used directly in this report, but was used in the supporting documentation. The software specifications are as follows:

- Program Name: MCNP
- Version/Revision Number: Version 4B2LV
- Status/Operating System: Qualified/HP-UX B.10.20
- Computer Software Configuration Item Number: 30033 V4B2LV
- Computer Type: HP 9000 Series Workstations
- CPU number: 700887

The MCNP software used was: (a) appropriate for the application of multiplication factor calculations, (b) used only within the range of validation as documented throughout References Briesmeister (1997) and CRWMS M&O (1998i), and (c) obtained from Software Configuration Management in accordance with appropriate procedures.

3.2 CLREG

The CLREG computer code (BSC 2002b) was used to calculate the critical limit (CL) for the benchmark experiments provided, and extend the range of applicability for the critical limit. The software specifications are as follows:

- Program Name: CLREG
- Version/Revision Number: V1.0
- Status/Operating System: Qualified/Windows 2000
- Software Tracking Number (STN) Number: 10528-1.0-01
- Computer Type: Personal Computer
- Computer Processing Unit (CPU) number: 150527

CLREG is a computer program that calculates sets of critical limits (critical limit functions) for waste packages under certain conditions. Each CL 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 explained by linear regression trending. Also inherent in each CL value is the statistical property of confidence for lower prediction limits and lower tolerance limits. The input and output files for the CLREG calculations are documented in Attachment III such that an independent repetition of the software use could be performed. The CLREG software used was:

(a) appropriate for the calculation of critical limits, (b) used only within the range of validation as documented in BSC (2002b), and (c) obtained from Software Configuration Management in accordance with appropriate procedures.

4. INPUTS

4.1 DATA AND PARAMETERS

4.1.1 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 for the various neutron interactions are used to determine the flow of the criticality calculation at each interaction site. 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 Briesmeister (1997, Appendix G).

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% 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 ZAIID identifier. The ZAIID 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 ZAIID nomenclature is available in Briesmeister (1997, Appendix G).

Calculations involving transport through the resonance region should 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 4-1 contains a listing of elements and isotopes selected for use in the criticality model. The following cross-section libraries were selected for use in the report *Selection of MCNP Cross Section Libraries* (CRWMS M&O 1998j). It should be noted that in application of the criticality model, the room temperature cross-section data will be used.

Table 4-1. Selected MCNP ZAIIDs for Various Elements and Isotopes

Element	Isotope	Cross Section Library ZAIID ^a	Element	Isotope	Cross Section Library ZAIID ^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

Table 4-1. Selected MCNP ZAIDs for Various Elements and Isotopes

Element	Isotope	Cross Section Library ZAID ^a	Element	Isotope	Cross Section Library ZAID ^a
Carbon	B-11	5011.56c		Sm-150	62150.50c
	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	67155.55c
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)		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
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

Table 4-1. Selected MCNP ZAIDs for Various Elements and Isotopes

Element	Isotope	Cross Section Library ZAID ^a	Element	Isotope	Cross Section Library ZAID ^a
Yttrium	Y-88	39088.35c	Plutonium	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		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	Americium	Pu-243	94243.60c (B-VI.2)
	Rh-105	45105.50c		Pu-244	94244.60c (B-VI.0)
Palladium	Pd-105	46105.50c		Am-241	95241.50c
	Pd-108	46108.50c	Curium	Am-242m	95242.50c
Silver	Ag-107	47107.60c (B-VI.0)		Am-243	95243.50c
	Ag-109	47109.60c (B-VI.0)		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
	I-127	53127.60c (T-2)		Cm-245	96245.35c
	I-129	53129.60c (B-VI.0)		Cm-246	96246.35c
Xenon	I-135	53135.50c		Cm-247	96247.35c
	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)
Cesium	Xe-135	54135.54c		Cf-252	98252.60c (B-VI.2)
	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)			

NOTE: ^a Information in parentheses “()” for the ENDF/B-VI cross-sections indicate which release

4.1.2 Criticality Benchmark Experiments

Criticality experiments were selected from a group of experiments that include laboratory critical experiments (LCEs) and commercial reactor criticals (CRCs). Numerous references were used as indicated in Section 7 along with descriptions of pertinent information regarding each of the experiments.

4.2 CRITERIA

This report provides information that can be used to address the following criteria:

- During the preclosure period, the disposal container/waste package shall be designed such that the effective multiplication factor (k_{eff}) is less than or equal to 0.95 under assumed accident conditions considering allowances for the bias in the method of calculation and the uncertainty in the experiments used to validate the method of calculation (BSC 2001, p. 16).

- During the postclosure period, the features, events, and processes considered in the performance assessment should represent a wide range of both beneficial and potentially adverse effects on performance (e.g., beneficial effects of radionuclide sorption and potentially adverse effects of fracture flow or a criticality event). Those features, events, and processes expected to materially affect compliance with 10 CFR 63.113 (b) or be potentially adverse to performance are included, while events (event classes or scenario classes that are very unlikely [less than one chance in 10,000 over 10,000 years]) can be excluded from the analysis (10 CFR 63.102 [j]).

4.3 CODES AND STANDARDS

The following standard is used as the basis of this report.

- ANSI/ANS-8.1-1998. *Nuclear Criticality Safety in Operations with Fissionable Material Outside Reactors*.

5. ASSUMPTIONS

Assumptions that were used in the supporting documentation for this report are provided in the various individual documents referenced by this report along with their basis and rationale.

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6. MODEL DISCUSSION

The criticality model applies the Monte Carlo method along with material cross-section data in evaluating the criticality potential of configurations of fissionable and other materials identified by the degradation analyses. The code system used to calculate k_{eff} is MCNP, which uses the "Monte Carlo" method for representing neutron transport. Neutron transport can best be described by Equation 6-1 (Duderstadt & Hamilton 1976, p. 113).

$$\frac{\partial n}{\partial t} + v\Omega \cdot \nabla n + v \Sigma_t n(r, E, \Omega, t) = \int_{4\pi} d\Omega' \int_0^\infty dE' v' \Sigma_s(E' \rightarrow E, \Omega' \rightarrow \Omega) n(r, E', \Omega', t) + s(r, E, \Omega, t) \quad (\text{Eq. 6-1})$$

where (a complete description of all variables is provided in Duderstadt & Hamilton [1976, pp. 103-114])

- 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 duplicate theoretically 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. Using appropriate material cross-section data in the criticality calculation is essential to obtaining credible results. 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.

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 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.

6.1 DISCUSSION OF UNCERTAINTIES

Due to a lack of prototypic spent-fuel critical experiments, and the range of potential configurations of waste package internal components over the regulatory period of the repository, different approaches are necessary in order to validate the criticality model in a piecemeal fashion. The establishment of the code bias can be made with results from a variety of benchmarks together to ensure adequate safety margin for applications using burnup credit in storage packages.

Sources and impacts of uncertainty involve the following:

- Not all isotopes in the selected MCNP cross section library are available at hot reactor temperatures, although U-235 is available at higher temperatures and so is U-238 which dominates the spent fuel inventory and resonance absorption. This uncertainty is inherent in the computed code bias.
- The use of an integral benchmark approach with regard to commercial reactor criticals (CRCs). The calculation of spent fuel isotopic material compositions produces uncertainty in the calculated spent fuel inventory that is used as input to MCNP. This uncertainty will be accounted for by the isotopic model and can be assessed as an additional penalty on the critical limit.
- Additional uncertainty is caused by the water scattering kernel. 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 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, but using the lower temperature kernel for applications against the bias.

6.2 DISCUSSION OF ALTERNATIVES

Alternate models were considered as well as alternate data sets for the criticality model.

6.2.1 Code Alternatives

The KENO code system (part of the SCALE code package [CRWMS M&O 2000]) was considered as an alternative code for criticality calculations. Due to it using a collapsed energy group structure for material cross-sections (versus continuous energy in MCNP), and earlier versions having a lack of flexibility in geometric modeling capabilities, all potential configurations of the waste package

internal configurations were not anticipated to be able to be represented, therefore it was not selected.

6.2.2 Data Set Alternatives

The criticality analysis model that will be applied in designing waste packages 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 availability of the commercial SNF isotopes. 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 6-1 lists these isotopes. The actinide ^{233}U from this table is not present in current generation commercial SNF. However, for long disposal time periods (tens of thousands of years), ^{233}U 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 1998b).

Table 6-1. 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	$^{242\text{m}}\text{Am}$
^{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 CRWMS M&O (1998c), using reactor operating history data from 4 different pressurized water reactors – Three Mile Island Unit 1 (TMI1), Crystal River Unit 3 (CR3), Sequoyah Unit 2 (SQ2), and McGuire Unit 1 (MG1). The reactor operating history information, pertinent details regarding assembly design schematics, and loading patterns were obtained from CRWMS M&O (1998d, 1998e, 1998f, and 1998g). Four different sets of burned fuel isotopes, in addition to O-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 U, Pu, and Am); and Actinide Only (consisting of 10 major actinide elements found in spent fuel). The isotope sets used are presented in Table 6-2.

Table 6-2. CRC Fuel Isotopes Set Description

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

NOTE: ^a BE = Best-Estimate; PI = Principal Isotope; PA = Principal Actinide; AO = Actinide Only

The CRC benchmark cases evaluated cover an initial enrichment range of 1.93 wt% U-235 to 4.167 wt% U-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 6-1 illustrates the k_{eff} values from the CRC benchmark results that were taken from CRWMS M&O (1998c, pp. 40-43). The results indicate, as expected, that as the number of spent fuel isotopes modeled increases, the scatter in the k_{eff} data decreases.

Figure 6-1. PWR CRC Eigenvalues

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7. VALIDATION

This section presents a systematic approach for validation of the calculational method used to determine the effective multiplication factor of a waste package. The validation approach is generally the same as given in ANSI/ANS 8.1, *Nuclear Criticality Safety in Operations with Fissionable Material Outside Reactors*. This section is organized as follows: 1) selected benchmark experiments and computational results, 2) bias and uncertainty calculation, and critical limits associated with the computer code used to calculate criticality, 3) establishment of the range of applicability of the benchmark experiments, and 4) the acceptance criteria used for criticality.

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 Range of Applicability (ROA).

Application of the criticality model will be in the analyses of a set of waste package configurations selected from the Master Scenarios which are discussed in YMP (2000, pp. 3-8 through 3-14). This report focuses on internal waste package configurations and parameters. The Range of Parameters (ROP) of the waste package configurations chosen should be within the parameters chosen for the ROA of the experiments. If the ROA includes the ROP, the next step would be to establish acceptance criteria. Critical limits will be determined and other margins or penalties will be used to determine if a particular configuration is critical. The term "penalty" is used in conjunction with extension of the ROA. The term "margin" is used to denote further reductions in the critical limits. The configurations to be validated for are as follows:

- The basket (other internal components [OIC]) is degraded, but the waste form is relatively intact (YMP 2000, p. 3-8, configurations IP-3a, b, c, d). For criticality to occur, several additional conditions are required: sufficient moderator is present, neutron absorber material is flushed from the waste package, and most of the fissionable material remains in the waste package. Configurations within this class arise from scenarios in which the basket containing the neutron absorber degrades before the waste form. They result from scenarios which involve the fissionable waste form (FWF) degrading at a much slower rate than the OICs. This configuration class will be referred to as *configuration #1* throughout the remainder of this document.
- Both basket and waste form are degraded simultaneously with the same three additional conditions (water, absorber removal, and fissionable material remaining) as configuration #1 above (YMP 2000, p. 3-8, configuration IP-2a). In general, this configuration will result in the fissionable material accumulating at the bottom of the waste package. Since both FWF and OIC 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 FWF and OIC. Intermediate configurations in which only the basket or the waste form is degraded first are covered by configuration classes 1 (above), or 3 (below). This configuration class will be referred to as *configuration #2* throughout the remainder of this document.

- The fissionable material from the waste form is mobilized and moved away from the neutron absorber, which remains in the largely intact basket (YMP 2000, p. 3-8, IP-1b). As with configuration #2, the fissionable material will most likely accumulate at the bottom of the waste package, but, unlike configuration #2, the physical opportunities for this transport and accumulation are limited because the basket is still largely intact. This configuration results from scenarios which involve the FWF degrading faster than the basket (OIC). An alternative configuration having these relative degradation rates is IP-1a (YMP 2000 p. 3-8), in which the fissionable component of the FWF does not move significantly after degradation. This configuration class will be referred to as *configuration #3* throughout the remainder of this document.
- Fissionable material accumulates at the bottom of the waste package, together with moderator provided either by water trapped in clay or by hydration of metal corrosion products, so that criticality can occur without standing water in the waste package (YMP 2000, p. 3-9, IP-4b, 5a, and 6a). The scenarios leading to this configuration class differ in that IP-4b (YMP 2000, p. 3-9) does not assume the neutron absorber has flushed from the waste package, but only assumes a relative displacement between fissionable material at the bottom of the waste package and neutron absorber distributed throughout the container. Configurations within this class can result from scenario groups which have penetrations in the bottom of the waste package, thus preventing standing water in the waste package. This flow-through removes soluble corrosion products, but leaves the insoluble corrosion products. This configuration class will be referred to as *configuration #4* throughout the remainder of this document.
- As with configuration #4 above, the moderator is provided by water trapped in clay, but in this case the fissionable material is distributed throughout a major fraction of the waste package's volume (YMP 2000, p. 3-9, IP-4a). This configuration class can only be reached if the FWF degrades faster than the OIC, so that the fissionable material remains in place to be locked in by its own hydration or by the hydration of OICs. This configuration class will be referred to as *configuration #5* throughout the remainder of this document.
- Waste form has degraded in place with OIC intact (YMP 2000, p. 3-8, IP-1a). This configuration class is of interest if the degradation of the waste form can distribute the fissionable material into a more reactive geometry than the intact waste form. This can happen with highly enriched research reactor SNF (CRWMS M&O 1998a). This configuration class will be referred to as *configuration #6* throughout the remainder of this document.

7.1 CRITICALITY EXPERIMENT SELECTION

The calculation method used to establish the criticality potential for a waste package needs to be validated against measured data that have been shown to be applicable to the package under consideration. This section provides brief descriptions of the benchmark experiments that have been selected to be utilized for the PWR criticality model validation.

Two types of experimental data are used in validating the criticality model. These are 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). It 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 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. Due to the waste package being 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 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 H/X ratio between the two systems, and causes a slight spectral shift.

The CRCs represent intact commercial SNF in known critical configurations. Although the CRC evaluations provide integral criticality benchmarks for SNF in a reactor, they do not provide separate benchmarks for isotopic concentrations of individual isotopes. The CRCs provide reasonable assurance that the initial isotope concentrations of SNF are known, which will be used as criticality benchmarks for SNF in an intact form. 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 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.

7.1.1 CRC Experiments

The CRC k_{eff} values were calculated using the best-estimate isotope set corresponding to those listed in Table 6-2. Each of the CRC benchmark cases used water scattering kernels corresponding to a temperature of 500K.

7.1.1.1 Crystal River Unit 3

The CR3 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 CR3 where the core thermal power varied between 2452 MWt and 2544 MWt (CRWMS M&O 1998d, pp. 5 and 280-289).

Table 7-1 provides some general information about the CR3 CRC experiments. The information includes the average burnup of the core in effective full power days (EFPD), the initial weight percent (wt%) 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 water-to-fuel volume ratio of 1.7 (CRWMS M&O 1998d, p. 26).

Table 7-1. General CR3 CRC Statepoint Information

Case	Cycle length to statepoint (EFPD, Cycle) ^a	Initial Enrichments (wt% U-235) ^a	Downtime (d) ^a	k_{eff} ^a	σ ^a	AENCF ^b (MeV)	CC ^c
CR1	0.0 (Cy 1A)	[1.93, 2.54, 2.83]	0.0	0.99601	0.00043	0.2344	1
CR2	268.8 (Cy 1B)	1.93, 2.54, 2.83, 2.00	195.3	0.99285	0.0004	0.2504	1
CR3	411.0 (Cy 1B)	1.93, 2.54, 2.83, 2.00	14.8	0.99502	0.00046	0.2518	1
CR4	0.0 (Cy 2)	2.54, [2.64], 2.83	97.0	0.99282	0.00044	0.2498	1
CR5	0.0 (Cy 3)	2.54, [2.62], 2.64, 2.83	164.0	0.99408	0.00045	0.2489	1
CR6	168.5 (Cy 3)	2.54, 2.62, 2.64, 2.83	16.8	0.99304	0.00045	0.2536	1
CR7	250.0 (Cy 3)	2.54, 2.62, 2.64, 2.83	12.3	0.99073	0.00045	0.2547	1
CR8	0.0 (Cy 4)	2.62, [2.62], 2.64, [2.95]	73.0	0.99134	0.00047	0.2499	1
CR9	228.1 (Cy 4)	2.62, 2.64, 2.95	15.2	0.99152	0.00046	0.2576	1
CR10	253.0 (Cy 4)	2.62, 2.64, 2.95	24.0	0.99603	0.00047	0.2568	1
CR11	0.0 (Cy 5)	2.62, 2.64, 2.95, [2.95, 3.29]	127.0	0.99479	0.00047	0.2475	1
CR12	388.5 (Cy 5)	2.62, 2.64, 2.95, 3.29	5.0	0.99805	0.00045	0.2605	1
CR13	0.0 (Cy 6)	2.62, 2.64, 2.95, 3.29, [3.49]	163.0	0.99561	0.00043	0.2513	1
CR14	96.0 (Cy 6)	2.62, 2.64, 2.95, 3.29, 3.49	168.9	0.99579	0.00047	0.2557	1
CR15	400.0 (Cy 6)	2.62, 2.64, 2.95, 3.29, 3.49	10.4	0.99273	0.00044	0.2612	1
CR16	0.0 (Cy 7)	2.54, 2.62, 2.64, 3.29, 3.49, [3.84]	113.0	0.99324	0.00052	0.2504	1
CR17	260.3 (Cy 7)	2.54, 2.62, 2.64, 3.29, 3.49, 3.84	18.9	0.99083	0.00045	0.2583	1
CR18	291.0 (Cy 7)	2.54, 2.62, 2.64, 3.29, 3.49, 3.84	39.5	0.99222	0.00049	0.2598	1
CR19	319.0 (Cy 7)	2.54, 2.62, 2.64, 3.29, 3.49, 3.84	109.5	0.98993	0.00047	0.2587	1

Table 7-1. General CR3 CRC Statepoint Information

Case	Cycle length to statepoint (EFPD, Cycle) ^a	Initial Enrichments (wt% U-235) ^a	Downtime (d) ^a	k_{eff} ^a	σ^a	AENCF ^b (MeV)	CC ^c
CR20	462.3 (Cy 7)	2.54, 2.62, 2.64, 3.29, 3.49, 3.84	2.2	0.99321	0.00042	0.2582	1
CR21	479.0 (Cy 7)	2.54, 2.62, 2.64, 3.29, 3.49, 3.84	7.2	0.99247	0.00046	0.2616	1
CR22	0.0 (Cy 8)	1.93, 2.62, 3.29, 3.49, 3.84, [3.94]	99.0	0.99039	0.00043	0.2532	1
CR23	97.6 (Cy 8)	1.93, 2.62, 3.29, 3.49, 3.84, 3.94	15.5	0.99021	0.00046	0.2572	1
CR24	139.8 (Cy 8)	1.93, 2.62, 3.29, 3.49, 3.84, 3.94	6.2	0.99063	0.00049	0.2582	1
CR25	404.0 (Cy 8)	1.93, 2.62, 3.29, 3.49, 3.84, 3.94	44.4	0.99054	0.00042	0.2615	1
CR26	409.6 (Cy 8)	1.93, 2.62, 3.29, 3.49, 3.84, 3.94	4.9	0.99067	0.00047	0.2610	1
CR27	515.5 (Cy 8)	1.93, 2.62, 3.29, 3.49, 3.84, 3.94	7.6	0.98772	0.00044	0.2643	1
CR28	0.0 (Cy 9)	1.93, 3.84, [3.90], 3.94	75.0	0.99208	0.00044	0.2546	1
CR29	158.8 (Cy 9)	1.93, 3.84, 3.90, 3.94	2.1	0.99311	0.0005	0.2584	1
CR30	219.0 (Cy 9)	1.93, 3.84, 3.90, 3.94	53.1	0.99078	0.00048	0.2597	1
CR31	363.1 (Cy 9)	1.93, 3.84, 3.90, 3.94	1.6	0.98837	0.00048	0.2635	1
CR32	0.0 (Cy 10)	3.84, 3.90, 3.94, [4.167]	55.0	0.99164	0.00052	0.2558	1
CR33	573.7 (Cy 10)	3.84, 3.90, 3.94, 4.167	16.4	0.98725	0.00048	0.2660	1

NOTE: ^a Values are from pp. 40 and 41 of CRWMS M&O (1998c)

^b Values are from pp. 64 through 66 of CRWMS M&O (1999b)

^c CC = configuration class applicability

7.1.1.2 Three Mile Island Unit 1

The TMI1 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 3 CRC experiments have been evaluated for TMI1 where the core thermal power was 2535 MWt (CRWMS M&O 1998g, pp. 5 and 65).

Table 7-2 provides some general information about the TMI1 CRC experiments. The information includes the average burnup of the core in EFPD, the initial weight percent (wt%) 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 water-to-fuel volume ratio of 1.7 (CRWMS M&O 1998g, p. 5).

Table 7-2. General TMI1 CRC Statepoint Information

Case	Cycle length to statepoint (EFPD, Cycle) ^a	Initial Enrichments (wt% U-235) ^a	Downtime (d) ^a	k _{eff} ^a	σ ^a	AENCF ^b (MeV)	CC ^c
TMI1	0.0 (Cy 1)	[2.06, 2.75, 3.05]	0.0	1.00141	0.00042	0.2353	1
TMI2	0.0 (Cy 5)	2.64, 2.85, [2.85]	2,420.0	0.99088	0.00046	0.2476	1
TMI3	114.4 (Cy 5)	2.64, 2.85	32.2	0.99162	0.00048	0.2498	1

NOTE: ^a Values are from p. 41 of CRWMS M&O (1998c)
^b Values are from pp. 64 through 66 of CRWMS M&O (1999b)
^c CC = configuration class applicability

7.1.1.3 Sequoyah Unit 2

The SQ2 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 3 CRC experiments have been evaluated for SQ2 (CRWMS M&O 1998c, p. 29).

Table 7-3 provides some general information about the SQ2 CRC experiments. The information includes the average burnup of the core in EFPD, the initial weight percent (wt%) 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 water-to-fuel volume ratio of 1.6 (CRWMS M&O 1998f, p. 7).

Table 7-3. General SQ2 CRC Statepoint Information

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

NOTE: ^a Values are from p. 41 of CRWMS M&O (1998c)
^b Values are from pp. 64 through 66 of CRWMS M&O (1999b)
^c CC = configuration class applicability

7.1.1.4 McGuire Unit 1

The MG1 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 6 CRC experiments have been evaluated for MG1 (CRWMS M&O 1998c, p. 25).

Table 7-4 provides some general information about the MG1 CRC experiments. The information includes the average burnup of the core in EFPD, the initial weight percent (wt%) 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 water-to-fuel volume ratio between 1.7 and 1.9 (CRWMS M&O 1998c, p. 27).

Table 7-4. General MG1 CRC Statepoint Information

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

NOTE: ^a Values are from p. 41 of CRWMS M&O (1998c)

^b Values are from pp. 64 through 66 of CRWMS M&O (1999b)

^c CC = configuration class applicability

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} and AENCF values for each of the LCEs described in the following subsections were taken from CRWMS M&O (1999c, Section 4).

In the subsequent tables the P/D term represents the pin pitch to pin outer diameter ratio, and the W/F term represents the unit cell moderator area to fuel area ratio.

7.1.2.1 Critical Configurations of Subcritical Clusters of 2.35 wt% Enriched UO₂ Rods in Water with Fixed Neutron Absorber Plates

Experiments with subcritical clusters of low-enrichment UO₂ 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 wt% ²³⁵U 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 7-5. 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 7-5. Clusters of 2.35 wt% UO₂ 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	1, 2, 5
exp2	Boral™	1.81	0.99842	0.00088	0.12469	1, 2, 3, 6
exp3	Type 6061 Aluminum	1.81	0.99898	0.00089	0.12172	1, 2, 3, 6
exp4	Type 304 Stainless Steel	1.81	1.00104	0.00087	0.12003	1, 2, 3, 6

7.1.2.2 Water-Reflected Fuel Rod Clusters in Square Pitched Arrays

A series of critical experiments with clusters of aluminum clad UO₂ 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 7-6 provides a brief description of the experiments which come from page 10 of NEA (1998, LEU-COMP-THERM-001). Each of the experiments used 2.35 wt% ²³⁵U enriched UO₂ fuel with an average loading of 17.08 g of ²³⁵U 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 7-6. 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	1, 2, 5, 6
Case 2	20 x 17, 3 clusters, 11.92 ± 0.04 cm separation	1.81	0.99445	0.00158	0.1223	1, 2, 5, 6
Case 3 ^b	20 x 16, 3 clusters, 8.41 ± 0.05 cm separation	1.81	0.99982	0.00159	0.12	1, 2, 5, 6
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	1, 2, 5, 6
Case 5	20 x 15, 3 clusters, 6.39 ± 0.05 cm separation	1.81	0.9931	0.00169	0.1204	1, 2, 5, 6
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	1, 2, 5, 6
Case 7	20 x 14, 3 clusters, 4.46 ± 0.10 cm separation	1.81	0.99261	0.00138	0.1211	1, 2, 5, 6
Case 8 ^c	19 x 6, 3 clusters, 7.57 ± 0.04 cm separation	1.81	0.99888	0.00151	0.1209	1, 2, 5, 6

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, p. 11 LEU-COMP-THERM-001).

^b The cluster separation referenced was 8.41 cm, but footnote (d) on p. 10 LEU-COMP-THERM-001 of NEA (1998), 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) on p. 10 LEU-COMP-THERM-001 of NEA (1998), 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 wt% Enriched UO₂ 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 wt% ²³⁵U enriched UO₂ fuel rods on a square pitch of 1.892 cm. The distinguishing characteristics of each experiment are given in Table 7-7.

Table 7-7. Clusters of 4.31 wt% UO₂ 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	1, 2, 3, 5, 6
exp6	lead	1.50	0.99675	0.00103	0.17662	1, 2, 3, 5, 6
exp7	stainless steel	1.50	0.99724	0.00111	0.1784	1, 2, 3, 5, 6

7.1.2.4 Critical Configurations with 4.31 wt% ²³⁵U Enriched UO₂ 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 wt% ²³⁵U uniformly enriched UO₂ 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 7-8.

Table 7-8. Configurations with 4.31 wt% UO₂ 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	0.0011	0.17735	1, 3, 4, 5, 6
exp9	1.89 cm, 1237, water with 2.55 g/l of boron	1.50	1.00827	0.00099	0.22171	1, 3, 4, 5, 6
exp10	1.715 cm, 509, non-borated water	1.36	1.0066	0.00174	0.2239	1, 3, 4, 5, 6
exp11	1.715 cm, 1192, water with 2.55 g/l of boron	1.36	1.00358	0.00157	0.26643	1, 3, 4, 5, 6

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 wt% ²³⁵U enriched UO₂ fuel with a 1.891 cm pitch. The neutron flux traps were created by positioning two plates of BoralTM 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 7-9.

Table 7-9. 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	1, 2, 4, 5, 6
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	1, 2, 4, 5, 6

7.1.2.6 Electric Power Research Institute 2.35 wt% 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). Two critical experiment configurations composed of water-moderated lattices of 2.35 wt% enriched UO₂ 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 7-10.

Table 7-10. EPRI 2.35 wt% UO₂ Critical Configurations

Exp ID	Description Pitch, # of Fuel Rods	P/D	k _{eff}	σ	AENCF (MeV)	CC
exp14	1.526 cm, 708 ^a	1.36	0.99593	0.00099	0.20945	1, 2, 5, 6
exp15	2.210 cm, 342	1.97	1.00074	0.00087	0.10984	1, 2, 5, 6

NOTES: ^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 NEA (1998) LEU-COMP-THERM-027, and consisted of a 14 x 14 array of 4.74 wt% enriched UO₂ 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 7-11. The experiment was a subcritical approach extrapolated to critical; the multiplication factor reached is within 0.1% of 1.000. The experiments were tests of the lead reflector effect.

Table 7-11. Lead-Reflected UO₂ 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	1, 2, 3, 5, 6

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 wt% ^{235}U enriched UO_2 fuel rods, 4.02 wt% ^{235}U enriched UO_2 fuel rods, combination 4 wt% Gd_2O_3 and 96 wt% (1.944 wt% ^{235}U 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 water-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 7-12.

Table 7-12. 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	1, 2, 5
ugd2	4808	0	0	0	16	0	137	1250.0	1.59	0.99945	0.00145	0.19828	1, 2, 5
ugd3	4788	0	20	0	0	0	153	1239.3	1.59	1.00054	0.00147	0.19948	1, 2, 5
ugd4	4788	0	20	0	16	0	137	1171.7	1.59	1.00193	0.0015	0.19985	1, 2, 5
ugd5	4780	0	28	0	0	0	153	1208.0	1.59	0.99955	0.00154	0.19752	1, 2, 5
ugd6	4780	0	28	0	16	0	137	1155.8	1.59	0.99996	0.00152	0.19775	1, 2, 5
ugd7	4780	0	28 ^b	0	0	0	153	1208.8	1.59	1.0041	0.00148	0.19675	1, 2, 5
ugd8	4772	0	36	0	0	0	153	1170.7	1.59	0.99929	0.00154	0.19756	1, 2, 5
ugd9	4772	0	36	0	16	0	137	1130.5	1.59	1.00135	0.00156	0.19873	1, 2, 5
ugd10	4772	0	36	0	0	16	137	1177.1	1.59	0.9979	0.00144	0.2011	1, 2, 5
ugd12	3920	888	0	0	0	0	153	1899.3	1.56	0.9994	0.00161	0.20965	1, 2, 5
ugd13	3920	888	0	16	0	0	137	1635.4	1.56	1.00049	0.00155	0.20841	1, 2, 5
ugd14	3920	860	28	0	0	0	153	1653.8	1.56	1.00066	0.00156	0.20416	1, 2, 5
ugd15	3920	860	28	16	0	0	137	1479.7	1.56	1.00158	0.00151	0.2056	1, 2, 5
ugd16	3920	852	36	0	0	0	153	1579.4	1.56	1.00335	0.00151	0.20648	1, 2, 5
ugd17	3920	852	36	16	0	0	137	1432.1	1.56	0.99912	0.00151	0.20341	1, 2, 5
ugd18	3676	944	0	0	0	0	180	1776.8	1.56	0.99876	0.0015	0.20851	1, 2, 5
ugd19	3676	928	16	0	0	0	180	1628.3	1.56	1.00133	0.00153	0.21011	1, 2, 5
ugd20	3676	912	32	0	0	0	180	1499.0	1.56	1.00322	0.00153	0.20698	1, 2, 5

NOTES: ^a Description column designations are as follows:

A - Number of 2.46 wt% ^{235}U fuel rods

B - Number of 4.02 wt% ^{235}U 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 UO₂ and PuO₂-UO₂ 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 UO₂ fuel with 5.74 wt% ²³⁵U enrichment, and mixed oxide (MOX) fuel containing 6.6 wt% PuO₂ and natural enriched UO₂ (Taylor 1965, p. A-1). This work was documented by Taylor (1965) and subsequently described by ORNL (1995). 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 7-13 presents a description of the various single-region experiments and Table 7-14 presents a description of the multi-region experiments.

Table 7-13. 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	1, 2, 5, 6
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	1, 2, 5, 6
ssr70	Fuel: MOX; Pitch: 1.3208 cm; Configuration: 22x23 square; Critical water height: 84.56 cm	1.54	0.99543	0.00072	0.2295	1, 2, 5, 6
ssr57	Fuel: MOX; Pitch: 1.4224 cm; Configuration: 19x19 square; Critical water height: 82.46 cm	1.66	0.99807	0.00075	0.1938	1, 2, 5, 6
ssr27	Fuel: MOX; Pitch: 1.4224 cm; Configuration: 21x21 square; Critical water height: 89.70 cm	1.66	0.99881	0.00082	0.2015	1, 2, 5, 6
ssr66	Fuel: MOX; Pitch: 1.8669 cm; Configuration: 13x13 square; Critical water height: 70.11 cm	2.18	1.00308	0.00073	0.1183	1, 2, 5, 6
ssr53	Fuel: MOX; Pitch: 2.0117 cm; Configuration: 12x12 square; Critical water height: 78.43 cm	2.35	1.00454	0.00066	0.1065	1, 2, 5, 6
ssr74	Fuel: MOX; Pitch: 2.6416 cm; Configuration: 11x11 square; Critical water height: 81.17 cm	3.08	1.00505	0.00068	0.079	1, 2, 5, 6

Table 7-14. 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	1, 2, 5, 6
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	1, 2, 5, 6

Table 7-14. Saxton Multi-Region Critical Configurations

Exp ID	Description	P/D	k _{eff}	σ	AENCF (MeV)	CC
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	1, 2, 5, 6
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	1, 2, 5, 6
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	1, 2, 5, 6
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	1, 2, 5, 6

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 B₄C rods and water, stainless steel sheets and water, borated aluminum sheets and water, or only water. The fuel rods were composed of 2.46 wt% ²³⁵U enriched UO₂ clad in Type 6061 aluminum with a diameter of 1.03 cm (Baldwin et al. 1979, p. 8-2). The B₄C rods were aluminum tubes filled with B₄C 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 7-15.

Table 7-15. Close Proximity Critical Benchmarks

Exp ID	Description	P/D	k _{eff}	σ	AENCF (MeV)	CC
core2	Assembly spacing (pin pitch): 0; # B ₄ C rods: 0; Metal between unit assemblies: N/A	1.59	1.00058	0.00159	0.19988	1, 2, 5, 6
core3	Assembly spacing (pin pitch): 1; # B ₄ C rods: 0; Metal between unit assemblies: N/A	1.59	1.00019	0.00148	0.18078	1, 2, 5, 6
core4	Assembly spacing (pin pitch): 1; # B ₄ C rods: 84; Metal between unit assemblies: N/A	1.59	0.9948	0.0015	0.17908	1, 2, 5, 6
core5	Assembly spacing (pin pitch): 2; # B ₄ C rods: 64; Metal between unit assemblies: N/A	1.59	0.99445	0.00153	0.16919	1, 2, 5, 6
core6	Assembly spacing (pin pitch): 2; # B ₄ C rods: 64; Metal between unit assemblies: N/A	1.59	0.99556	0.00152	0.17216	1, 2, 5, 6
core7	Assembly spacing (pin pitch): 3; # B ₄ C rods: 34; Metal between unit assemblies: N/A	1.59	0.99463	0.00151	0.15963	1, 2, 5, 6
core8	Assembly spacing (pin pitch): 3; # B ₄ C rods: 34; Metal between unit assemblies: N/A	1.59	0.98895	0.00149	0.16496	1, 2, 5, 6
core9	Assembly spacing (pin pitch): 4; # B ₄ C rods: 0; Metal between unit assemblies: N/A	1.59	0.99298	0.00144	0.15528	1, 2, 5, 6
core10	Assembly spacing (pin pitch): 3; # B ₄ C rods: N/A; Metal between unit assemblies: None	1.59	0.99511	0.00148	0.16036	1, 2, 5, 6

Table 7-15. Close Proximity Critical Benchmarks

Exp ID	Description	P/D	k _{eff}	σ	AENCF (MeV)	CC
core11	Assembly spacing (pin pitch): 1; # B ₄ C rods: N/A; Metal between unit assemblies: SS	1.59	0.99699	0.00148	0.17893	1, 2, 5, 6
core12	Assembly spacing (pin pitch): 2; # B ₄ C rods: N/A; Metal between unit assemblies: SS	1.59	0.99549	0.00151	0.16671	1, 2, 5, 6
core13	Assembly spacing (pin pitch): 1; # B ₄ C rods: N/A; Metal between unit assemblies: B/AI set 5	1.59	0.99933	0.00151	0.18075	1, 2, 5, 6
core15	Assembly spacing (pin pitch): 1; # B ₄ C rods: N/A; Metal between unit assemblies: B/AI set 3	1.59	0.99107	0.00157	0.18348	1, 2, 5, 6
core16	Assembly spacing (pin pitch): 2; # B ₄ C rods: N/A; Metal between unit assemblies: B/AI set 3	1.59	0.99041	0.0015	0.16952	1, 2, 5, 6
core17	Assembly spacing (pin pitch): 1; # B ₄ C rods: N/A; Metal between unit assemblies: B/AI set 2	1.59	0.99365	0.00151	0.18187	1, 2, 5, 6
core18	Assembly spacing (pin pitch): 2; # B ₄ C rods: N/A; Metal between unit assemblies: B/AI set 2	1.59	0.9947	0.0015	0.16855	1, 2, 5, 6
core19	Assembly spacing (pin pitch): 1; # B ₄ C rods: N/A; Metal between unit assemblies: B/AI set 1	1.59	0.99383	0.00153	0.18354	1, 2, 5, 6
core20	Assembly spacing (pin pitch): 2; # B ₄ C rods: N/A; Metal between unit assemblies: B/AI set 1	1.59	0.99392	0.00151	0.16933	1, 2, 5, 6
core21	Assembly spacing (pin pitch): 3; # B ₄ C rods: N/A; Metal between unit assemblies: B/AI set 1	1.59	0.9916	0.0014	0.16225	1, 2, 5, 6

7.1.2.11 Electric Power Research Institute Mixed Oxide Critical Configurations

ORNL (1995) describes criticality tests with mixed oxide fuel performed for the Electric Power Research Institute. Six critical experiment configurations composed of unborated and borated water moderated lattices of 2 wt% PuO₂ (8 wt% ²⁴⁰Pu)/98 wt% UO₂ (natural) 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 Pu/²³⁵U (2.79) bounds that calculated for such fuel (1.01) (ORNL 1995). 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 7-16.

Table 7-16. 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	1, 2, 5, 6
exp23	Pitch =1.778 cm, 761 fuel rods, 680.9 ppm borated water moderator	1.39	1.0005	0.00169	0.27397	1, 2, 5, 6
exp24	Pitch =2.210 cm, 197 fuel rods, unborated water moderator	1.72	1.00302	0.00171	0.16128	1, 2, 5, 6
exp25	Pitch =2.210 cm, 761 fuel rods, 1090.4 ppm borated water moderator	1.72	1.00835	0.00161	0.18944	1, 2, 5, 6
exp26	Pitch =2.515 cm, 160 fuel rods, unborated water moderator	1.96	1.00709	0.0016	0.13192	1, 2, 5, 6
exp27	Pitch =2.515 cm, 689 fuel rods, 767.2 ppm borated water moderator	1.96	1.00752	0.00155	0.15372	1, 2, 5, 6

7.1.2.12 Critical Triangular Lattice of MOX & UO₂ 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 PuO₂-UO₂ and UO₂ fuel rods. The fuel rods were placed in a uniform distribution with a Pu/²³⁵U ratio approximating that of a 20,000 MWd/MTU burnup. Each PuO₂-UO₂ fuel rod was surrounded by six UO₂ fuel rods with a triangular lattice pitch. The UO₂ rods were 4.31 wt% ²³⁵U enriched, and the MOX fuel was 2 wt% PuO₂ and 98 wt% natural UO₂. Information for this experiment is provided in Table 7-17.

Table 7-17. Critical Configuration of MOX and UO₂ 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	1, 2, 5

NOTE: ^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 the *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 NEA (1998), Volume VI and are listed in Table 7-18.

Table 7-18. Configurations Incorporating Mixed Plutonium and Natural Uranium Nitrate Solutions

Exp ID	Description	k_{eff}	σ	AENCF (MeV)	CC
MIX-SOL-THERM-001 Water Reflected Annular Cylindrical Tank with Central Bottle and Annular Inserts					
PNL3187	102.19 g Pu/l, 365.20 g U/l, 2% B ₄ C Concrete Annulus, No Bottle, Critical Height: 48.55 cm, H/Pu-239 (annular tank) = 234, 91.118 wt% Pu-239 in Pu	0.99821	0.00116	0.04158	2, 3, 4, 5, 6
PNL3391	103.37 g Pu/l, 363.66 g U/l, 0% B ₄ C Concrete Annulus, Bottle 2, Critical Height: 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	2, 3, 4, 5, 6
PNL3492	103.37 g Pu/l, 363.66 g U/l, 1% B ₄ C Concrete Annulus, Bottle 2, Critical Height: 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	2, 3, 4, 5, 6
PNL3593	107.91 g Pu/l, 379.55 g U/l, 6% B ₄ C Concrete Annulus, Bottle 2, Critical Height: 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	2, 3, 4, 5, 6
PNL3694	108.27 g Pu/l, 380.41 g U/l, No Concrete Annulus, Bottle 2, Critical Height: 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	2, 3, 4, 5, 6
PNL3795	195.61 g Pu/l, 6.5 g U/l, 2% B ₄ C Concrete Annulus, Bottle 3, Critical Height: 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	2, 3, 4, 5, 6
PNL3896	110.13 g Pu/l, 3.8 g U/l, 2% B ₄ C Concrete Annulus, Bottle 3, Critical Height: 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	2, 3, 4, 5, 6
PNL3897	58.30 g Pu/l, 2.3 g U/l, 2% B ₄ C Concrete Annulus, Bottle 3, Critical Height: 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	2, 3, 4, 5, 6
PNL3898	72.74 g Pu/l, 247.33 g U/l, 2% B ₄ C Concrete Annulus, Bottle 2, Critical Height: 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	2, 3, 4, 5, 6
PNL3808	47.08 g Pu/l, 161.72 g U/l, 2% B ₄ C Concrete Annulus, Bottle 2, Critical Height: 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	2, 3, 4, 5, 6
PNL3999	73.64 g Pu/l, 250.30 g U/l, Polyethylene with Cd Cover Annulus, Bottle 2, Critical Height: 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	2, 3, 4, 5, 6
PNL5300	74.25 g Pu/l, 251.64 g U/l, Solid Polyethylene with Cd Cover Center, Critical Height: 104.62 cm, H/Pu-239 (annular tank) = 346, 91.117 wt% Pu-239 in Pu	1.0067	0.00105	0.02917	2, 3, 4, 5, 6

Table 7-18. Configurations Incorporating Mixed Plutonium and Natural Uranium Nitrate Solutions

Exp ID	Description	k_{eff}	σ	AENCF (MeV)	CC
MIX-SOL-THERM-002 Water Reflected Cylindrical Tank With a 68.68 cm Inner Diameter (ID), 91.102 wt% Pu-239 in Pu					
PNL1158	11.83 g Pu/l, 11.05 g U/l, Critical Height: 76.80 cm, H/Pu-239 = 2,403	1.00686	0.00067	0.00393	2, 3, 4, 5, 6
PNL1159	11.73 g Pu/l, 10.78 g U/l, Critical Height: 83.14 cm, H/Pu-239 = 2,435	1.00558	0.00064	0.0038	2, 3, 4, 5, 6
PNL1161	12.19 g Pu/l, 41.04 g U/l, Critical Height: 81.72 cm, H/Pu-239 = 2,317	1.00751	0.00066	0.00597	2, 3, 4, 5, 6
MIX-SOL-THERM-003 Water/Polyethylene Reflected Cylindrical Tank With Various Diameters, 93.95 wt% Pu-239 in Pu					
awre1	101.3 g Pu/l, 228.5 g U/l, ID = 25.425 cm, Critical Height: 56.31 cm, H/Pu-239 = 239	1.01511	0.0012	0.03133	2, 3, 4, 5, 6
awre2	101.3 g Pu/l, 228.5 g U/l, ID = 30.62 cm, Critical Height: 29.89 cm, H/Pu-239 = 239	1.01167	0.00117	0.03206	2, 3, 4, 5, 6
awre3	101.3 g Pu/l, 228.5 g U/l, ID = 37.99 cm, Critical Height: 21.17 cm, H/Pu-239 = 239	1.01028	0.00114	0.03183	2, 3, 4, 5, 6
awre4	101.3 g Pu/l, 228.5 g U/l, ID = 50.72 cm, Critical Height: 16.05 cm, H/Pu-239 = 239	1.00486	0.00111	0.03228	2, 3, 4, 5, 6
awre5	31.58 g Pu/l, 71.3 g U/l, ID = 30.62 cm, Critical Height: 46.18 cm, H/Pu-239 = 847	1.00875	0.00101	0.01062	2, 3, 4, 5, 6
awre6	31.58 g Pu/l, 71.3 g U/l, ID = 37.99 cm, Critical Height: 28.24 cm, H/Pu-239 = 847	1.01337	0.00108	0.01053	2, 3, 4, 5, 6
awre7	31.58 g Pu/l, 71.3 g U/l, ID = 50.72 cm, Critical Height: 20.39 cm, H/Pu-239 = 847	1.0064	0.00102	0.01089	2, 3, 4, 5, 6
awre8	18.61 g Pu/l, 42.2 g U/l, ID = 37.99 cm, Critical Height: 72.86 cm, H/Pu-239 = 1461	1.01255	0.00091	0.00684	2, 3, 4, 5, 6
awre9	18.61 g Pu/l, 42.2 g U/l, ID = 50.72 cm, Critical Height: 33.59 cm, H/Pu-239 = 1461	1.00977	0.00088	0.00684	2, 3, 4, 5, 6
awre10	17.50 g Pu/l, 39.6 g U/l, ID = 50.72 cm, Critical Height: 37.16 cm, H/Pu-239 = 1556	1.00839	0.00081	0.00648	2, 3, 4, 5, 6
MIX-SOL-THERM-004 Cylindrical Tank With a 35.39 cm ID and either Water Reflector, Concrete Reflector, or No Reflector, 91.118 wt% Pu-239 in Pu					
PNL1577	172.56 g Pu/l, 262.79 g U/l, No Reflector, Critical Height: 57.97 cm, H/Pu-239 = 137	0.99645	0.00128	0.05956	2, 3, 4, 5, 6
PNL1678	172.82 g Pu/l, 262.55 g U/l, Water Reflector, Critical Height: 28.93 cm, H/Pu-239 = 136	0.99976	0.00115	0.05069	2, 3, 4, 5, 6
PNL1783	173.22 g Pu/l, 262.88 g U/l, Concrete Reflector, Critical Height: 30.60 cm, H/Pu-239 = 136	0.99976	0.00115	0.05386	2, 3, 4, 5, 6
PNL1868	118.71 g Pu/l, 173.98 g U/l, Concrete Reflector, Critical Height: 27.03 cm, H/Pu-239 = 214	1.00247	0.00119	0.03416	2, 3, 4, 5, 6
PNL1969	119.04 g Pu/l, 174.67 g U/l, Water Reflector, Critical Height: 25.26 cm, H/Pu-239 = 213	0.99967	0.00111	0.0336	2, 3, 4, 5, 6

Table 7-18. Configurations Incorporating Mixed Plutonium and Natural Uranium Nitrate Solutions

Exp ID	Description	k_{eff}	σ	AENCF (MeV)	CC
PNL2070	118.90 g Pu/l, 174.53 g U/l, No Reflector, Critical Height: 41.08 cm, H/Pu-239 = 214	0.99925	0.00115	0.03743	2, 3, 4, 5, 6
PNL2565	41.69 g Pu/l, 63.38 g U/l, No Reflector, Critical Height: 44.46 cm, H/Pu-239 = 664	1.00363	0.00112	0.01295	2, 3, 4, 5, 6
PNL2666	41.89 g Pu/l, 63.65 g U/l, Water Reflector, Critical Height: 28.11 cm, H/Pu-239 = 660	1.00337	0.00105	0.0116	2, 3, 4, 5, 6
PNL2767	41.83 g Pu/l, 63.55 g U/l, Concrete Reflector, Critical Height: 29.36 cm, H/Pu-239 = 661	1.00629	0.00113	0.01197	2, 3, 4, 5, 6

7.1.3.2 Plutonium Nitrate Solutions

The experiments involving plutonium are from NEA (1998, Volume I) and are listed in Table 7-19.

Table 7-19. Configurations Incorporating Plutonium Nitrate Solutions

Exp ID	Description	k_{eff}^a	σ	AENCF (MeV)	CC
PU-SOL-THERM-001 Water Reflected 11.5-Inch Diameter Spheres, 0.049-inch thick shell of Type 304L Stainless Steel, 4.57 wt% Pu-240 in Pu, 95.12 wt% Pu-239 in Pu					
pust1t1	73.0 g Pu/liter, Critical Mass: 945 gm, H/Pu-239 = 371	1.00995	0.00102	0.01252	2, 3, 4, 5, 6
pust1t2	96.0 g Pu/liter, Critical Mass: 1243 gm, H/Pu-239 = 272	1.01109	0.001	0.01702	2, 3, 4, 5, 6
pust1t3	119.0 g Pu/liter, Critical Mass: 1541 gm, H/Pu-239 = 216	1.01396	0.00094	0.02159	2, 3, 4, 5, 6
pust1t4	132.0 g Pu/liter, Critical Mass: 1709 gm, H/Pu-239 = 190	1.00643	0.00104	0.02397	2, 3, 4, 5, 6
pust1t5	140.0 g Pu/liter, Critical Mass: 1813 gm, H/Pu-239 = 180	1.01014	0.00101	0.02479	2, 3, 4, 5, 6
pust1t6	268.7 g Pu/liter, Critical Mass: 3480 gm, H/Pu-239 = 91	1.00831	0.00104	0.04809	2, 3, 4, 5, 6
PU-SOL-THERM-003 Water Reflected 13-Inch Diameter Spheres, 0.050-inch thick shell of Type 347 Stainless Steel Unless Otherwise Indicated					
pu003-1	33.32 g Pu/liter, Critical Mass: 631 gm, H/Pu-239 = 788, 1.76 wt% Pu-240	1.00962	0.00091	0.00623	2, 3, 4, 5, 6
pu003-2	34.32 g Pu/liter, Critical Mass: 650 gm, H/Pu-239 = 756, 1.76 wt% Pu-240	1.00885	0.00091	0.00651	2, 3, 4, 5, 6
pu003-3	37.43 g Pu/liter, Critical Mass: 709 gm, H/Pu-239 = 699, 3.12 wt% Pu-240	1.01228	0.00092	0.00693	2, 3, 4, 5, 6
pu003-4	38.12 g Pu/liter, Critical Mass: 722 gm, H/Pu-239 = 682, 3.12 wt% Pu-240	1.00965	0.00094	0.0072	2, 3, 4, 5, 6

Table 7-19. Configurations Incorporating Plutonium Nitrate Solutions

Exp ID	Description	k_{eff}^a	σ	AENCF (MeV)	CC
pu003-5	40.65 g Pu/liter, Critical Mass: 770 gm, H/Pu-239 = 627, 3.12 wt% Pu-240	1.01393	0.00092	0.00785	2, 3, 4, 5, 6
pu003-6	44.09 g Pu/liter, Critical Mass: 835 gm, H/Pu-239 = 563, 3.12 wt% Pu-240	1.01214	0.00091	0.00845	2, 3, 4, 5, 6
pu003-7	35.98 g Pu/liter, Critical Mass: 649 gm, H/Pu-239 = 738, 3.12 wt% Pu-240, 20 Gauge 2S Al Shell	1.01369	0.00093	0.00678	2, 3, 4, 5, 6
pu003-8	36.81 g Pu/liter, Critical Mass: 664 gm, H/Pu-239 = 714, 3.12 wt% Pu-240, 20 Gauge 2S Al Shell	1.01175	0.00095	0.00703	2, 3, 4, 5, 6
PU-SOL-THERM-004 Water Reflected 14-Inch Diameter Spheres, 0.050-inch thick shell of Type 347 Stainless Steel					
pu004-1	26.27 g Pu/liter, Critical Mass: 621 gm, H/Pu-239 = 987, 0.54 wt% Pu-240	1.01134	0.00088	0.00524	2, 3, 4, 5, 6
pu004-2	26.31 g Pu/liter, Critical Mass: 622 gm, H/Pu-239 = 977, 0.54 wt% Pu-240	1.00448	0.00082	0.00541	2, 3, 4, 5, 6
pu004-3	27.20 g Pu/liter, Critical Mass: 643 gm, H/Pu-239 = 935, 0.54 wt% Pu-240	1.00916	0.00087	0.00538	2, 3, 4, 5, 6
pu004-4	28.09 g Pu/liter, Critical Mass: 664 gm, H/Pu-239 = 889, 0.54 wt% Pu-240	1.00712	0.00086	0.00561	2, 3, 4, 5, 6
pu004-5	27.58 g Pu/liter, Critical Mass: 652 gm, H/Pu-239 = 942, 1.76 wt% Pu-240	1.00753	0.00091	0.00543	2, 3, 4, 5, 6
pu004-6	28.60 g Pu/liter, Critical Mass: 676 gm, H/Pu-239 = 927, 3.12 wt% Pu-240	1.00862	0.00087	0.00564	2, 3, 4, 5, 6
pu004-7	29.57 g Pu/liter, Critical Mass: 699 gm, H/Pu-239 = 892, 3.12 wt% Pu-240	1.01248	0.0009	0.0056	2, 3, 4, 5, 6
pu004-8	29.95 g Pu/liter, Critical Mass: 708 gm, H/Pu-239 = 869, 3.12 wt% Pu-240	1.00778	0.00086	0.0062	2, 3, 4, 5, 6
pu004-9	31.60 g Pu/liter, Critical Mass: 747 gm, H/Pu-239 = 805, 3.12 wt% Pu-240	1.00965	0.00089	0.00619	2, 3, 4, 5, 6
pu04-10	35.36 g Pu/liter, Critical Mass: 836 gm, H/Pu-239 = 689, 3.12 wt% Pu-240	1.00987	0.00092	0.00715	2, 3, 4, 5, 6
pu04-11	39.38 g Pu/liter, Critical Mass: 931 gm, H/Pu-239 = 592, 3.12 wt% Pu-240	1.0095	0.00092	0.00805	2, 3, 4, 5, 6
pu04-12	29.44 g Pu/liter, Critical Mass: 696 gm, H/Pu-239 = 893, 3.12 wt% Pu-240	1.01108	0.00087	0.00594	2, 3, 4, 5, 6
pu04-13	29.27 g Pu/liter, Critical Mass: 692 gm, H/Pu-239 = 903, 3.43 wt% Pu-240	1.00856	0.00091	0.00579	2, 3, 4, 5, 6
PU-SOL-THERM-005 Water Reflected 14-Inch Diameter Spheres, 0.050-inch thick shell of Type 347 Stainless Steel					
pu005-1	29.65 g Pu/liter, Critical Mass: 701 gm, H/Pu-239 = 903, 4.05 wt% Pu-240	1.0086	0.00088	0.00571	2, 3, 4, 5, 6
pu005-2	30.54 g Pu/liter, Critical Mass: 722 gm, H/Pu-239 = 868, 4.05 wt% Pu-240	1.00908	0.00088	0.00589	2, 3, 4, 5, 6

Table 7-19. Configurations Incorporating Plutonium Nitrate Solutions

Exp ID	Description	k_{eff}^a	σ	AENCF (MeV)	CC
pu005-3	31.43 g Pu/liter, Critical Mass: 743 gm, H/Pu-239 = 834, 4.05 wt% Pu-240	1.01116	0.00091	0.0062	2, 3, 4, 5, 6
pu005-4	33.54 g Pu/liter, Critical Mass: 793 gm, H/Pu-239 = 765, 4.05 wt% Pu-240	1.01197	0.00093	0.00664	2, 3, 4, 5, 6
pu005-5	36.04 g Pu/liter, Critical Mass: 852 gm, H/Pu-239 = 694, 4.05 wt% Pu-240	1.01367	0.0009	0.00723	2, 3, 4, 5, 6
pu005-6	38.49 g Pu/liter, Critical Mass: 910 gm, H/Pu-239 = 633, 4.05 wt% Pu-240	1.0102	0.00095	0.00766	2, 3, 4, 5, 6
pu005-7	40.91 g Pu/liter, Critical Mass: 967 gm, H/Pu-239 = 581, 4.05 wt% Pu-240	1.01073	0.00094	0.00838	2, 3, 4, 5, 6
pu005-8	30.58 g Pu/liter, Critical Mass: 723 gm, H/Pu-239 = 869, 4.40 wt% Pu-240	1.00799	0.00091	0.00593	2, 3, 4, 5, 6
pu005-9	31.85 g Pu/liter, Critical Mass: 753 gm, H/Pu-239 = 825, 4.40 wt% Pu-240	1.01023	0.00089	0.00631	2, 3, 4, 5, 6
PU-SOL-THERM-007 Water Reflected Partly Filled 11.5-Inch Diameter Spheres, 0.049-inch thick shell of Type 304L Stainless Steel, 4.67 wt% Pu-240, 95.059 wt% Pu-239 in Pu					
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	2, 3, 4, 5, 6
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	2, 3, 4, 5, 6
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	2, 3, 4, 5, 6
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	2, 3, 4, 5, 6
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	2, 3, 4, 5, 6
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	2, 3, 4, 5, 6
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	2, 3, 4, 5, 6
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	2, 3, 4, 5, 6
PU-SOL-THERM-009 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					

Table 7-19. Configurations Incorporating Plutonium Nitrate Solutions

Exp ID	Description	k_{eff}^a	σ	AENCF (MeV)	CC
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	2, 3, 4, 5, 6
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	2, 3, 4, 5, 6
pust9-3	9.457 g Pu/liter, Critical Volume: 949.1 liters, Full Sphere, H/Pu-239 = 2803	1.02176	0.00089	0.00246	2, 3, 4, 5, 6
PU-SOL-THERM-0010 Water Reflected Cylinders, 0.062-inch thick shell of Type 347 stainless steel, 2.9 wt% Pu-240 in Pu					
pu10091	99.09 g Pu/liter, Inner Radius (IR) = 11.4264 cm, Critical Height: 30.7086 cm, Critical Mass: 1249 g, H/Pu-239 = 267	1.02337	0.00101	0.01675	2, 3, 4, 5, 6
pu10092	73.92 g Pu/liter, IR = 11.4264 cm, Critical Height: 35.4076 cm, Critical Mass: 1073 g, H/Pu-239 = 357	1.02091	0.00097	0.01299	2, 3, 4, 5, 6
pu10093	54.53 g Pu/liter, IR = 11.4264 cm, Critical Height: 44.5770 cm, Critical Mass: 997 g, H/Pu-239 = 484	1.01316	0.00097	0.00994	2, 3, 4, 5, 6
pu10111	54.53 g Pu/liter, IR = 13.9684 cm, Critical Height: 25.6032 cm, Critical Mass: 856 g, H/Pu-239 = 485, Extra 0.065 inch layer of stainless steel placed around cylinder	1.01879	0.00099	0.01001	2, 3, 4, 5, 6
pu10112	47.21 g Pu/liter, IR = 13.9684 cm, Critical Height: 28.1686 cm, Critical Mass: 815 g, H/Pu-239 = 558, Extra 0.065 inch layer of stainless steel placed around cylinder	1.01543	0.00098	0.00873	2, 3, 4, 5, 6
pu10113	47.21 g Pu/liter, IR = 13.9684 cm, Critical Height: 27.0764 cm, Critical Mass: 784 g, H/Pu-239 = 558	1.01615	0.00092	0.00852	2, 3, 4, 5, 6
pu10114	41.73 g Pu/liter, IR = 13.9684 cm, Critical Height: 32.6390 cm, Critical Mass: 835 g, H/Pu-239 = 606	1.00903	0.00091	0.0079	2, 3, 4, 5, 6
pu10115	36.90 g Pu/liter, IR = 13.9684 cm, Critical Height: 43.0022 cm, Critical Mass: 973 g, H/Pu-239 = 665	1.01069	0.00093	0.00755	2, 3, 4, 5, 6
pu10116	63.99 g Pu/liter, IR = 13.9684 cm, Critical Height: 22.8092 cm, Critical Mass: 895 g, H/Pu-239 = 414	1.01992	0.00101	0.01114	2, 3, 4, 5, 6
pu10117	48.98 g Pu/liter, IR = 13.9684 cm, Critical Height: 25.9588 cm, Critical Mass: 780 g, H/Pu-239 = 535	1.01146	0.00092	0.00879	2, 3, 4, 5, 6
pu10121	48.75 g Pu/liter, IR = 15.2390 cm, Critical Height: 22.3520 cm, Critical Mass: 799 g, H/Pu-239 = 543	1.0156	0.00097	0.00896	2, 3, 4, 5, 6
pu10122	42.29 g Pu/liter, IR = 15.2390 cm, Critical Height: 25.2476 cm, Critical Mass: 779 g, H/Pu-239 = 618	1.01616	0.00095	0.00776	2, 3, 4, 5, 6
pu10123	36.52 g Pu/liter, IR = 15.2390 cm, Critical Height: 28.4734 cm, Critical Mass: 758 g, H/Pu-239 = 728	1.02352	0.00094	0.00691	2, 3, 4, 5, 6

Table 7-19. Configurations Incorporating Plutonium Nitrate Solutions

Exp ID	Description	k_{eff}^a	σ	AENCF (MeV)	CC
pu10124	31.14 g Pu/liter, IR = 15.2390 cm, Critical Height: 33.4264 cm, Critical Mass: 759 g, H/Pu-239 = 850	1.01642	0.00087	0.0061	2, 3, 4, 5, 6
PU-SOL-THERM-0011 Unreflected 16- & 18-Inch Diameter Spheres, 0.050 inch thick shell of Type 347 stainless steel, 0.020 inch thick Cd Cover on the 18-inch sphere, 4.2 wt% Pu-240 in Pu					
pu11161	34.96 g Pu/liter, IR = 20.1206 cm, Critical Mass: 1194 g, H/Pu-239 = 765	1.01661	0.00103	0.00738	2, 3, 4, 5, 6
pu11162	36.22 g Pu/liter, IR = 20.1206 cm, Critical Mass: 1237 g, H/Pu-239 = 736	1.02377	0.00101	0.00777	2, 3, 4, 5, 6
pu11163	38.13 g Pu/liter, IR = 20.1206 cm, Critical Mass: 1302 g, H/Pu-239 = 691	1.02224	0.00101	0.00827	2, 3, 4, 5, 6
pu11164	38.16 g Pu/liter, IR = 20.1206 cm, Critical Mass: 1303 g, H/Pu-239 = 682	1.01688	0.00105	0.00845	2, 3, 4, 5, 6
pu11165	43.43 g Pu/liter, IR = 20.1206 cm, Critical Mass: 1483 g, H/Pu-239 = 575	1.01338	0.00104	0.00973	2, 3, 4, 5, 6
pu11181	22.35 g Pu/liter, IR = 22.6974 cm, Critical Mass: 1095 g, H/Pu-239 = 1208	1.00169	0.00089	0.00505	2, 3, 4, 5, 6
pu11182	23.27 g Pu/liter, IR = 22.6974 cm, Critical Mass: 1140 g, H/Pu-239 = 1151	1.0068	0.00088	0.00549	2, 3, 4, 5, 6
pu11183	23.10 g Pu/liter, IR = 22.6974 cm, Critical Mass: 1132 g, H/Pu-239 = 1158	1.00336	0.00097	0.00514	2, 3, 4, 5, 6
pu11184	23.82 g Pu/liter, IR = 22.6974 cm, Critical Mass: 1167 g, H/Pu-239 = 1100	1.00285	0.00088	0.00547	2, 3, 4, 5, 6
pu11185	25.20 g Pu/liter, IR = 22.6974 cm, Critical Mass: 1235 g, H/Pu-239 = 1039	1.01131	0.00093	0.00593	2, 3, 4, 5, 6
pu11186	27.49 g Pu/liter, IR = 22.6974 cm, Critical Mass: 1347 g, H/Pu-239 = 908	1.00796	0.00097	0.00633	2, 3, 4, 5, 6
pu11187	23.94 g Pu/liter, IR = 22.6974 cm, Critical Mass: 1173 g, H/Pu-239 = 1103	1.00792	0.00088	0.00548	2, 3, 4, 5, 6

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 reason is unknown at this time, but since the calculated values are over-predictions of a critical system, this is considered conservative with respect to criticality safety applications.

7.1.3.3 Low-Enrichment Uranium Solutions

The first set of experiments involving low-enrichment uranium are from NEA (1998), Volume IV, the second set (case prefix "LEUJ") are from work at the Japan Atomic Energy Research Institute (Miyoshi et al. 1997), and the third set (case prefix SPHU9) are cases that look at UO_3-H_2O critical solutions (Wittekind 1992, p. 43). These experiments are listed in Table 7-20.

Table 7-20. Configurations Incorporating Low-Enrichment Uranium Solutions

Exp ID	Description	k_{eff}	σ	AENCF (MeV)	CC
LEU-SOL-THERM-002 174 Liter Spherical Tank of 4.9% Enriched UO_2F_2 Solutions, 34.399 cm Radius, 0.1588 cm thick 1100 Aluminum Shell					
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	2, 3, 4, 5, 6
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	2, 3, 4, 5, 6
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	2, 3, 4, 5, 6
Cylindrical Tank With a 59.0 cm ID, 0.3 cm thick stainless steel SS 304, U-235 Enrichment of 9.97 wt%					
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	2, 3, 4, 5, 6
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	2, 3, 4, 5, 6
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	2, 3, 4, 5, 6
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	2, 3, 4, 5, 6
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	2, 3, 4, 5, 6
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	2, 3, 4, 5, 6
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	2, 3, 4, 5, 6
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	2, 3, 4, 5, 6
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	2, 3, 4, 5, 6
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	2, 3, 4, 5, 6
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	2, 3, 4, 5, 6

Table 7-20: Configurations Incorporating Low-Enrichment Uranium Solutions

Exp ID	Description	k_{eff}	σ	AENCF (MeV)	CC
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	2, 3, 4, 5, 6
UO ₃ -H ₂ O Solution Experiments					
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	2, 3, 4, 5, 6
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	2, 3, 4, 5, 6
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	2, 3, 4, 5, 6
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	2, 3, 4, 5, 6
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	2, 3, 4, 5, 6
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	2, 3, 4, 5, 6
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	2, 3, 4, 5, 6
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	2, 3, 4, 5, 6
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	2, 3, 4, 5, 6
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	2, 3, 4, 5, 6
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	2, 3, 4, 5, 6
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	2, 3, 4, 5, 6

NOTE: ^a For the UO₃-H₂O 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 UO₃-H₂O solution experiments the calculated k_{∞} value is the bottom number

^c For the UO₃-H₂O solution experiments the top number represents experimental uncertainty

^d For the UO₃-H₂O 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 wt% enriched uranyl fluoride and is taken from NEA (1998), LEU-SOL-THERM-001 (LST-001). This experiment used the SHEBA-II (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 7-21.

Table 7-21. Configurations Incorporating Uranyl Fluoride Solutions

Exp ID	Description	k_{eff}	σ	AENCF (MeV)	CC
Ist1-1	Average solution density: 2.1092 g/cm ³ , Average uranium density: 0.9783 g/cm ³ , Average U-235 enrichment: 4.9977 atom percent, H/X: 453.9	1.01069	0.00085	0.0523	2, 3, 4, 5, 6

7.2 BIAS AND UNCERTAINTY

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. Usually, it is difficult to distinguish between bias and uncertainty or the difference between measurement and calculational bias and uncertainty, therefore they are all taken together.

Modeling and inputs for computing the effective neutron multiplication factor for a critical experiment with a criticality code often induce bias in the resulting k_{eff} value. These k_{eff} values deviate from the expected result ($k_{\text{eff}} = 1$) from 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.

An essential element of validating the methods and models 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 waste package 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.

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 2000, pp. 3-8 through 3-14]). 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. A CL function may be expressed as a regression-based function of neutronic and/or physical variable(s). In application, a CL function could also be a single value, reflecting a conservative result over the range of applicability for the waste form characterized.

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 CLs 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 CL function.

The purpose of the CL 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 CL 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 7-1 displays two general processes for establishing CL 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 CL 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 CL. 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 (DFTL) method, discussed in YMP (2000, pp. 3-56 and 3-57), are "non-trending" methods.

Figure 7-1. Process for Calculating Critical Limits

Source: YMP 2000, p. 3-53

The regression or “trending” methods use statistical tolerance values based on linear regression techniques to establish a CL 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 2000, p. 3-52). 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 CL. The lower uniform tolerance band (LUTB) method, discussed in YMP (2000, pp. 3-55 and 3-56), trends a single parameter against k_{eff} . Multiple regression methods that trend multiple parameters against k_{eff} may also be used to establish the tolerance-limit CL function. In either single or multiple situations, the regression trend that produces the lowest CL is defined to be the more conservative regression. This report currently only uses single parameter regression methods.

In all calculations of CL 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 CL for cases in which the best estimate of the bias trend would result in a CL greater than 1.0. The treatment of this element is discussed below in the context of each method used to establish the basic CL function.

The critical limit is estimated such that a calculated k_{eff} below this limit is considered subcritical, and a system is considered acceptably subcritical if a calculated k_{eff} plus calculational uncertainties lies below this limit. In equation notation,

$$k_S + \Delta k_S < \text{CL} \quad (\text{Eq. 7-1})$$

where

k_S = the calculated multiplication factor of a system to be considered for criticality
 Δk_S = the uncertainty in the value of k_S .

The CL function is defined as,

$$f(x) = k_C(x) - \Delta k_C(x) \quad (\text{Eq. 7-2})$$

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.
 $\Delta k_C(x)$ = 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, CL is estimated as a function ($f[\text{CL}]$) of a parameter(s). Because both $\Delta k_C(x)$ and $k_C(x)$ can vary with this parameter, the CL 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

$$\beta = k_C - 1 \quad (\text{Eq. 7-3})$$

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 CL 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.

7.2.1 Statistical Analyses

The following discussion addresses the statistical analyses that were performed for this report. Explicit, detailed statistical analyses and tests will be performed in a future revision in order to address issues including, but not limited to, goodness-of-fit, normality of residuals, collinearity, and other tests deemed necessary for a complete statistical evaluation.

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 (UO_2 and MOX based fuel)
- Uranium Solution LCEs
- Pu Solution LCEs

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

With the Student's t-test for two groups it can be determined, with 95% confidence, whether subsets have different mean values, and thus should not be analyzed together. The equality test requires computing the statistic " T " in Equation 7-4.

$$T = \frac{\bar{Y}_1 - \bar{Y}_2}{\sqrt{\frac{(n-1)S_{y1}^2 + (m-1)S_{y2}^2}{n+m-2}} \sqrt{\frac{1}{n} + \frac{1}{m}}} \quad (\text{Eq. 7-4})$$

where the $\bar{Y}$ values are the calculated multiplication factor averages for each subset, n and m are the number of observations for each subset, and the S_{y1}^2 and S_{y2}^2 values represent the variances for each subset as shown in Equations 7-5 and 7-6.

$$S_{y1}^2 = \frac{\sum_{i=1,n} (Y_i - \bar{Y}_1)^2}{n-1} \quad (\text{Eq. 7-5})$$

$$S_{y2}^2 = \frac{\sum_{i=1,m} (Y_i - \bar{Y}_2)^2}{m-1} \quad (\text{Eq. 7-6})$$

The “T” statistic is compared to the Student’s t-distribution with 95% 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 7-22 presents the test results.

Table 7-22. Equality Test Statistic Results

Subsets	UO ₂ and MOX LCEs					
	Sample Size	Average k _{eff}	Variance	T statistic	t _{α/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					
U Solutions	28	1.0028	2.512E-04	-3.4257	1.9780	N
Pu 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’s 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 7-7 along with the statistical parameters in Equations 7-8 and 7-9.

$$T = b \sqrt{\frac{(n-2)S_{xx}}{SS_R}} \quad (\text{Eq. 7-7})$$

where

b comes from the fitted linear regression equation

$$S_{xx} = \sum_{i=1,n} (x_i - \bar{x})^2 \quad (\text{Eq. 7-8})$$

and

$$SS_R = \sum_{i=1,n} (y_i - a - bx_i)^2 \quad (\text{Eq. 7-9})$$

The test statistic is compared to the Student’s t-distribution with 95% 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% confidence, trends due to the randomness of the data are eliminated.

7.2.2.1 Trending Evaluation

Trending against various parameters were performed in order to determine correlations between characteristics and the calculated multiplication factors for each subset. Depending on the type of benchmark, different parameters were trended against to determine which exhibit the strongest trends. The regression statistics for the trend evaluations are presented in Tables 7-23 through 7-26 for each of the subsets, and illustrated in Figures 7-2 through 7-15.

Table 7-23. 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

NOTE: ^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 7-24. UO₂ and MOX LCE Trending Parameter Results

Trend Parameter	N	Slope	Intercept	S _{xx}	SS _R	r	T	t _{α/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 7-25. Uranium Solution Trending Parameter Results

Trend Parameter	N	Slope	Intercept	S _{xx}	SS _R	r	T	t _{α/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 7-26. Pu Solution Trending Parameter Results

Trend Parameter	N	Slope	Intercept	S _{xx}	SS _R	r	T	t _{α/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 7-2. CRC Subset with AENCF as Trending Parameter

Figure 7-3. CRC Subset with Core Average Burnup as Trending Parameter

Figure 7-4. CRC Subset with Soluble Boron Concentration as Trending Parameter

Figure 7-5. CRC Subset with ALF as Trending Parameter

Figure 7-6. UO₂ and MOX LCE Subset with AENCF as Trending Parameter

Figure 7-7. UO₂ and MOX LCE Subset with P/D as Trending Parameter

Figure 7-8. UO₂ and MOX LCE Subset with Pin Pitch as Trending Parameter

Figure 7-9. UO₂ and MOX LCE Subset with Water to Fuel Volume Ratio as Trending Parameter

Figure 7-10. Uranium Solution Subset with AENCF as Trending Parameter

Figure 7-11. Uranium Solution Subset with H/X as Trending Parameter

Figure 7-12. Uranium Solution Subset with ALF as Trending Parameter

Figure 7-13. Plutonium Solution Subset with AENCF as Trending Parameter

Figure 7-14. Plutonium Solution Subset with H/X as Trending Parameter

Figure 7-15. Plutonium Solution Subset with ALF as Trending Parameter

7.2.3 Critical Limit Determination

The CL for a waste package 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. The CL is calculated by CLREG only when a trending regression is identified as statistically significant. If no trend is identified, then the NDTL or the DFTL method is used as previously discussed in Section 7.2.

CLREG is a computer program that calculates sets of CLs (CL functions) for waste packages under certain conditions. Each CL 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. Also inherent in each CL value is the statistical property of confidence for lower prediction limits and lower tolerance limits. A complete discussion of the statistical methodology for CLREG is provided in BSC (2002b).

CLs 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 CL from experiments applicable to a particular configuration class is then selected as 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 7-16 through 7-18, with the selected CL values

presented in Table 7-27 for each of the subsets. The results presented in Table 7-27 were generated for a 95% confidence level covering 99.5% of the population.

Table 7-27. Critical Limits for Experiment Subsets

Subset	Trend Parameter	CL
CRCs	Core Average Burnup (BU)	$CL = -2.403E-4 \cdot BU + 0.9858$
Lattice LCEs	Pin Pitch (P)	$CL = 7.0175E-03 \cdot P + 0.9677$ ($1.32 \text{ cm} \leq P \leq 1.89 \text{ cm}$); $CL = 0.982$ ($1.89 \text{ cm} < P \leq 2.64 \text{ cm}$) ^a
UO ₂ Solutions	None	0.952 ^b
Pu Solutions	AENCF	0.980 ($2.46E-03 \text{ MeV} \leq \text{AENCF} \leq 5.07E-02 \text{ MeV}$)

NOTE: ^a Upper limit set at 0.982 since no positive bias credit is taken

^b Calculated using the NDTL method with 95% confidence level covering 99% of the population.

Figure 7-16. Critical Limit Plot for CRC Experiment Subset

It should be noted that in burnup credit applications, the system multiplication factor will be calculated using the principal isotope set for material compositions which inherently adds an additional bias on the calculated k_{eff} of about 0.015.

Figure 7-17. Critical Limit Plot for Lattice LCE Subset

Figure 7-18. Critical Limit Plot for Pu Solution LCE Subset

7.3 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 in 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 (2000, pp. 3-8 through 3-14).

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.

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 7-19 illustrates the neutron flux spectral characteristics that were compared for a representative 21 PWR waste package (WP), a CRC statepoint, two MOX LCEs - SSR53 (12x12 PuO₂ lattice) and EXP22 (12x12 PuO₂ Lattice) - and one fresh fuel LCE (SSR48 UO₂ lattice).

Figure 7-19. 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 7-20. A 21-assembly area of the core was modeled in a fully flooded, intact waste package configuration as shown in Figure 7-20. 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 16.358 GWd/MTU through 34.416 GWd/MTU, and initial enrichments of 2.62 through 3.49 wt% U-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.

Figure 7-20. 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 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 7-21. 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, etc.), when compared to the waste package (WP), the results indicate that CRCs are just as adequate for benchmarks and more closely represents the reaction rates for burned fuel in a storage package configuration.

Figure 7-21. Thermal Region Reaction Ratio Comparison

Overall the range of parameters covered by the current set of benchmark experiments are summarized in Table 7-28.

Table 7-28. Experiment Parameter Summary

Subset	Number of Experiments	Range of Parameters
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
Pu Solutions	107	Initial enrichment (wt% ²³⁹ Pu): 91.1 through 99.5; H/X: 91 through 2803; AENCF (MeV): 2.46E-03 through 5.07E-02; Applicable to homogeneous mixtures

7.4 ACCEPTANCE CRITERIA

The acceptance criteria are determined by the final generation of a loading curve for the waste package. The process for determining the acceptance criteria is illustrated in Figure 7-22. The development of the loading curve will be to meet the requirements of the CL which are based on the values reported in Table 7-28. This will determine which spent fuel assemblies are acceptable for loading.

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 extension of the range of applicability (EROA) (Δk_{EROA}), will be subtracted from the critical limit, therefore setting a new CL for a prescribed parameter range.

The acceptance criteria for a waste package system is as follows:

$$k_s + \Delta k_s < \text{CL} - \Delta k_{\text{EROA}} - \Delta k_{\text{ISO}} \quad (\text{Eq. 7-10})$$

where,

k_s = calculated k_{eff} for the system

Δk_s = the standard deviation of k_s about the average combined collision, absorption, and track-length estimate due to the Monte Carlo calculation statistics

Δk_{ISO} = an additional bias and uncertainty resulting from isotopic model validation that will be subtracted from the CL

An example for extending the ROA based on burnup is provided in Attachment II. This extension was calculated using CLREG.

The following are the current acceptance criteria commercial SNF must meet to be considered with the criticality model for burnup credit applications:

- Assembly average initial enrichment range of 1.93 through 4.17 wt% ^{235}U
- A waste package average burnup range of 0.0 through 33.0 GWd/MTU
- Fuel pin pitches between 1.26 cm and 2.64 cm

Figure 7-22. Process for Establishing Criticality Acceptance Criteria

7.5 FUTURE ACTIVITIES

The following provides a listing of outstanding issues that are under consideration to be investigated which help provide additional support for validation of the criticality model:

- If geochemical analyses define parameter ranges for configurations within a configuration class beyond those already evaluated, additional benchmarks will be evaluated to encompass those ranges.
- Detailed statistical analyses and tests will be performed in order to address issues including but not limited to goodness-of-fit, normality of residuals, collinearity, among other tests for a more complete statistical evaluation. Also, multiple regressions that trend multiple parameters will be investigated.
- Additional investigation of experiments that consistently exhibit high (above 1.01) eigenvalues will be made to determine the cause(s).
- Additional trending parameters characterizing system leakage, spectrum, interstitial poison effects, and benchmark applicability will be investigated.

8. CONCLUSIONS

This report presented a set of benchmark experiments that cover a range of the potential configurations PWR assemblies stored in a waste package may take. The major parameters covered by the benchmark experiments were burnup, initial enrichment, spectrum, and geometry. Critical limits were calculated for subsets of the total benchmark experiments that can be used for a given configuration class, based on statistical analyses. Based on the benchmark experiment results presented throughout Section 7.1 in Tables 7-1 through 7-21, this report concludes that the criticality model is a valid tool for calculating the multiplication factor for the various waste package configurations that may exist over time in the geologic repository. Critical limits were statistically derived from the benchmark experiments and separated into subset applicability for different configuration classes in Section 7.2, and a specified range of applicability was provided in Section 7.3.

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10. ATTACHMENTS

The description of the attachments is listed in Table 10-1.

Table 10-1. Attachment Listing

Attachment	No. 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 input and output files contained in Attachment IV
IV	N/A	Compact disc attachment containing CLREG 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 2002b).

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

Ind Var	Keff(cc)	Pred Keff	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	Keff(cc)	Pred Keff	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
1.87E+00	1.003	1.000	0.991	0.981	0.980

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

Ind Var	Keff(cc)	Pred Keff	PreClos CL	LUTB CL	Bonf LTL
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. Pu Solution Experiments with AENCF as Trend Parameter

Ind Var	Keff(cc)	Pred Keff	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

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

Ind Var	Keff(cc)	Pred Keff	PreClos CL	LUTB CL	Bonf LTL
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
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

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

Ind Var	Keff(cc)	Pred Keff	PreClos CL	LUTB CL	Bonf LTL
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 2002b).

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 wt% ^{235}U , 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.

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

Ind Var	Keff(cc)	Pred Keff	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

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

Ind Var	Keff(cc)	Pred Keff	PreClos CL	LUTB CL	Bonf LTL
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

Figure II-1. Example of EROA

ATTACHMENT III

This attachment contains a listing of the CLREG 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	07:10a	Input file for CRC subset using burnup as the trend parameter
crcbu01out.csv	Excel	3,861	9/09/2002	07:12a	Output file for CRC subset using burnup as the trend parameter
crcbu01util	ASCII	3,186	9/09/2002	07:12a	CLREG generated utility file for CRC subset using burnup as the trend parameter
latlcepitch.csv	Excel	1,875	8/13/2002	03:52p	Input file for lattice LCE subset using pitch as the trend parameter
latlcepitchout.csv	Excel	7,053	8/13/2002	04:04p	Output file for lattice LCE subset using pitch as the trend parameter
latlcepitchutil	ASCII	4,900	8/13/2002	04:04p	CLREG generated utility file for lattice LCE subset using pitch as the trend parameter
pusolaencf.csv	Excel	2,651	8/13/2002	03:54p	Input file for Pu solution subset using AENCF as trend parameter
pusolaencfout.csv	Excel	9,069	8/13/2002	04:07p	Output file for Pu solution subset using AENCF as trend parameter
pusolaencfutil	ASCII	5,979	8/13/2002	04:07p	CLREG generated utility file for Pu solution subset using AENCF as trend parameter
crceroaout.csv	Excel	4,553	9/09/2002	07:20a	Output file for extension of the range of applicability example
crceroa.csv	Excel	1,125	9/09/2002	07:19a	Input file for extension of the range of applicability example
crceroautil	ASCII	3,546	9/09/2002	07:20a	CLREG generated utility file for extension of the range of applicability example

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1. QA: QA

SPECIAL INSTRUCTION SHEET

Page: 1 of: 1

Complete Only Applicable Items

file list
3-21-03 nfc

This is a placeholder page for records that cannot be scanned.

2. Record Date 3/13/03 2/3/03 dc 5-27-03		3. Accession Number AT-TO: DOC, 20030319.0001	
4. Author Name(s) John M. Scaglione		5. Author Organization Risk & Criticality/ESP	
6. Title/Description Criticality Model Report			
7. Document Number(s) MDL-EBS-NU-000003			8. Version Designator Rev. 00 ICN 01
9. Document Type Model Report		10. Medium CD ROM	
11. Access Control Code General K10 5-24-03 PUB			
12. Traceability Designator N/A K10 5-24-03 DC 34795			
13. Comments			

THIS IS AN ELECTRONIC
ATTACHMENT