

BSC

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DISCLAIMER

The Calculations contained in this document were developed by Bechtel SAIC Company, LLC (BSC) and are intended solely for the use of BSC in its work for the Yucca Mountain Project.

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1. PURPOSE

The objective of this calculation is to provide the uncertainty term for fission products and minor actinides which contributes to the determination of the critical limit for burnup credit calculations. The scope of this calculation covers PWR and BWR spent nuclear fuel (SNF).

This activity supports the Criticality Department's validation of burnup credit. The intended use of these results is in future Criticality Department calculations and analyses.

Limitations of this evaluation are as follows:

- Calculations are based upon PWR and BWR waste package baskets containing stainless steel/boron neutron absorber material (BSC 2005 [DIRS 174180]).

2. REFERENCES

This section presents the references used in this calculation. The document input reference system (DIRS) number is listed first, and then the corresponding reference.

2.1 DESIGN INPUTS

174180 BSC (Bechtel SAIC Company) 2005. *Reactivity Effect of Cross Section Uncertainty for Burnup Credit Validation*. CAL-DSU-NU-000011 REV 00A. Las Vegas, Nevada: Bechtel SAIC Company. ACC: DOC.20050525.0001.

177701 Gauld, I.C. and Mueller, D.E. 2005. *Evaluation of Cross-Section Sensitivities in Computing Burnup Credit Fission Product Concentrations*. ORNL/TM-2005/48. Oak Ridge, Tennessee: Oak Ridge National Laboratory. ACC: MOL.20060912.0060.

2.2 DESIGN CONSTRAINTS

2.2.1 EG-PRO-3DP-G04B-00037, Rev. 1. *Calculations and Analyses*. Las Vegas, Nevada: Bechtel SAIC Company. ACC: ENG.20060414.0007.

2.2.2 IT-PRO-0011, Rev. 0, ICN 0. *Software Management*. Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: DOC.20060301.0007.

2.3 DESIGN OUTPUTS

None.

2.4 SOFTWARE CODES

None.

3. ASSUMPTIONS

3.1 ASSUMPTIONS THAT REQUIRE VERIFICATION

None.

3.2 ASSUMPTIONS THAT DO NOT REQUIRE VERIFICATION

3.2.1 Linear Perturbation of Reactivity Effects

Assumption: The sensitivity of changes in reactivity to changes in isotopics engendered by cross-section uncertainty is treated as a linear function.

Rationale: The rationale for this assumption is that the reactivity effects of fission products and minor actinides are relatively small compared to the effects of uranium and plutonium in SNF. In addition, the reactivity effects (Δk_{worth}) of cross-section uncertainties were computed (BSC 2005 [DIRS 174180], Attachment III, Effects of Xsec Uncertainty PWR.xls) individually for each isotope and the sum of these effects was less than the composite effect of Principal Isotope fission products and minor actinides (actinides other than U and Pu, which are Np-237, Am-241, Am-242m, and Am-243) taken together in a single calculation. Thus, the calculation of reactivity effects assuming a linear behavior for perturbations of the cross-section values is conservative.

Use in the Calculation: This assumption was used in Sections 6.2 and 6.4.

3.2.2 Sensitivities of Minor Actinides

Assumption: A sensitivity of 1.0 was assigned to each minor actinide. The sensitivities of minor actinides are not provided in Gauld and Mueller 2005 [DIRS 177701]; only fission products are addressed.

Rationale: The rationale for this assumption is that the numerical value of sensitivities includes negative terms related to isotopic depletion and that omission of these terms is conservative. The positive value of 1.0 indicates that if an absorber cross section is reduced by its uncertainty, an equivalent reduction of the isotopic content results.

Use in the Calculation: This assumption was used in Section 6.1 and 6.4.

3.2.3 Sensitivities of PWR and BWR SNF

Assumption: The sensitivities of PWR and BWR SNF are equal. Gauld and Mueller 2005 [DIRS 177701] provides sensitivities evaluated only for PWR SNF.

Rationale: The isotopic sensitivities are dependent upon radioactive decay and neutron capture reactions of isotopes, which are independent of the fuel type.

Use in the Calculation: This assumption was used in Section 6.1 and 6.4.

4. METHODOLOGY

4.1 QUALITY ASSURANCE

This calculation is prepared in accordance with *Calculations and Analyses* (Reference 2.2.1). This calculation does not concern structures, systems, or components that are important to safety, important to waste isolation, or are quality level 1. Therefore, no additional reviews are required.

4.2 USE OF SOFTWARE

4.2.1 EXCEL

- Software Title: Excel
- Version/Revision number: Microsoft® Excel 2003 SP-2
- Computer Environment: Software is installed on a DELL OptiPlex GX620 personal computer, DOE Management and Operating Contractor (M&O) Property tag number YMP003943, running Microsoft Windows XP, Service Pack 2.

Microsoft Excel for Windows, Version 2003 SP-2, is used in calculations and analysis to manipulate the inputs using standard mathematical expressions and operations. It is also used to tabulate and chart results. The user-defined formulas, inputs, and results are documented in sufficient detail to allow an independent repetition of computations. Thus, Microsoft Excel is used only as a worksheet and not as a software routine. Microsoft Excel 2003 SP-2 is an exempt software product in accordance with *Software Management* (Reference 2.2.2, Subsection 1.4.1).

The spreadsheet files for the Excel calculations are documented in Attachment I.

4.3 SENSITIVITY CALCULATION METHODOLOGY

The bias and uncertainty for criticality calculations including fission products and minor actinides must be determined as part of the validation process for burnup credit. The bias is determined elsewhere via critical experiments such as Commercial Reactor Criticals (CRCs). CRCs do not facilitate determination of the uncertainty introduced by the inclusion of fission products and minor actinides, and a propagation of errors methodology based upon uncertainties tabulated in the Evaluated Nuclear Data Files (ENDF/B) is employed in the *Reactivity Effects of Cross Section Uncertainties for Burnup Credit Validation* report (BSC 2005 [DIRS 174180]). The direct effect of cross section uncertainties upon k_{eff} is evaluated by BSC 2005 [DIRS 174180], but cross section uncertainties also propagate to isotopic content uncertainties. A study of isotopic effects (Gauld and Mueller 2005 [DIRS 177701]) provides the relative sensitivity of isotopic contents to uncertainties in cross sections, and these sensitivities are used to scale the reactivity effects determined by BSC 2005 [DIRS 174180].

5. LIST OF ATTACHMENTS

Attachment #	Title	Number of Pages
I	CD Listing	1
II	One Compact Disc	N/A

6. BODY OF CALCULATION

6.1 ISOTOPIC SENSITIVITIES

This section provides a description of the isotopic sensitivities of fission products and minor actinides.

The relative isotopic sensitivity to a change in cross section is expressed as:

$$S_i = \frac{\partial N_i / N_i}{\partial \sigma_i / \sigma_i} \quad (\text{Eq. 1})$$

where

S_i = the sensitivity of the concentration of isotope_{*i*} to uncertainty in cross section

∂N_i = change in number density of isotope_{*i*}

N_i = Number density of isotope_{*i*}

$\partial \sigma_i$ = change in cross section of isotope_{*i*}

σ_i = cross section of isotope_{*i*}

A relative sensitivity of 1.0 would indicate that the concentration of an isotope is as sensitive as the cross section, i.e. a 10 percent change in cross section would result in a ten percent change in the isotopic concentration. Fission product and minor actinide concentrations have sensitivities less than one because if the cross section were to decrease, the isotope would have fewer neutron capture reactions during irradiation in a reactor, which would result in a larger concentration of that isotope upon discharge from the reactor. Thus a neutron capture reaction has a negative sensitivity while parent isotope decay has a positive sensitivity. Relative sensitivities for fission products are presented in Gauld and Mueller 2005 [DIRS 177701]. The values of the relative sensitivities for each fission product and minor actinide are provided in Table 1 for each reaction, i.e., isotope decay of the parent, producing the daughter isotope and neutron capture removing the isotope. The total sensitivity for each isotope is calculated by summing the reaction sensitivity values. Relative sensitivity values for minor actinides were not provided in Gauld and Mueller 2005 [DIRS 177701] and are set to the value of 1.0.

Table 1: Isotope Relative Sensitivities

Reactivity Effect of Cross Section Uncertainties Upon Isotopic Compositions

Isotope	Reaction	S	Reaction	S	Reaction	S	Reaction	S	Reaction	S	Reaction	S	Reaction	S	S _{Total}	
1	Mo-95	Zr-94	2.52E-04	nb-94	4.14E-08	Zr-95	-4.56E-04	Nb-95	-9.96E-04	Nb-95m	-6.00E-06		Mo-95	-6.70E-02	-0.0653	
2	Tc-99	Mo-98	4.17E-03	Tc-98	8.68E-09	Mo-99	-9.64E-05						Tc-99	-1.26E-01	-0.1217	
3	Sm-149	Pm-147	2.79E-01	Nd-148	2.77E-02	Pm-148	8.77E-02	Pm-148m	6.21E-02	Sm-148	1.28E-02	Pm-149	-1.31E-02	Sm-149	-1.00E+00	-0.5176
4	Ru-101	Mo-100	3.16E-03	Ru-100	1.16E-03								Ru-101	-5.68E-02	-0.0525	
5	Rh-103	Ru-102	5.26E-03	Rh-102	5.09E-09	Ru-103	-3.72E-03	Rh-103 (f,y)	1.16E-13				Rh-103	-4.64E-01	-0.4550	
6	Ag-109	Pd-108	1.20E-01	Pd-108(f,y)	-2.16E-08	Pd-109	-1.06E-04	Ag-109(f,y)	-2.15E-07				Ag-109	-3.85E-01	-0.2649	
7	Nd-143	Ce-142	2.30E-03	Pr-142	5.21E-06	Nd-142	6.28E-04	Ce-143	-8.70E-05	Pr-143	-5.92E-03		Nd-143	-4.59E-01	-0.4501	
8	Nd-145	Nd-143	2.56E-03	Ce-144	1.52E-03	Nd-144	1.07E-02						Nd-145	-1.53E-01	-0.1382	
9	Sm-147	Nd-146	4.32E-03	Nd-147	-1.78E-02	Pm-147	-3.63E-01	Pm-147(f,y)	2.10E-05				Sm-147	-3.30E-01	0.0551	
		(20 y)	7.06E-03		-1.98E-02		-4.79E-01		-7.74E-06					-1.11E-01	0.3949	
10	Sm-150	Nd-148	1.57E-02	Pm-148	6.89E-02	Pm-148m	6.01E-02	Sm-149	-3.24E-03	Pm-150	-9.42E-06		Sm-150	-1.78E-01	-0.0301	
11	Sm-151	Sm-149	-2.13E-03	Nd-150	1.42E-02	Sm-150	4.07E-01	Pm-151	-2.73E-03				Sm-151	-9.90E-01	-0.5639	
12	Sm-152	Sm-150	2.37E-01	Sm-151	1.60E-02								Sm-152	-7.30E-01	-0.4770	
13	Eu-151												Eu-151	-1	-1.0000	
14	Eu-153	Sm-151	2.32E-02	Sm-152	3.19E-01	Eu-152m	1.54E-06	Sm-153	-6.51E-03				Eu-153	-5.52E-01	-0.2033	
15	Gd-155	Eu-153	4.77E-01	Eu-154	-5.58E-02	Gd-154	1.74E-01	Eu-155	-7.77E-01				Gd-155	-1.01E+00	0.4738	
16	Cs-133	Xe-132	1.49E-03	Xe-132(f,y)	-7.16E-07	Cs-132	1.14E-10	I-133	-4.90E-05	Xe-133	-4.57E-03	Xe-133m	-5.68E-05	Cs-133	-1.79E-01	-0.1728
17	Np-237	Am-241	1												1.0000	
18	Am-241	Pu-240	1												1.0000	
19	Am-242m	Am-241	1												1.0000	
20	Am-243	Am-242m	1												1.0000	

Notes:

1. ORNL 2005 values are at 42 GWd/MTU - BSC 2004 values are at 40 GWd/MTU
 2. Sensitivities of an Isotope to Itself are Always Negative Due to Coupling of Cross Section and Isotopic Effects
 3. Sensitivities of an Isotope to Neutron Capture by Precursors may be Positive or Negative. Absolute Value is Summed Due to Independence of These Nuclides
 4. Sensitivities for Minor Actinides are Conservative Estimates Applying a Maximum Value of 1.0
 5. Sensitivity for Eu-151 is scaled from Gd-155, Sm-149, and Sm-151 Isotope Burn-Out Sensitivities which have Similar Cross Section Magnitudes
- Reference: Gauld, I.C. and Mueller, D.E., 2005 [DIRS 177701]

6.2 LINEAR PERTURBATION OF REACTIVITY EFFECTS

The reactivity effects of isotopic uncertainties are assumed to be linearly dependent upon the change in cross section of each isotope. The reactivity effect of isotopic uncertainty for a given isotope is:

$$(\Delta k_i)_{\text{Iso}} = S_i * (\Delta k_i)_{\text{Xsec}} \quad (\text{Eq. 2})$$

where

$(\Delta k_i)_{\text{Iso}}$ = the reactivity effect of isotopic uncertainty of isotope_i

S_i = the relative sensitivity of isotope_i from Table 1

$(\Delta k_i)_{\text{Xsec}}$ = the reactivity effect of cross section uncertainty of isotope_i

6.3 CROSS SECTION UNCERTAINTIES AND REACTIVITY EFFECTS

The values of cross section uncertainties are presented in BSC 2005 ([DIRS 174180], Tables 1 and 2) as Confidence Factors, which are fraction of the cross section that could be included in a burnup credit reactivity calculation after twice the evaluated uncertainty has been removed. The reactivity effects of the cross section uncertainties are presented in Table 13 of BSC 2005 [DIRS 174180] for each individual isotope, evaluated in both PWR and BWR waste package basket designs. These results are summarized in Table 2 for PWR and Table 3 for BWR SNF.

Table 2: PWR Reactivity Effect for Cross Section Uncertainties

Nuclide	Confidence Factor	(21-PWR Waste Package)		$\frac{\Delta k_U}{\Delta k_{Worth}}$ (%)
		Isotope Δk_{Worth}	Isotope Δk_U	
Mo-95	0.80	-0.00187	0.00027	0.2
Tc-99	0.90	-0.00424	0.00081	0.7
Sm-149	0.90	-0.01545	0.00130	1.2
Ru-101	0.26	-0.00100	0.00030	0.2
Rh-103	0.90	-0.01158	0.00074	0.7
Ag-109	0.94	-0.00200	0.00014	0.2
Nd-143	0.92	-0.01630	0.00105	0.9
Nd-145	0.58	-0.00315	0.00136	1.2
Sm-147	0.34	-0.00198	0.00092	0.8
Sm-150	0.88	-0.00178	0.00014	0.2
Sm-151	0.96	-0.01071	0.00063	0.6
Sm-152	0.96	-0.00444	0.00005	0.2
Eu-151	0.98	-0.00036	0.00023	0.2
Eu-153	0.96	-0.00342	0.00036	0.3
Gd-155	0.96	-0.00706	0.00081	0.7
Np-237	0.68	-0.00578	0.00303	2.7
Am-241	0.74	-0.01241	0.00322	2.9
Am-242m	1.22	0.00023	0.00054	0.5
Am-243	0.82	-0.00174	0.00060	0.5
Total Δk_{Worth}		-0.1050	Percent Reactivity Effect	15.0

Reference: BSC 2005 [DIRS 174180], Tables 1, 2 and 13

Table 3: BWR Reactivity Effect for Cross Section Uncertainties

Nuclide	(44-BWR Waste Package)		Δk_U	Δk_{Worth}
	Confidence Factor	Isotope Δk_{Worth}		
Mo-95	0.80	-0.00150	0.00013	0.2
Tc-99	0.90	-0.00319	0.00038	0.4
Sm-149	0.90	-0.03286	0.00285	2.7
Ru-101	0.26	-0.00134	0.00098	0.9
Rh-103	0.90	-0.00861	0.00064	0.6
Ag-109	0.94	-0.00186	0.00057	0.5
Nd-143	0.92	-0.00927	0.00063	0.6
Nd-145	0.58	-0.00225	0.00074	0.7
Sm-147	0.34	-0.00166	0.00104	1.0
Sm-150	0.88	-0.00110	-0.00023	0.2
Sm-151	0.96	-0.01287	0.00050	0.5
Sm-152	0.96	-0.00254	-0.00015	0.2
Eu-151	0.98	-0.00060	-0.00016	0.2
Eu-153	0.96	-0.00281	0.00020	0.2
Gd-155	0.96	-0.00613	0.00006	0.2
Np-237	0.68	-0.00581	0.00195	1.8
Am-241	0.74	-0.01021	0.00265	2.5
Am-242m	1.22	0.00032	0.00022	0.2
Am-243	0.82	-0.00130	0.00027	0.3
Total Δk_{Worth}		-0.1056	Percent Reactivity Effect	13.9

Reference: BSC 2005 [DIRS 174180], Tables 1, 2 and 13

6.4 REACTIVITY EFFECTS OF ISOTOPIC UNCERTAINTY

The reactivity effects of isotopic uncertainty are engendered by cross section uncertainty in the depletion calculations that calculate the isotopic changes to the fuel during irradiation in a reactor. Applying Equation 2 to the Δk value for each isotope of Tables 2 and 3 produces the reactivity effects of isotopic uncertainty presented in Tables 4 and 5 for PWR and BWR SNF respectively. Note that the percent Δk_U values in Tables 4 and 5 are normalized by the Total Δk_{Worth} values presented in Tables 2 and 3 respectively. The reactivity effects of isotopic uncertainties, 5.0 percent for PWR and 2.5 percent for BWR, are less than the reactivity effects of cross section uncertainties, 15 percent and 13.9 percent, as expected because of the negative reaction sensitivities.

Table 4: PWR Reactivity Effect for Isotopic Uncertainties

(21-PWR Waste Package)			
	S	Isotopic Δk_U	$\frac{\Delta k_U}{\Delta k_{Worth}}$ (%)
Mo-95	-0.0653	-0.00002	0.0
Tc-99	-0.1217	-0.00010	-0.1
Sm-149	-0.5176	-0.00067	-0.6
Ru-101	-0.0525	-0.00002	0.0
Rh-103	-0.4550	-0.00034	-0.3
Ag-109	-0.2649	-0.00004	0.0
Nd-143	-0.4501	-0.00047	-0.4
Nd-145	-0.1382	-0.00019	-0.2
Sm-147	0.0551	0.00005	0.0
Sm-150	-0.0301	0.00000	0.0
Sm-151	-0.5639	-0.00036	-0.3
Sm-152	-0.4770	-0.00002	0.0
Eu-151	-1.0000	-0.00023	-0.2
Eu-153	-0.2033	-0.00007	-0.1
Gd-155	0.4738	0.00038	0.4
Np-237	1.0000	0.00303	2.9
Am-241	1.0000	0.00322	3.1
Am-242m	1.0000	0.00054	0.5
Am-243	1.0000	0.00060	0.6
		Percent Reactivity Effect	5.0

Table 5: BWR Reactivity Effect for Isotopic Uncertainties

(44-BWR Waste Package)			
	S	Isotopic Δk_U	Δk_U Δk_{Worth} (%)
Mo-95	-0.0653	-0.00001	0.0
Tc-99	-0.1217	-0.00005	0.0
Sm-149	-0.5176	-0.00148	-1.4
Ru-101	-0.0525	-0.00005	0.0
Rh-103	-0.4550	-0.00029	-0.3
Ag-109	-0.2649	-0.00015	-0.1
Nd-143	-0.4501	-0.00028	-0.3
Nd-145	-0.1382	-0.00010	-0.1
Sm-147	0.0551	0.00006	0.1
Sm-150	-0.0301	0.00001	0.0
Sm-151	-0.5639	-0.00028	-0.3
Sm-152	-0.4770	0.00007	0.1
Eu-151	-1.0000	0.00016	0.2
Eu-153	-0.2033	-0.00004	0.0
Gd-155	0.4738	0.00003	0.0
Np-237	1.0000	0.00195	1.8
Am-241	1.0000	0.00265	2.5
Am-242m	1.0000	0.00022	0.2
Am-243	1.0000	0.00027	0.3
		Percent Reactivity Effect	2.5

6.5 OVERALL REACTIVITY EFFECT OF CROSS SECTION AND ISOTOPIC UNCERTAINTIES

The PWR and BWR reactivity effects for cross section uncertainties (Tables 2 and 3) are summed with the PWR and BWR reactivity effects for isotopic uncertainties (Tables 4 and 5) respectively to produce the overall reactivity effect of cross section and isotopic uncertainties. The overall reactivity effect of cross section and isotopic uncertainties is thus 20.0 percent for PWRs and 16.4 percent for BWRs. The overall reactivity effect of uncertainties is to reduce the benefit of fission products and minor actinides for burnup credit calculations by these percentages.

The uncertainty terms that can be applied are obtained by multiplying the percent reactivity effect by the total reactivity worth of fission products and minor actinides. For PWR SNF, Table 2 shows that the total reactivity worth is -0.1050 , so 20.0 percent of this value produces an

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uncertainty term penalty factor of 0.021. For BWR SNF, Table 3 shows that the total reactivity worth is -0.1056 , so 16.4 percent of this value produces an uncertainty term penalty factor of 0.017.

7. RESULTS

The results of this calculation are listed as follows:

- The PWR reactivity effect of isotopic uncertainties is 5.0 percent ΔkU , which when added to the reactivity effect of cross section uncertainties of 15.0 percent, yields an overall reactivity effect of 20.0 percent.
- The BWR reactivity effect of isotopic uncertainties is 2.5 percent ΔkU , which when added to the reactivity effect of cross section uncertainties of 13.9 percent, yields an overall reactivity effect of 16.4 percent.
- The overall reactivity effect of uncertainties is to reduce the benefit of fission products and minor actinides for burnup credit calculations by these percentages.
- The penalty factor for PWR SNF to accommodate cross section and isotopic uncertainties of fission products and minor actinides was calculated to be 0.021
- The penalty factor for BWR SNF to accommodate cross section and isotopic uncertainties of fission products and minor actinides was calculated to be 0.017

The EXCEL spreadsheet for the calculations of this evaluation is provided electronically in Attachment II.

All outputs are reasonable compared to the inputs, and the results of this calculation are suitable for their intended use.

Title: Reactivity Effects of Isotopic Uncertainty for Burnup Credit Validation

Document Identifier: 000-00C-WHS0-01500-000-00A

Page I-1 of 1

Attachment I: Attachment CD Listing

This attachment contains a listing and description of the files contained on the attachment CD of this report (Attachment II). The CD was written using ROXIO Easy CD Creator 5 Basic installed on DOE M&O Property tag number YMP000960 central processing unit, and can be viewed on most standard CD-ROM drives. The file attributes on the CD are as follows:

<u>Filename</u>	<u>File Size (kilobytes)</u>	<u>File Date</u>	<u>File Time</u>	<u>Description</u>
Reactivity Effects of Isotopic Uncertainties.xls	138	9/28/2006	5:35p	Archive containing EXCEL spreadsheet

There is 1 file (and no folders) contained on the CD.

OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT
SPECIAL INSTRUCTION SHEET

1. QA: N/A
Page 1 of 1

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

2. Record Date
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13. Comments
1 ORIGINAL
1 COPY

VALIDATION OF COMPLETE FILE TRANSFER. ALL FILES COPIED. SOFTWARE USED IS MS EXCEL

THIS IS AN ELECTRONIC
ATTACHMENT

XREF

MOL.20061205.0155

DEC 06 2006

T Church

MD5 Validation

dir

Volume in drive D is volume_1
Volume Serial Number is 063B-8D34

Directory of D:\

09/28/2006 05:35p	141,312	Reactivity Effects of Isotopic
Uncertainties.xls		
1 File(s)	141,312	bytes

Total Files Listed:		
1 File(s)	141,312	bytes
0 Dir(s)	0	bytes free