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Evaluation of Cross-Section Sensitivities in Computing Burnup Credit Fission Product Concentrations

August 2005

Prepared by
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CONTENTS

Page

LIST OF FIGURES

LIST OF TABLES

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ABSTRACT

U.S. Nuclear Regulatory Commission Interim Staff Guidance 8 (ISG-8) for burnup credit covers actinides only, a position based primarily on the lack of definitive critical experiments and adequate radiochemical assay data that can be used to quantify the uncertainty associated with fission product credit. The accuracy of fission product neutron cross sections is paramount to the accuracy of criticality analyses that credit fission products in two respects: (1) the microscopic cross sections determine the reactivity worth of the fission products in spent fuel and (2) the cross sections determine the reaction rates during irradiation and thus influence the accuracy of predicted final concentrations of the fission products in the spent fuel. This report evaluates and quantifies the importance of the fission product cross sections in predicting concentrations of fission products proposed for use in burnup credit. The study includes an assessment of the major fission products in burnup credit and their production precursors. Finally, the cross-section importances, or sensitivities, are combined with the importance of each major fission product to the system eigenvalue (k_{eff}) to determine the net importance of cross sections to k_{eff}. The importances established the following fission products, listed in descending order of priority, that are most likely to benefit burnup credit when their cross-section uncertainties are reduced: ^{151}Sm, ^{103}Rh, ^{155}Eu, ^{150}Sm, ^{152}Sm, ^{153}Eu, ^{154}Eu, and ^{143}Nd.

1. INTRODUCTION

Implementation of burnup credit to allow credit for fission product absorption is currently being evaluated in the United States. The accuracy of neutron cross sections is paramount to the accuracy of criticality analyses that credit the absorption of the fission products in two respects: (1) the microscopic cross sections determine the reactivity worth of the fission products in spent fuel and (2) the cross sections define the reaction rates during irradiation and thus influence the final concentrations of the fission products in spent nuclear fuel (SNF). The nuclides under consideration include the dominant absorbing fission products in the fuel. These nuclides typically include, but are not limited to, ^{95}Mo, ^{99}Tc, ^{101}Ru, ^{103}Rh, ^{109}Ag, ^{133}Cs, ^{143}Nd, ^{145}Nd, ^{147}Sm, $^{149\text{-}152}$Sm, ^{155}Gd, and ^{153}Eu (ref. 1). These nuclides are referred to in this work as burnup credit fission products.

A careful review and evaluation of the microscopic cross sections for these fission products are being performed at Oak Ridge National Laboratory. Improved cross sections will enhance the ability to accurately predict the reactivity effect associated with fission product absorption and the isotopic concentrations in the spent fuel, thus improving the ability to accurately predict the total reactivity worth of each fission product.

The concentrations of fission products, however, are determined not only by the cross sections of the fission products of direct importance to criticality but also by the cross sections of the precursor nuclides in the production chains. Therefore, any review of cross sections must include not only the burnup credit fission products but also the potentially important production precursors. While the cross sections for a particular burnup credit fission product may be accurately known and validated for criticality safety, its predicted *concentration* in spent fuel may be in error due to uncertainties in the cross sections of precursor nuclides that lead to the production of the nuclide of interest.

This report describes work to identify precursor fission product cross sections with high importance to the production of the burnup credit fission products. The objective is to identify those fission products (in addition to the primary fission products in burnup credit) for which a reevaluation of their cross sections and a subsequent reduction in cross section uncertainty would improve the prediction of the fission product concentrations in SNF.

2. METHODS

Each burnup credit fission product was evaluated to determine the sensitivity of the predicted concentration to the fission product cross sections. This evaluation included the sensitivity of not only the cross section of the burnup credit fission product itself but also the cross sections of all precursor nuclides. The sensitivity was determined using the relative sensitivity coefficients of the microscopic cross sections with respect to the predicted concentration of each fission product. A relative sensitivity coefficient of 1.0 means that a 1% relative change in the cross-section value will result in a corresponding change in the predicted concentration of 1%. The coefficients, therefore, directly reflect the relative importance of data parameters to the results of a computer simulation.

The coefficients were calculated using a version of the ORIGEN-S isotope generation and depletion code[2] that was processed using the GRESS (GRadient Enhanced Software System) code.[3] GRESS is an automatic differentiation preprocessor that inserts mathematical operations into the Fortran source code to calculate and propagate partial derivatives through the code during the burnup simulation using the chain rule method.[4] The GRESS code was used previously[5] with ORIGEN-S to perform sensitivity calculations for high-burnup fuel investigations. The sensitivity coefficients (S) were derived using the derivatives of the fission product concentrations calculated by GRESS with respect to each of the precursor nuclide cross sections ($\delta n/\delta\sigma$) and the computed time-dependent fission product concentrations. Because the fission product concentrations change dramatically during irradiation, the sensitivity coefficients are burnup and time dependent. The coefficients were therefore calculated as a function of burnup, up to a maximum burnup in this study of about 43,000 MWd/MTU. In many cases the burnup credit fission products are stable; therefore, the coefficients typically do not change appreciably after discharge from the reactor. For those fission products that do change appreciably, notably ^{155}Gd and ^{147}Sm, the coefficients were tabulated at cooling times of 5 years and 20 years after discharge from a reactor.

3. RESULTS

The relative sensitivity coefficients for each major burnup credit fission product are tabulated in Tables 1 through 15 using burnup intervals of about 4000 MWd/MTU. The coefficients represent the relative importance of the fission product cross sections to the predicted concentration of each burnup credit fission product. These coefficients are tabulated with respect to the cross section of the fission product itself and also with respect to the cross sections of the dominant precursor nuclides. The coefficients were evaluated only with respect to the radiative capture cross sections in this work. The capture cross-section sensitivities are identified by the heading $\sigma(n,\gamma)$ in the tables. When neutron capture leads to the production of a metastable-state nuclide, the sensitivity of the branching fraction is also listed (labeled with the table heading $F\gamma$).

As noted previously, the sensitivity coefficients for many fission products do not change appreciably after discharge. For these nuclides, the coefficients are listed during irradiation and after irradiation with a decay time of 1 year after discharge from the reactor. For other nuclides exhibiting a strong dependence on the decay time, the coefficients are listed at times of 5 years and 20 years after discharge.

A change in the cross-section value for a particular fission product may act to either increase or decrease the predicted concentration of a burnup credit fission product. A negative coefficient means that an increase in the cross section will decrease the concentration of the burnup credit fission product, whereas a positive coefficient means that an increase in the cross section will increase the concentration. The objective of this study was to determine the impact of cross-section errors on the computed fission product concentrations. Whether the error increased or decreased the computed concentration was not at issue, only the magnitude of the error. Thus, the magnitude (absolute value) of the coefficient, not the sign, was used to establish the cross-section importance rankings for burnup credit.

The relative sensitivity coefficients for each burnup credit fission product are illustrated in Fig. 1. For illustrative purposes, the figure uses the tabulated coefficients for 43,000-MWd/MTU burnup. The figure shows the magnitude (absolute value) of the coefficients for cross sections of both the fission product itself (blue) and precursor nuclides (yellow, green, and orange). The fission products are plotted in order of the importance of the total cross-section sensitivity to the predicted final concentration. Note that the total sensitivities ($|S|$) plotted in Fig. 1 represent the sum of all partial sensitivities (absolute values) that can contribute to the error in the predicted concentrations. The plotted sensitivities therefore represent a maximum error since the values do not consider the potential for offsetting errors.

The figure shows that the concentrations of many fission products are most sensitive to their own cross sections. The figure shows that ^{133}Cs, ^{145}Nd, ^{99}Tc, ^{95}Mo, and ^{101}Ru exhibit relatively low cross-section sensitivities, with relative coefficients of less than about 0.2 for typical SNF: that is, an error of 10% in all of these fission product cross sections will yield an error in the predicted isotopic concentrations of less than 2%. Thus, an error in the cross section for these fission products must be large in order to have a pronounced adverse impact on the predicted concentration.

The other fission products (^{103}Rh, ^{109}Ag, ^{143}Nd, $^{147,149\text{-}152}$Sm, ^{155}Gd, and ^{153}Eu) display larger cross-section sensitivities. However, as stated, most fission products are sensitive only to their own cross sections: that is, the role of fission product precursors is minor. The notable exceptions are ^{151}Sm, ^{155}Gd, ^{153}Eu, and ^{147}Sm, which exhibit a significant sensitivity to the cross sections of precursor fission products. The major precursors, with sensitivity coefficients listed in parentheses, are ^{150}Sm ($S = 0.40$), ^{155}Eu ($S = -0.95$), ^{152}Sm ($S = 0.32$), and ^{147}Pm ($S = -0.48$), respectively. The reason for the large sensitivity to the precursor fission products is that production by neutron capture, and not directly by fission, is a dominant production route. These fission products are discussed separately.

Table 1. Relative sensitivity coefficients for ^{95}Mo

Burnup (MWd/MTU)	**^{94}Zr σ(n,γ)**	**^{94}Nb σ(n,γ)**	**^{95}Zr σ(n,γ)**	**^{95}Nb σ(n,γ)**	**^{95m}Nb σ(n,γ)**	**^{95}Mo σ(n,γ)**
4,256	5.58E−06	2.37E−09	−6.80E−05	−2.27E−04	−4.26E−06	−1.44E−03
8,512	1.99E−05	3.95E−09	−1.78E−04	−5.00E−04	−4.58E−06	−5.16E−03
12,768	3.77E−05	6.21E−09	−2.52E−04	−6.39E−04	−4.72E−06	−9.96E−03
17,024	5.88E−05	9.13E−09	−3.02E−04	−7.22E−04	−4.87E−06	−1.57E−02
21,280	8.29E−05	1.27E−08	−3.38E−04	−7.80E−04	−5.03E−06	−2.23E−02
25,536	1.10E−04	1.70E−08	−3.66E−04	−8.29E−04	−5.21E−06	−2.97E−02
29,792	1.41E−04	2.20E−08	−3.91E−04	−8.74E−04	−5.40E−06	−3.79E−02
34,048	1.74E−04	2.78E−08	−4.14E−04	−9.16E−04	−5.60E−06	−4.69E−02
38,304	2.11E−04	3.42E−08	−4.35E−04	−9.56E−04	−5.80E−06	−5.66E−02
42,560	2.52E−04	4.14E−08	−4.56E−04	−9.96E−04	−6.00E−06	−6.70E−02
1-year decay	2.91E−04	4.13E−08	−4.74E−04	−9.48E−04	−5.70E−06	−6.06E−02

Table 2. Relative sensitivity coefficients for ^{99}Tc

Burnup (MWd/MTU)	**^{98}Mo σ(n,γ)**	**^{98}Tc σ(n,γ)**	**^{99}Mo σ(n,γ)**	**^{99}Tc σ(n,γ)**
4,256	1.45E−04	4.60E−10	−6.82E−05	−4.73E−03
8,512	4.46E−04	1.30E−09	−7.22E−05	−1.44E−02
12,768	7.70E−04	2.15E−09	−7.44E−05	−2.48E−02
17,024	1.13E−03	3.03E−09	−7.69E−05	−3.60E−02
21,280	1.52E−03	3.94E−09	−7.96E−05	−4.83E−02
25,536	1.96E−03	4.87E−09	−8.27E−05	−6.17E−02
29,792	2.44E−03	5.83E−09	−8.59E−05	−7.62E−02
34,048	2.97E−03	6.79E−09	−8.93E−05	−9.19E−02
38,304	3.55E−03	7.74E−09	−9.29E−05	−1.09E−01
42,560	4.17E−03	8.68E−09	−9.64E−05	−1.26E−01
1-year decay	4.19E−03	8.65E−09	−9.65E−05	−1.26E−01

Table 3. Relative sensitivity coefficients for ^{101}Ru

Burnup (MWd/MTU)	**^{100}Mo σ(n,γ)**	**^{100}Ru σ(n,γ)**	**^{101}Ru σ(n,γ)**
4,256	1.17E−04	1.66E−06	−2.11E−03
8,512	3.56E−04	1.59E−05	−6.44E−03
12,768	6.12E−04	4.67E−05	−1.11E−02
17,024	8.90E−04	9.81E−05	−1.61E−02
21,280	1.20E−03	1.75E−04	−2.16E−02
25,536	1.53E−03	2.84E−04	−2.76E−02
29,792	1.89E−03	4.30E−04	−3.41E−02
34,048	2.29E−03	6.22E−04	−4.12E−02
38,304	2.71E−03	8.64E−04	−4.88E−02
42,560	3.16E−03	1.16E−03	−5.68E−02
1-year decay	3.16E−03	1.16E−03	−5.68E−02

Table 4. Relative sensitivity coefficients for ^{103}Rh

Burnup (MWd/MTU)	^{102}Ru σ(n,γ)	^{102}Rh σ(n,γ)	^{103}Ru σ(n,γ)	^{103}Rh σ(n,γ)	^{103}Rh Fγ
4,256	1.55E−04	1.39E−09	−9.19E−04	−1.64E−02	0.00E+00
8,512	5.13E−04	2.11E−09	−1.88E−03	−5.46E−02	1.23E−14
12,768	9.15E−04	2.79E−09	−2.31E−03	−9.75E−02	4.61E−14
17,024	1.36E−03	3.39E−09	−2.56E−03	−1.44E−01	8.69E−14
21,280	1.85E−03	3.90E−09	−2.76E−03	−1.92E−01	1.24E−13
25,536	2.40E−03	4.33E−09	−2.95E−03	−2.44E−01	1.50E−13
29,792	3.00E−03	4.67E−09	−3.13E−03	−2.98E−01	1.63E−13
34,048	3.68E−03	4.91E−09	−3.32E−03	−3.53E−01	1.60E−13
38,304	4.43E−03	5.05E−09	−3.52E−03	−4.09E−01	1.43E−13
42,560	5.26E−03	5.09E−09	−3.72E−03	−4.64E−01	1.16E−13
1-year decay	5.58E−03	4.67E−09	−3.79E−03	−4.26E−01	6.85E−14

Table 5. Relative sensitivity coefficients for ^{109}Ag

Burnup (MWd/MTU)	^{108}Pd σ(n,γ)	^{108}Pd Fγ	^{109}Pd σ(n,γ)	^{109}Ag σ(n,γ)	^{109}Ag Fγ
4,256	6.44E−03	−9.14E−09	−7.01E−05	−1.89E−02	0.00E+00
8,512	1.58E−02	−8.52E−09	−7.17E−05	−5.30E−02	−3.33E−10
12,768	2.55E−02	−9.33E−09	−7.42E−05	−8.86E−02	−3.30E−09
17,024	3.60E−02	−1.06E−08	−7.73E−05	−1.26E−01	−1.06E−08
21,280	4.75E−02	−1.20E−08	−8.11E−05	−1.66E−01	−2.37E−08
25,536	6.01E−02	−1.37E−08	−8.53E−05	−2.08E−01	−4.41E−08
29,792	7.37E−02	−1.55E−08	−9.01E−05	−2.51E−01	−7.30E−08
34,048	8.83E−02	−1.75E−08	−9.51E−05	−2.96E−01	−1.11E−07
38,304	1.04E−01	−1.96E−08	−1.00E−04	−3.40E−01	−1.59E−07
42,560	1.20E−01	−2.16E−08	−1.06E−04	−3.85E−01	−2.15E−07
1-year decay	1.20E−01	1.77E−08	−1.06E−04	−3.85E−01	−2.16E−07

Table 6. Relative sensitivity coefficients for ^{133}Cs

Burnup (MWd/MTU)	^{132}Xe σ(n,γ)	^{132}Xe Fγ	^{132}Cs σ(n,γ)	^{133}I σ(n,γ)	^{133}Xe σ(n,γ)	^{133m}Xe σ(n,γ)	^{133}Cs σ(n,γ)
4,256	3.93E−05	−1.64E−07	4.15E−11	−3.61E−05	−3.01E−03	−3.62E−05	−6.80E−03
8,512	1.28E−04	−1.81E−07	5.05E−11	−3.71E−05	−3.34E−03	−3.99E−05	−2.06E−02
12,768	2.28E−04	−2.14E−07	5.87E−11	−3.80E−05	−3.48E−03	−4.17E−05	−3.54E−02
17,024	3.43E−04	−2.56E−07	6.66E−11	−3.92E−05	−3.60E−03	−4.35E−05	−5.14E−02
21,280	4.76E−04	−3.08E−07	7.43E−11	−4.05E−05	−3.74E−03	−4.54E−05	−6.89E−02
25,536	6.29E−04	−3.69E−07	8.22E−11	−4.20E−05	−3.89E−03	−4.74E−05	−8.78E−02
29,792	8.04E−04	−4.41E−07	9.01E−11	−4.37E−05	−4.05E−03	−4.96E−05	−1.08E−01
34,048	1.01E−03	−5.23E−07	9.81E−11	−4.54E−05	−4.22E−03	−5.19E−05	−1.30E−01
38,304	1.23E−03	−6.15E−07	1.06E−10	−4.72E−05	−4.39E−03	−5.43E−05	−1.54E−01
42,560	1.49E−03	−7.16E−07	1.14E−10	−4.90E−05	−4.57E−03	−5.68E−05	−1.79E−01
1-year decay	1.50E−03	8.80E−08	1.14E−10	−4.91E−05	−4.57E−03	−5.70E−05	−1.77E−01

Table 7. Relative sensitivity coefficients for ^{143}Nd

Burnup (MWd/MTU)	^{142}Ce $\sigma(n,\gamma)$	^{142}Pr $\sigma(n,\gamma)$	^{142}Nd $\sigma(n,\gamma)$	^{143}Ce $\sigma(n,\gamma)$	^{143}Pr $\sigma(n,\gamma)$	^{143}Nd $\sigma(n,\gamma)$
4,256	5.48E−05	2.82E−08	2.74E−07	−6.23E−05	−2.93E−03	−1.52E−02
8,512	2.02E−04	2.17E−07	4.16E−06	−6.43E−05	−4.01E−03	−5.49E−02
12,768	3.63E−04	4.77E−07	1.49E−05	−6.61E−05	−4.30E−03	−9.53E−02
17,024	5.43E−04	8.04E−07	3.53E−05	−6.81E−05	−4.51E−03	−1.38E−01
21,280	7.48E−04	1.21E−06	6.87E−05	−7.06E−05	−4.71E−03	−1.85E−01
25,536	9.83E−04	1.72E−06	1.20E−04	−7.34E−05	−4.93E−03	−2.34E−01
29,792	1.25E−03	2.36E−06	1.94E−04	−7.65E−05	−5.15E−03	−2.87E−01
34,048	1.56E−03	3.14E−06	2.98E−04	−7.98E−05	−5.40E−03	−3.43E−01
38,304	1.91E−03	4.08E−06	4.40E−04	−8.33E−05	−5.65E−03	−4.00E−01
42,560	2.30E−03	5.21E−06	6.28E−04	−8.70E−05	−5.92E−03	−4.59E−01
1-year decay	2.36E−03	5.37E−06	6.14E−04	−8.75E−05	−5.93E−03	−4.49E−01

Table 8. Relative sensitivity coefficients for ^{145}Nd

Burnup (MWd/MTU)	^{143}Nd $\sigma(n,\gamma)$	^{144}Ce $\sigma(n,\gamma)$	^{144}Nd $\sigma(n,\gamma)$	^{145}Nd $\sigma(n,\gamma)$
4,256	2.73E−06	1.25E−04	2.67E−05	−5.67E−03
8,512	1.89E−05	3.45E−04	2.43E−04	−1.74E−02
12,768	6.82E−05	5.37E−04	6.70E−04	−2.99E−02
17,024	1.76E−04	7.10E−04	1.31E−03	−4.35E−02
21,280	3.53E−04	8.69E−04	2.19E−03	−5.84E−02
25,536	6.10E−04	1.02E−03	3.32E−03	−7.47E−02
29,792	9.55E−04	1.16E−03	4.72E−03	−9.24E−02
34,048	1.39E−03	1.28E−03	6.41E−03	−1.11E−01
38,304	1.93E−03	1.41E−03	8.40E−03	−1.32E−01
42,560	2.56E−03	1.52E−03	1.07E−02	−1.53E−01
1-year decay	2.55E−03	1.52E−03	1.07E−02	−1.53E−01

Table 9. Relative sensitivity coefficients for ^{147}Sm

Burnup (MWd/MTU)	^{146}Nd $\sigma(n,\gamma)$	^{147}Nd $\sigma(n,\gamma)$	^{147}Pm $\sigma(n,\gamma)$	^{147}Pm $F\gamma$	^{147}Sm $\sigma(n,\gamma)$
4,256	1.08E−04	−8.72E−03	−1.75E−02	0.00E+00	−9.58E−03
8,512	3.83E−04	−1.33E−02	−5.60E−02	−4.79E−07	−3.28E−02
12,768	6.87E−04	−1.40E−02	−9.50E−02	−2.03E−06	−5.83E−02
17,024	1.02E−03	−1.45E−02	−1.34E−01	−3.68E−06	−8.68E−02
21,280	1.40E−03	−1.50E−02	−1.72E−01	−4.30E−06	−1.19E−01
25,536	1.84E−03	−1.54E−02	−2.11E−01	−3.38E−06	−1.54E−01
29,792	2.34E−03	−1.60E−02	−2.50E−01	−6.01E−07	−1.93E−01
34,048	2.91E−03	−1.65E−02	−2.88E−01	4.20E−06	−2.36E−01
38,304	3.57E−03	−1.71E−02	−3.26E−01	1.17E−05	−2.82E−01
42,560	4.32E−03	−1.78E−02	−3.63E−01	2.10E−05	−3.30E−01
Decay time					
5 years	6.77E−03	−1.96E−02	−4.66E−01	−4.67E−06	−1.34E−01
20 years	7.06E−03	−1.98E−02	−4.79E−01	−7.74E−06	−1.11E−01

Table 10. Relative sensitivity coefficients for ^{149}Sm

Burnup (MWd/MTU)	**^{147}Pm σ(n,γ)**	**^{148}Nd σ(n,γ)**	**^{148}Pm σ(n,γ)**	**^{148m}Pm σ(n,γ)**	**^{148}Sm σ(n,γ)**	**^{149}Pm σ(n,γ)**	**^{149}Sm σ(n,γ)**
4,256	3.10E−02	1.62E−03	1.01E−02	1.04E−02	2.44E−05	−7.86E−03	−1.00E+00
8,512	1.30E−01	4.55E−03	3.04E−02	3.21E−02	3.30E−04	−8.00E−03	−1.00E+00
12,768	1.97E−01	7.32E−03	4.59E−02	4.60E−02	9.37E−04	−8.40E−03	−1.00E+00
17,024	2.44E−01	1.01E−02	5.83E−02	5.59E−02	1.83E−03	−8.94E−03	−1.00E+00
21,280	2.74E−01	1.28E−02	6.81E−02	6.24E−02	3.00E−03	−9.57E−03	−1.00E+00
25,536	2.91E−01	1.57E−02	7.57E−02	6.63E−02	4.45E−03	−1.03E−02	−1.00E+00
29,792	2.96E−01	1.86E−02	8.12E−02	6.80E−02	6.17E−03	−1.10E−02	−1.00E+00
34,048	3.03E−01	2.14E−02	8.45E−02	6.43E−02	8.11E−03	−1.17E−02	−1.00E+00
38,304	2.93E−01	2.45E−02	8.67E−02	6.36E−02	1.04E−02	−1.24E−02	−1.00E+00
42,560	2.79E−01	2.77E−02	8.77E−02	6.21E−02	1.28E−02	−1.31E−02	−1.00E+00
1-year decay	2.77E−01	2.80E−02	8.84E−02	6.28E−02	7.28E−03	−1.31E−02	−5.69E−01

Table 11. Relative sensitivity coefficients for ^{150}Sm

Burnup (MWd/MTU)	**^{148}Nd σ(n,γ)**	**^{148}Pm σ(n,γ)**	**^{148m}Pm σ(n,γ)**	**^{149}Sm σ(n,γ)**	**^{150}Pm σ(n,γ)**	**^{150}Sm σ(n,γ)**
4,256	8.23E−04	4.19E−03	4.52E−03	1.16E−01	−5.31E−06	−7.53E−03
8,512	2.39E−03	1.65E−02	1.92E−02	3.02E−02	−5.07E−06	−2.24E−02
12,768	3.91E−03	2.67E−02	3.00E−02	1.38E−02	−5.27E−06	−3.78E−02
17,024	5.44E−03	3.55E−02	3.85E−02	6.36E−03	−5.60E−06	−5.42E−02
21,280	7.00E−03	4.33E−02	4.54E−02	2.03E−03	−6.04E−06	−7.16E−02
25,536	8.60E−03	5.01E−02	5.08E−02	−8.28E−04	−6.57E−06	−9.02E−02
29,792	1.03E−02	5.60E−02	5.50E−02	−2.84E−03	−7.18E−06	−1.10E−01
34,048	1.20E−02	6.10E−02	5.75E−02	−2.59E−03	−7.87E−06	−1.32E−01
38,304	1.38E−02	6.53E−02	5.91E−02	−2.95E−03	−8.63E−06	−1.54E−01
42,560	1.57E−02	6.89E−02	6.01E−02	−3.24E−03	−9.42E−06	−1.78E−01
1-year decay	1.57E−02	6.89E−02	6.01E−02	−3.24E−03	−9.43E−06	−1.78E−01

Table 12. Relative sensitivity coefficients for ^{151}Sm

Burnup (MWd/MTU)	**^{149}Sm σ(n,γ)**	**^{150}Nd σ(n,γ)**	**^{150}Sm σ(n,γ)**	**^{151}Pm σ(n,γ)**	**^{151}Sm σ(n,γ)**
4,256	2.21E−03	6.89E−04	1.89E−02	−3.06E−03	−4.42E−01
8,512	1.99E−03	2.39E−03	7.26E−02	−2.99E−03	−8.50E−01
12,768	1.37E−03	4.21E−03	1.31E−01	−2.92E−03	−9.55E−01
17,024	6.65E−04	5.98E−03	1.88E−01	−2.89E−03	−9.78E−01
21,280	−9.25E−05	7.65E−03	2.41E−01	−2.87E−03	−9.84E−01
25,536	−8.63E−04	9.19E−03	2.87E−01	−2.85E−03	−9.86E−01
29,792	−1.62E−03	1.06E−02	3.28E−01	−2.83E−03	−9.87E−01
34,048	−1.73E−03	1.19E−02	3.61E−01	−2.80E−03	−9.88E−01
38,304	−1.94E−03	1.31E−02	3.88E−01	−2.77E−03	−9.89E−01
42,560	−2.13E−03	1.42E−02	4.07E−01	−2.73E−03	−9.90E−01
1-year decay	−2.08E−03	1.45E−02	3.98E−01	−2.79E−03	−9.68E−01

Table 13. Relative sensitivity coefficients for ^{152}Sm

Burnup (MWd/MTU)	^{150}Sm σ(n,γ)	^{151}Sm σ(n,γ)	^{152}Sm σ(n,γ)
4,256	4.44E−03	2.61E−01	−4.42E−02
8,512	2.28E−02	1.89E−01	−1.28E−01
12,768	4.51E−02	1.16E−01	−2.14E−01
17,024	6.99E−02	7.53E−02	−3.01E−01
21,280	9.65E−02	5.25E−02	−3.85E−01
25,536	1.25E−01	3.86E−02	−4.67E−01
29,792	1.54E−01	2.96E−02	−5.43E−01
34,048	1.83E−01	2.35E−02	−6.13E−01
38,304	2.11E−01	1.92E−02	−6.76E−01
42,560	2.37E−01	1.60E−02	−7.30E−01
1-year decay	2.37E−01	1.60E−02	−7.30E−01

Table 14. Relative sensitivity coefficients for ^{153}Eu

Burnup (MWd/MTU)	^{151}Sm σ(n,γ)	^{152}Sm σ(n,γ)	^{152m}Eu σ(n,γ)	^{153}Sm σ(n,γ)	^{153}Eu σ(n,γ)
4,256	2.38E−02	9.98E−02	6.92E−07	−4.11E−03	−3.63E−02
8,512	6.87E−02	2.78E−01	2.08E−06	−4.29E−03	−9.83E−02
12,768	7.45E−02	3.79E−01	2.42E−06	−4.45E−03	−1.55E−01
17,024	6.68E−02	4.27E−01	2.35E−06	−4.65E−03	−2.10E−01
21,280	5.68E−02	4.42E−01	2.18E−06	−4.89E−03	−2.66E−01
25,536	4.74E−02	4.36E−01	2.00E−06	−5.17E−03	−3.24E−01
29,792	3.94E−02	4.16E−01	1.84E−06	−5.48E−03	−3.81E−01
34,048	3.29E−02	3.88E−01	1.71E−06	−5.81E−03	−4.39E−01
38,304	2.75E−02	3.54E−01	1.61E−06	−6.16E−03	−4.96E−01
42,560	2.32E−02	3.19E−01	1.54E−06	−6.51E−03	−5.52E−01
1-year decay	2.31E−02	3.18E−01	1.48E−06	−6.52E−03	−5.47E−01

Table 15. Relative sensitivity coefficients for ^{155}Gd

Burnup (MWd/MTU)	^{153}Eu σ(n,γ)	^{154}Eu σ(n,γ)	^{154}Gd σ(n,γ)	^{155}Eu σ(n,γ)	^{155}Gd σ(n,γ)
4,256	1.68E−02	1.52E−02	4.69E−04	−3.56E−01	−6.96E−01
8,512	1.90E−01	1.40E−01	8.50E−03	−7.50E−01	−1.03E+00
12,768	3.78E−01	2.28E−01	2.40E−02	−8.12E−01	−1.04E+00
17,024	5.03E−01	2.44E−01	4.35E−02	−8.24E−01	−1.03E+00
21,280	5.63E−01	2.14E−01	6.46E−02	−8.30E−01	−1.03E+00
25,536	5.81E−01	1.63E−01	8.64E−02	−8.30E−01	−1.02E+00
29,792	5.72E−01	1.06E−01	1.09E−01	−8.24E−01	−1.02E+00
34,048	5.47E−01	4.85E−02	1.31E−01	−8.13E−01	−1.02E+00
38,304	5.14E−01	−5.68E−03	1.53E−01	−7.97E−01	−1.01E+00
42,560	4.77E−01	−5.58E−02	1.74E−01	−7.77E−01	−1.01E+00
Decay time					
5 years	4.43E−01	1.17E−01	1.95E−03	−9.47E−01	−1.13E−02
20 years	4.43E−01	1.18E−01	1.08E−03	−9.48E−01	−6.28E−03

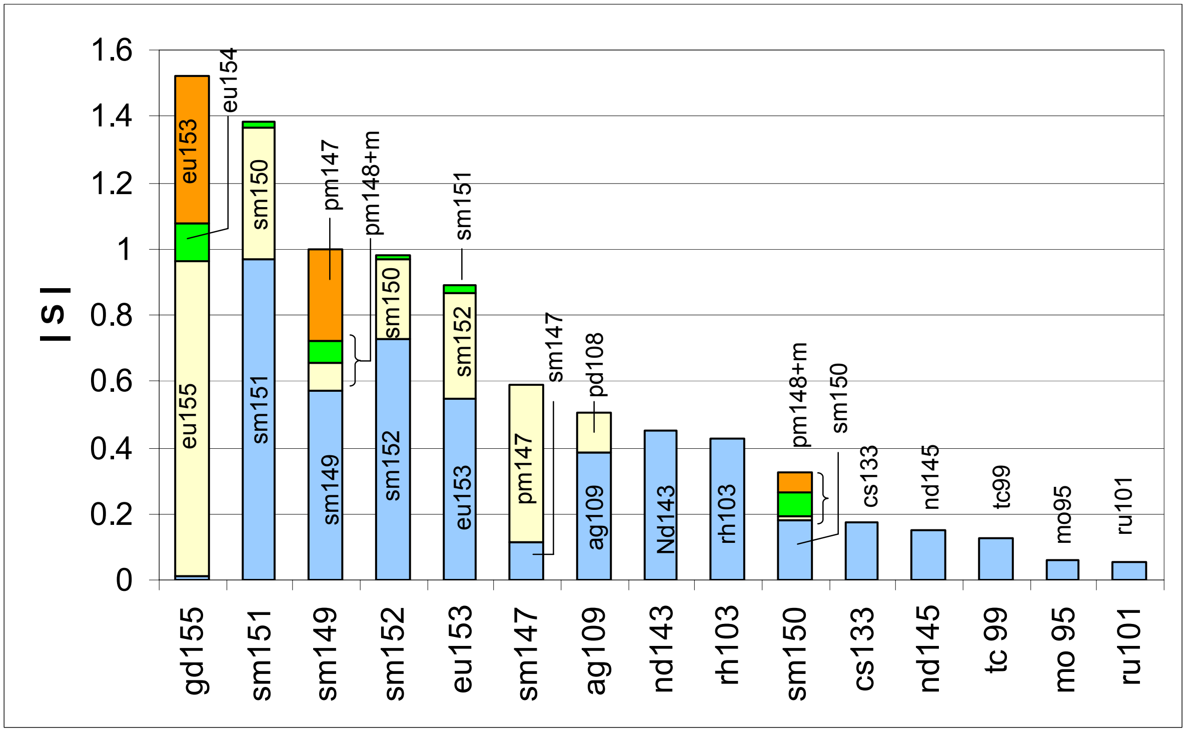

Fig. 1. Relative sensitivity coefficients (5 years after discharge) of burnup credit fission product isotopic concentrations to the cross section of the fission product itself (shown in blue) and cross sections of precursor nuclides (shown in yellow, green, and orange).

3.1 GADOLINIUM-155

After removal of spent fuel from the reactor, the production of ^{155}Gd is almost entirely from the decay of ^{155}Eu. Thus, the ^{155}Gd concentration in SNF exhibits almost no sensitivity to the value of its own cross section *after discharge*. The highest sensitivities are to ^{155}Eu (S = −0.95) and to ^{153}Eu (S = 0.44). Gadolinium-155 is also a high-ranking fission product in burnup credit that is not predicted well. It is typically underpredicted by about 25% (ref. 6). Thus, the ^{155}Eu cross section is a strong candidate for reevaluation. The ^{153}Eu cross section is addressed separately below.

3.2 SAMARIUM-151

The concentration of ^{151}Sm in SNF is strongly influenced by its own cross section (S = −0.97) but also exhibits a high sensitivity to the cross section of ^{150}Sm (S = 0.40) caused by the significant production route from ^{150}Sm capture. An evaluation of the importance of ^{151}Sm in burnup credit (e.g., see ref. 6) indicates that it is one of the largest fission product absorbers. Further evaluation of current benchmarking of isotopic predictions (e.g., see ref. 6) also indicates that ^{151}Sm is substantially overpredicted (about 30% on average). Therefore, both ^{150}Sm and ^{151}Sm are potential candidates for cross-section reevaluation.

3.3 EUROPIUM-153

The concentration of ^{153}Eu in SNF is influenced by the cross sections of ^{153}Eu (S = −0.55) and ^{152}Sm (S = 0.32). Europium-153 is a moderately important fission product and, as shown above, is an important precursor for ^{155}Gd. Current benchmarks indicate that it is predicted very well using current cross-section data, and thus a reevaluation of the cross section would likely be of moderate benefit in reducing uncertainties in burnup credit analyses that credit fission product absorption. This result also implies that errors in the cross section of ^{155}Eu are a likely cause for the observed underprediction in the computed concentration of ^{155}Gd (see ^{155}Gd discussion in Section 3.1).

3.4 SAMARIUM-147

Samarium-147 exhibits the highest sensitivity (after discharge) to ^{147}Pm (S = −0.48) and to lesser extent its own cross section (S = −0.13 after 5 years, and S = −0.11 after 20 years cooling). Samarium-147 is another fission product of moderate importance in burnup credit. It is also very well predicted using existing data, and thus a reevaluation of the cross section would likely be of limited benefit to fission product burnup credit.

4. DISCUSSION

Cross-section sensitivities are a key piece of information that can be used to help identify and prioritize which cross sections need to be reevaluated. However, there are several other factors that should also be considered in determining the priority of cross-section measurements.

The first factor is the relative reactivity worth of the affected fission product nuclide (i.e., the relative importance of the fission product as it impacts the k_{eff} in a burnup credit criticality assessment). Greatly improving the ability to calculate the concentration of a fission product with a very low reactivity worth will not enhance the effectiveness of burnup credit. Conversely, a modest improvement in the ability to calculate the concentration of a high-worth fission product may have significant impact. The reactivity sensitivity factors are the differential change in system k_{eff} due to a change in the macroscopic cross sections $(\delta k/k)/(\delta n/n)$. The fission product sensitivity factors were calculated for a Generic Burnup Credit cask[7] using the SCALE TSUNAMI-3D calculation sequence.[8,9] These values are used as weighting factors in the determination of priority or ranking of cross sections to be examined.

The second factor to be considered is how well the current data and methods accurately predict fission product concentrations. If calculated concentrations for a fission product are already very close to the expected or measured values, there is little incentive to perform reviews of the cross sections related to generation of that fission product. A measure of how well the compositions of fission product nuclides may be calculated is available from the data published in Table 5 of ref. 6. The column in Table 5 labeled $\overline{X}$ contains the average of the measured concentrations divided by the calculated concentrations for each fission product nuclide. A value of 1.0 means the measured and calculated compositions are equal. A useful weight factor then is the absolute value of the difference between 1.0 and the $\overline{X}$ value from Table 5. This quantity is referred to as the "best estimate bias," or BEB, in Table 16 of this report. The factor ultimately used to establish the priority ranking is the product of the sensitivity coefficients $(\delta k/k)/(\delta\sigma/\sigma)$ and the BEB. This factor therefore represents a nuclide weighting that includes the ability to predict the fission product concentrations with existing cross-section data and the importance of the fission product to absorption in a criticality assessment.

The reactivity sensitivity factors and the BEB fraction are used in Table 16 with the cross-section sensitivity values discussed in the previous section to develop a proposed priority or ranking for which cross sections should be reviewed.

Based on the important fission products identified and the cross-section sensitivities and reactivity worth for these nuclides, the following priority fission products are recommended for review in descending order of importance: ^{151}Sm, ^{103}Rh, ^{155}Eu, ^{150}Sm, ^{152}Sm, ^{153}Eu, ^{154}Eu, and ^{143}Nd. Medium-importance fission products include ^{99}Tc, ^{150}Nd, ^{149}Sm, ^{133}Cs, ^{147}Pm, ^{148}Pm, and ^{148m}Pm.

Table 16. Prioritization of cross-section review for burnup credit

Nuclide	Cross section	Burnup credit nuclide	Sensitivity of number density to cross sections (δn/n)/(δσ/σ)	Sensitivity of k_{eff} to number density (δk/k)/(δn/n)	Sensitivity of k_{eff} to cross sections (δk/k)/(δσ/σ)	Best est. bias (BEB) $\lvert(1 - \overline{X})\rvert$	Σ {BEB * |(δk/k)/(δσ/σ)|}	Nuclide rank
^{151}Sm	(n,γ)	^{151}Sm	−9.68E−01	−7.53E−03	7.29E−03	0.223	1.64E−03	1
^{151}Sm	(n,γ)	^{152}Sm	1.60E−02	−2.92E−03	−4.67E−05	0.249		
^{151}Sm	(n,γ)	^{153}Eu	2.31E−02	−1.92E−03	−4.44E−05	0.034		
^{103}Rh	(n,γ)	^{103}Rh	−4.26E−01	−8.24E−03	3.51E−03	0.269	9.45E−04	2
^{103}Rh	Fγ	^{103}Rh	6.85E−14	−8.24E−03	−5.65E−16	0.269		
^{155}Eu	(n,γ)	^{155}Gd	−9.47E−01	−3.42E−03	3.24E−03	0.287	9.30E−04	3
^{150}Sm	(n,γ)	^{151}Sm	3.98E−01	−7.53E−03	−3.00E−03	0.223	8.56E−04	4
^{150}Sm	(n,γ)	^{152}Sm	2.37E−01	−2.92E−03	−6.92E−04	0.249		
^{150}Sm	(n,γ)	^{150}Sm	−1.78E−01	−1.28E−03	2.28E−04	0.066		
^{152}Sm	(n,γ)	^{152}Sm	−7.30E−01	−2.92E−03	2.13E−03	0.249	5.51E−04	5
^{152}Sm	(n,γ)	^{153}Eu	3.18E−01	−1.92E−03	−6.12E−04	0.034		
^{153}Eu	(n,γ)	^{155}Gd	4.43E−01	−3.42E−03	−1.52E−03	0.287	4.71E−04	6
^{153}Eu	(n,γ)	^{153}Eu	−5.47E−01	−1.92E−03	1.05E−03	0.034		
^{154}Eu	(n,γ)	^{155}Gd	1.17E−01	−3.42E−03	−4.01E−04	0.287	1.15E−04	7
^{143}Nd	(n,γ)	^{143}Nd	−4.49E−01	−1.12E−02	5.03E−03	0.012	6.03E−05	8
^{143}Nd	(n,γ)	^{145}Nd	2.55E−03	−2.16E−03	−5.50E−06	0.004		
^{99}Tc	(n,γ)	^{99}Tc	−1.26E−01	−2.80E−03	3.53E−04	0.156	5.51E−05	9
^{150}Nd	(n,γ)	^{151}Sm	1.45E−02	−7.53E−03	−1.09E−04	0.223	2.44E−05	10
^{149}Sm	(n,γ)	^{149}Sm	−5.69E−01	−1.47E−02	8.35E−03	0.002	2.05E−05	11
^{149}Sm	(n,γ)	^{151}Sm	−2.08E−03	−7.53E−03	1.57E−05	0.223		
^{149}Sm	(n,γ)	^{150}Sm	−3.24E−03	−1.28E−03	4.16E−06	0.066		
^{133}Cs	(n,γ)	^{133}Cs	−1.77E−01	−3.73E−03	6.60E−04	0.024	1.59E−05	12
^{102}Ru	(n,γ)	^{103}Rh	5.58E−03	−8.24E−03	−4.60E−05	0.269	1.24E−05	13
^{155}Gd	(n,γ)	^{155}Gd	−1.13E−02	−3.42E−03	3.87E−05	0.287	1.11E−05	14
^{147}Pm	(n,γ)	^{149}Sm	2.77E−01	−1.47E−02	−4.07E−03	0.002	8.95E−06	15
^{147}Pm	(n,γ)	^{147}Sm	−4.66E−01	−1.75E−03	8.15E−04	0.001		
^{147}Pm	Fγ	^{147}Sm	−4.67E−06	−1.75E−03	8.16E−09	0.001		
^{148}Pm	(n,γ)	^{149}Sm	8.84E−02	−1.47E−02	−1.30E−03	0.002	8.43E−06	16
^{148}Pm	(n,γ)	^{150}Sm	6.89E−02	−1.28E−03	−8.84E−05	0.066		
^{103}Ru	(n,γ)	^{103}Rh	−3.79E−03	−8.24E−03	3.12E−05	0.269	8.41E−06	17
^{148m}Pm	(n,γ)	^{149}Sm	6.28E−02	−1.47E−02	−9.22E−04	0.002	6.93E−06	18
^{148m}Pm	(n,γ)	^{150}Sm	6.01E−02	−1.28E−03	−7.71E−05	0.066		
^{151}Pm	(n,γ)	^{151}Sm	−2.79E−03	−7.53E−03	2.10E−05	0.223	4.69E−06	19
^{148}Nd	(n,γ)	^{149}Sm	2.80E−02	−1.47E−02	−4.11E−04	0.002	2.15E−06	20
^{148}Nd	(n,γ)	^{150}Sm	1.57E−02	−1.28E−03	−2.01E−05	0.066		
^{154}Gd	(n,γ)	^{155}Gd	1.95E−03	−3.42E−03	−6.68E−06	0.287	1.92E−06	21
^{98}Mo	(n,γ)	^{99}Tc	4.19E−03	−2.80E−03	−1.17E−05	0.156	1.83E−06	22
^{145}Nd	(n,γ)	^{145}Nd	−1.53E−01	−2.16E−03	3.30E−04	0.004	1.32E−06	23
^{143}Pr	(n,γ)	^{143}Nd	−5.93E−03	−1.12E−02	6.64E−05	0.012	7.97E−07	24
^{153}Sm	(n,γ)	^{153}Eu	−6.52E−03	−1.92E−03	1.25E−05	0.034	4.26E−07	25
^{133}Xe	(n,γ)	^{133}Cs	−4.57E−03	−3.73E−03	1.71E−05	0.024	4.09E−07	26
^{149}Pm	(n,γ)	^{149}Sm	−1.31E−02	−1.47E−02	1.92E−04	0.002	3.85E−07	27

Table 16. (continued)

Nuclide	**Cross section**	**Burnup credit nuclide**	**Sensitivity of number density to cross sections (δn/n)/(δσ/σ)**	**Sensitivity of k_{eff} to number density (δk/k)/(δn/n)**	**Sensitivity of k_{eff} to cross sections (δk/k)/(δσ/σ)**	**Best est. bias (BEB) $\lvert(1 - \overline{X})\rvert$**	**Σ {BEB * |(δk/k)/(δσ/σ)|}**	**Nuclide rank**
^{142}Ce	(n,γ)	^{143}Nd	2.36E−03	−1.12E−02	−2.64E−05	0.012	3.17E−07	28
^{147}Sm	(n,γ)	^{147}Sm	−1.34E−01	−1.75E−03	2.34E−04	0.001	2.34E−07	29
^{148}Sm	(n,γ)	^{149}Sm	7.28E−03	−1.47E−02	−1.07E−04	0.002	2.14E−07	30
^{132}Xe ^{132}Xe	(n,γ) Fγ	^{133}Cs ^{133}Cs	1.50E−03 8.80E−08	−3.73E−03 −3.73E−03	−5.60E−06 −3.28E−10	0.024 0.024	1.34E−07	31
^{144}Nd	(n,γ)	^{145}Nd	1.07E−02	−2.16E−03	−2.31E−05	0.004	9.23E−08	32
^{142}Nd	(n,γ)	^{143}Nd	6.14E−04	−1.12E−02	−6.87E−06	0.012	8.25E−08	33
^{99}Mo	(n,γ)	^{99}Tc	−9.65E−05	−2.80E−03	2.70E−07	0.156	4.22E−08	34
^{147}Nd	(n,γ)	^{147}Sm	−1.96E−02	−1.75E−03	3.43E−05	0.001	3.43E−08	35
^{144}Ce	(n,γ)	^{145}Nd	1.52E−03	−2.16E−03	−3.28E−06	0.004	1.31E−08	36
^{146}Nd	(n,γ)	^{147}Sm	6.77E−03	−1.75E−03	−1.18E−05	0.001	1.18E−08	37
^{143}Ce	(n,γ)	^{143}Nd	−8.75E−05	−1.12E−02	9.80E−07	0.012	1.18E−08	38
^{133m}Xe	(n,γ)	^{133}Cs	−5.70E−05	−3.73E−03	2.13E−07	0.024	5.10E−09	39
^{133}I	(n,γ)	^{133}Cs	−4.91E−05	−3.73E−03	1.83E−07	0.024	4.40E−09	40
^{150}Pm	(n,γ)	^{150}Sm	−9.43E−06	−1.28E−03	1.21E−08	0.066	7.98E−10	41
^{142}Pr	(n,γ)	^{143}Nd	5.37E−06	−1.12E−02	−6.01E−08	0.012	7.21E−10	42
^{152m}Eu	(n,γ)	^{153}Eu	1.48E−06	−1.92E−03	−2.85E−09	0.034	9.68E−11	43
^{102}Rh	(n,γ)	^{103}Rh	4.67E−09	−8.24E−03	−3.85E−11	0.269	1.04E−11	44
^{98}Tc	(n,γ)	^{99}Tc	8.65E−09	−2.80E−03	−2.42E−11	0.156	3.78E−12	45
^{132}Cs	(n,γ)	^{133}Cs	1.14E−10	−3.73E−03	−4.25E−13	0.024	1.02E−14	46
^{109}Ag ^{109}Ag	(n,γ) Fγ	^{109}Ag ^{109}Ag	−3.85E−01 −2.16E−07	−1.11E−03 −1.11E−03	4.28E−04 2.40E−10			47
^{95}Mo	(n,γ)	^{95}Mo	−6.06E−02	−1.46E−03	8.84E−05			48
^{100}Mo	(n,γ)	^{101}Ru	3.16E−03	−8.95E−04	−2.83E−06			49
^{94}Nb	(n,γ)	^{95}Mo	4.13E−08	−1.46E−03	−6.03E−11			50
^{95}Nb	(n,γ)	^{95}Mo	−9.48E−04	−1.46E−03	1.38E−06			51
^{95m}Nb	(n,γ)	^{95}Mo	−5.70E−06	−1.46E−03	8.32E−09			52
^{108}Pd ^{108}Pd	(n,γ) Fγ	^{109}Ag ^{109}Ag	1.20E−01 1.77E−08	−1.11E−03 −1.11E−03	−1.33E−04 −1.97E−11			53
^{109}Pd	(n,γ)	^{109}Ag	−1.06E−04	−1.11E−03	1.18E−07			54
^{100}Ru	(n,γ)	^{101}Ru	1.16E−03	−8.95E−04	−1.04E−06			55
^{101}Ru	(n,γ)	^{101}Ru	−5.68E−02	−8.95E−04	5.08E−05			56
^{94}Zr	(n,γ)	^{95}Mo	2.91E−04	−1.46E−03	−4.25E−07			57
^{95}Zr	(n,γ)	^{95}Mo	−4.74E−04	−1.46E−03	6.92E−07			58

5. RECOMMENDATIONS

Establishing a priority ranking list for a reevaluation of burnup credit fission product cross sections should consider (1) the importance of the fission product in burnup credit (i.e., reactivity worth), (2) the importance of the cross section in the prediction of the fission product concentrations, and (3) the accuracy of existing data based on known isotopic measurements. Ref. 6 documents the relative importance of the fission products at several burnups and provides a summary of isotopic assay data demonstrating the current accuracy of computation methods to predict nuclide concentrations. Table 16, presented in Section 4 of this report, combines these factors to produce a relative ranking for which cross sections relevant to burnup credit should be reevaluated.

Review of the current isotopic assay benchmark results indicates that the fission products exhibiting the most discrepant results in comparisons with isotopic assay measurements include ^{155}Gd, ^{151}Sm, ^{152}Sm, ^{103}Rh, and ^{99}Tc. Assessment of the cross sections related to the generation and loss of these nuclides are therefore considered to be of highest priority. Note that no isotopic validation data are available for ^{95}Mo, ^{101}Ru, and ^{109}Ag, precluding an evaluation of the accuracy of existing cross sections. Based on the important fission products identified and the cross-section sensitivities for these nuclides, the following priority fission products are recommended in descending order of importance: ^{151}Sm, ^{103}Rh, ^{155}Eu, ^{150}Sm, ^{152}Sm, ^{153}Eu, ^{154}Eu, and ^{143}Nd. Medium-importance fission products include ^{99}Tc, ^{150}Nd, ^{149}Sm, ^{133}Cs, ^{147}Pm, ^{148}Pm, and ^{148m}Pm.

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