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Review of the Palisades Pressure Vessel Accumulated Fluence Estimate and of the Least Squares Methodology Employed

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Abstract

This report provides a review of the Palisades submittal to the Nuclear Regulatory Commission requesting endorsement of their accumulated neutron fluence estimates based on a least squares adjustment methodology. This review highlights some minor issues in the applied methodology and provides some recommendations for future work. The overall conclusion is that the Palisades fluence estimation methodology provides a reasonable approach to a "best estimate" of the accumulated pressure vessel neutron fluence and is consistent with the state-of-the-art analysis as detailed in community consensus ASTM standards.

Acknowledgment

The author wishes to express his appreciation to Professor John Williams, University of Arizona, and Dr. Igor Remec, Oak Ridge National Laboratory, for productive discussions that helped in the formulation of this review.

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Executive Summary

The following observations can be made following a review of the 4/4/96 Palisades Nuclear Regulatory Commission (NRC) submittal, the 6/26/97 compilation of all Requests for Additional Information (RAIs) submitted after 4/4/96, and the NRC interim Safety Evaluation Report (SER):

- The Palisades analysis represents a dosimetry-community consensus "best estimate" fluence and conforms to state-of-the-art practices.
- The difference between the calculated M/C values and the "spectrum-adjusted" M/C values is within the expected range of variation seen in the comparison of benchmark fields. It is also consistent with the international consensus statements on the state-of-the-art for computing of reactor pressure vessel neutron fluence.
- The fidelity of the dosimetry cross sections is not responsible for any significant observed discrepancy in the M/C ratios.
- The ^{235}U spectrum uncertainty can probably explain at least 5-7% of the observed M/C discrepancy between the $^{54}Fe(n,p)$ & $^{58}Ni(n,p)$ and $^{63}Cu(n,\alpha)$ reaction rates.
- The Palisades dosimetry measurements appear to be very consistent and to exhibit a low dispersion. The scatter in the data is consistent with the Palisades statements on the measurement uncertainty.
- The Winfrith Iron benchmark C/E data show that, while the calculations through iron overpredict the Φ_{1MeV} neutron fluence through thick iron, they underpredict the transmitted fluence through thin iron. This observation is subject to some caveats but may relate to what is seen in the Palisades C/E analysis.

The Palisades accumulated fluence estimates conform to technically sound community consensus standards. The fluence estimate appears to be consistent with the requirements of ASTM standard E-900 and NRC Regulatory Guide 1.99. The estimate also appears to be consistent with the intent of 10 Code of Federal Regulations (CFR) 50.61 and the basis for the Pressurized Thermal Shock (PTS) rule.

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Review of the Palisades Pressure Vessel Accumulated Fluence Estimate and of the Least Squares Methodology Employed

1. Scope of Review

The Consumers Energy Palisades Nuclear Plant asked the author to provide an independent review of their application of measurements in estimating the neutron fluence in the reactor pressure vessel and in meeting the intent of the Nuclear Regulatory Commission (NRC) 10 Code of Federal Regulations (CFR) 50.61 Pressurized Thermal Shock (PTS) rule for pressure vessel embrittlement. The depth of this review is to be consistent with a level of effort of 80 man-hours. Specific questions included:

- Is the method used by Westinghouse (the Palisades primary contractor on fluence issues) technically sound?
- Is it consistent with the basis for the PTS rule?
- Has Palisades communicated clearly and where would further explanations be useful?

Palisades provided a packet of material for the review that consisted of two three-ring binders of documentation. This information included the 4/4/96 submittal to the NRC, their 6/26/97 submittal, which is a compilation of all Requests for Additional Information (RAIs) submitted after 4/4/96, and the NRC 12/20/96 interim Safety Evaluation Report (SER). This review is to be based upon the materials provided in the Palisades packet of materials and upon background information the reviewer possesses based on his past experience. Additional background information could be made available upon request by the reviewer from Consumers Power Company (CPC). The initial Palisades submittal to the NRC requested a 25% decrease in the estimate of the accumulated pressure vessel fluence based on a least squares analysis of all available fluence information. The NRC's interim SER accepted an 8% reduction based on the changes made in the transport calculations, but disallowed all best estimate adjustments related to the use of the nuclear power plant measurements.

2. Overall Impression

My overall reaction is that the Palisades fluence estimation methodology provides a reasonable approach to a "best estimate" of the accumulated pressure vessel neutron fluence and is consistent with the community consensus as I know it.

My views of the community consensus have been formed in my position as chairman of the ASTM E10.05 subcommittee on Nuclear Radiation Metrology, as a member of the Symposium Committee which organizes the International Reactor Dosimetry conferences, and in my professional work characterizing the neutron spectrum for various configurations of research reactors and compiling community-consensus dosimetry cross sections and uncertainty data. My background includes expertise in radiation transport calculations (Monte Carlo as well as discrete ordinate methods) as well as expertise in dosimetry measurements and spectrum adjustment techniques. Because of this background I was asked by the DOE to review the recent OECD/NEA Nuclear Science Committee Task Force Report on Computing Radiation Dose to Reactor Pressure Vessel and Internals [NEA97] and to provide the draft for the U.S. contribution.

Some comments and recommendations are made in the following sections. I do not consider any of my comments or questions to be of a nature that would cast significant question on the methodology or conclusions presented in the Palisades material that I have reviewed.

3. Discrepancy Between the Calculated and Measured Reaction Rates

The NRC suggests that one possible explanation of the discrepancy between the experimental activity measurements (cavity and surveillance) and the DORT calculations is the use of inaccurate $^{54}Fe(n,p)$ and $^{58}Ni(n,p)$ dosimetry cross sections (Reference [SE255], page 9). Their words are:

> **"The in-vessel high energy and low energy dosimeters indicate a substantial difference in M/C fluence bias; M/C = 1.0 +/- 0.03 versus M/C = 0.86 +/- 0.02, respectively. In the CPC/W analysis this difference is assumed to be due to a spectrum dependent error in the DORT calculations which results in an exact calculation above E > 4.0 MeV and an overprediction for E < 4.0 MeV. ... While this conclusion may be correct, several other possible explanations for the observed 1.00/0.86 difference between the high/low-energy M/C bias that would not require a reduction in the DORT calculated fluence are identified. These include: (1) the use of erroneously low dosimeter cross sections for the Fe-54 and Ni-58 in the interpretation of the measurement, and/or (2) errors in the Fe-54 and Ni-58 measurements."**

I strongly disagree with this conjecture. With regard to the first alternative, the $^{54}Fe(n,p)$ and $^{58}Ni(n,p)$ have been considered to be Category I candidate reactions [Zi79] for many years and recent analysis clearly supports their inclusion as Category I reactions [Gr97a, Gr97b]. A Category I reaction for reactor neutron dosimetry is defined [Vl77] as a reaction: (a) for which the energy-dependent cross sections are well known over their response range in standard neutron fields; and (b) for which calculated reaction rates in the standard fields are consistent with the measured reaction rates.

3.1 ^{54}Fe(n,p) and ^{58}Ni(n,p) Cross Sections

These two dosimetry cross sections are very well characterized and validated in standard neutron fields. They also have validated energy-dependent uncertainty files. Tables 1 and 2 show the calculated-to-experimental (C/E) agreement for these reactions in the standard fission benchmark fields. Figures 1 and 2 show the C/E ratios for a wide range of dosimetry reactions in these fields. In the ^{252}Cf standard field the C/E uncertainty (including the effect of the spectrum uncertainty, the cross section uncertainty, and the activity measurement uncertainty) is 2.6% for the ^{54}Fe(n,p) reaction and 2.84% for the ^{58}Ni(n,p) reaction with C/E values of 1.014 and 0.9806, respectively. In the ^{235}U thermal fission neutron standard field the total uncertainties are 5.9% and 7.17%, respectively, with C/E values of 0.9965 and 0.9742. The major contributor to the ^{235}U field uncertainty is the uncertainty of the fission neutron spectrum even in this standard field.

If one looks for uncertainty in the Palisades analysis, the radiation transport cross sections are **much more** suspect and do not typically even have complete energy-dependent covariance files. No ENDF/B-VI covariance data are available for the cross sections used in the transport calculations - as opposed to reactions used for dosimetry applications. Limited ENDF/B-V covariance data for transport cross sections (elastic and inelastic components) are available on some materials as part of the COVFILS library. Some sensitivity calculations on the importance of the transport cross sections are available.

3.2 ^{63}Cu(n,α) Cross Section

The dosimetry sensor which was found to be in conflict with the ^{54}Fe(n,p) and ^{58}Ni(n,p) sensors in the NRC response is the ^{63}Cu(n,α) sensor. This is also a Category I reaction and, as seen in Tables 1 and 2, has also been well validated in the standard neutron fields. Thus the conflict between the Palisades dosimetry measurements is not easily ascribed to the uncertainty in the dosimetry cross sections. The dosimetry cross section validation is **MUCH** more complete than that for the radiation transport calculations. The transport methods and data were, in fact, validated by comparison with measured activities in carefully controlled environments. You can not call these dosimetry cross sections into question without also invalidating the various light water reactor (LWR) benchmarks used to validate the transport cross sections.

Some individuals have cited the cross section comparison plots in Reference [Gr93] to support this conjecture regarding the large uncertainty in the ^{54}Fe(n,p)^{54}Mn and ^{58}Ni(n,p)^{58}Co reaction cross sections. As the author of this reference I can state that this is a misrepresentation of the data presented in the report. The report attempts to show the variation in existing cross section libraries - **if the users do not pay careful attention to the source and fidelity of the cross section evaluation**. When one considers only recent dosimetry-quality evaluations, the ^{58}Ni(n,p) and ^{54}Fe(n,p) cross sections have very consistent cross sections as reflected in the various national cross section nuclear data files. Table 3 compares the spectrum-averaged cross sections from various modern dosimetry

Table 1: Uncertainty of Dosimetry Cross Sections in the ^{252}Cf Standard Fission Field

	Dosimetry Reaction	Median Resp. Energy, E_{50} (MeV)	^{252}Cf Fission Cross Section			^{252}Cf Fission Uncertainty			
			Calc. (mb)	Expt. (mb)	C/E	Spect. Unc. (%)	Xsec. Unc. (%)	Expt. Unc. (%)	C/E Unc. (%)
reactions in Palisades dosimetry									
1	$^{59}Co(n,\gamma)^{60}Co$	1.045	6.062	6.971	0.8697	0.709	4.71	5.00	6.90
2*	$^{235}U(n,f)FP$	1.690	1218.	1210.	1.007	0.0764	0.319	1.20	1.24
3	$^{237}Np(n,f)FP$	2.069	1335.	1361.	0.9810	0.231	9.21	1.58	9.35
4+	$^{238}U(n,f)FP$	2.751	315.4	325.7	0.9684	0.398	0.535	1.63	1.76
5*	$^{58}Ni(n,p)^{58}Co$	4.097	115.3	117.6	0.9806	0.720	2.41	1.30	2.84
6*	$^{54}Fe(n,p)^{54}Mn$	4.259	88.13	86.88	1.014	0.783	2.09	1.34	2.60
7	$^{46}Ti(n,p)^{46}Sc$	5.878	12.33	14.09	0.8751	1.18	2.47	1.76	3.26
8*	$^{63}Cu(n,\alpha)^{60}Co$	7.252	0.6784	0.6891	0.9845	1.39	2.38	1.98	3.39
other related dosimetry reactions									
9*	$^{93}Nb(n,n')^{93m}Nb$	2.693	142.7	150.6	0.9475	0.355	2.99	3.00	4.25
10*	$^{47}Ti(n,p)^{47}Sc$	3.826	19.38	19.29	1.005	0.619	3.78	1.66	4.18
11*	$^{59}Co(n,2n)^{58}Co$	12.98	0.4228	0.4056	1.042	3.28	2.61	2.52	4.89
Category I reactions are shaded dark as depicted in this table footer and indicated with a *									
Potential category I reactions are lightly shaded as depicted in this table footer and indicated with a +									

quality cross section evaluations using the 620-group (unadjusted) neutron spectrum interpolated (via the CPC/W methodology) from the Palisades in-vessel capsule (W290-9) cycle 9 calculation. The table entries also include the cross section uncertainty obtained by convolving the cross section covariance (when it was given in an evaluation) with the neutron spectrum. This table confirms the consistency and the small variation among the community-consensus values for these cross sections in the applicable neutron environments.

When dosimetry-quality cross section evaluations with associated covariance matrices are considered, the $^{54}Fe(n,p)^{54}Mn$ reaction W290-9 spectrum-averaged cross section has a mean value of 0.2793×10^{-1} +/- 0.34%. This is very consistent with the variation seen in the individual cross section evaluations and their associated uncertainty of ~2%. I emphasize that this uncertainty is only the cross section contribution and that this uncertainty term is not a simple spectrum-averaged uncertainty using only the diagonal covariance terms, but is produced by a proper convoluting of the total cross section covariance matrix (including the off-diagonal terms) with the W290-9 surveillance capsule calculated spectrum using techniques detailed in Reference [Gr96]. The $^{58}Ni(n,p)^{58}Co$ reaction shows similar good consistency with a spectrum-averaged cross section of 0.3614×10^{-1} +/- 1.03%. This is consistent with the individual evaluation uncertainty estimates which range from ~2% to ~6%. The $^{63}Cu(n,\alpha)^{60}Co$ reaction also shows good consistency with the individual evaluations and their associated uncertainty estimates, but has a larger variation than the other Category I reactions. The problem here is attributed to the ENDF/B-V evaluation,

which is the oldest evaluation considered here. This ENDF/B-V evaluation is the outlier among the evaluations, but it also has a large (~5%) uncertainty, so this datapoint does not seriously disagree with the other evaluations.

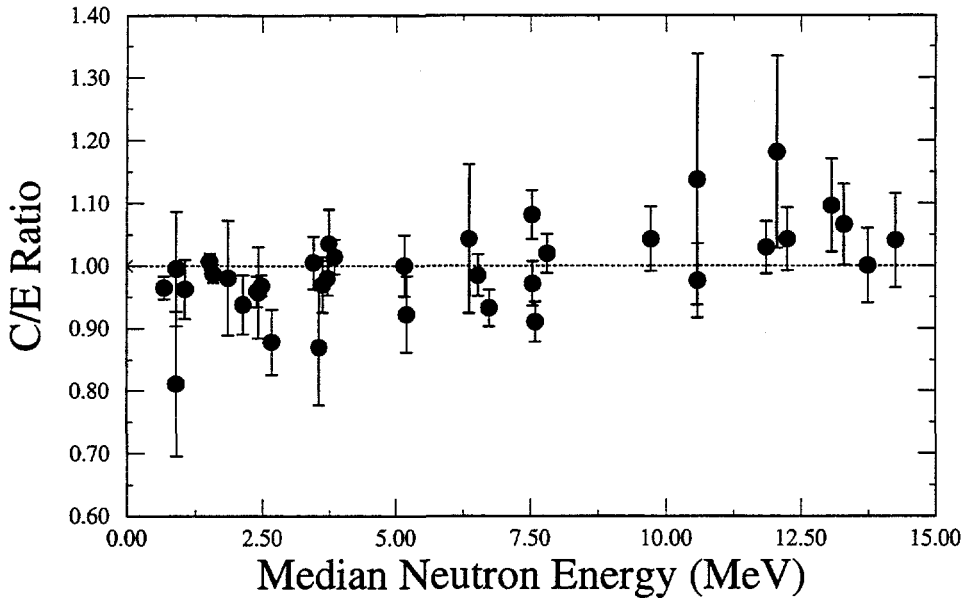

Figure 1: C/E Ratio for ^{252}Cf Standard Fission Field

3.3 ^{46}Ti(n,p) Cross Section

The NRC response did not say much specifically about the ^{46}Ti(n,p) reaction, but it is the other high energy threshold reaction used in the Palisade's adjustment. The ^{46}Ti(n,p)^{46}Sc reaction is **NOT** a Category I reaction. It shows significant C/E problems in standard benchmark spectra. Older ENDF/B-V dosimetry libraries for this reaction had a good C/E. The new libraries (GLUCS-93 and IRDF-90 evaluations and the recommended cross sections as reflected in the SNLRML compilation used in the Palisades analysis) show poor agreement for this cross section in benchmark fields while the new evaluations show a much smaller uncertainty than for older ENDF/B-V libraries. The problems with the ^{46}Ti(n,p) reaction are being examined now by the dosimetry cross section community [Gr97b]. This reaction is **VERY** suspect.

Table 4 shows a compilation of the available experimental and calculated ^{46}Ti(n,p) spectrum-averaged cross sections in the ^{252}Cf benchmark standard fission field. These data clearly indicate the problems with this cross section. The Zolatarev ^{46}Ti(n,p)^{46}Sc evaluation, included in Table 4 but not considered in Reference [Gr93], is still being studied by the author. Of the remaining cross section evaluations, the GLUCS93 evaluation appears to have the highest fidelity. A work-around for the C/E problems with this dosimetry cross section, suggested for use [Gr97b] until the situation is clarified, is to use the new GLUCS/IRDF-90 cross section but to use the older (larger) ENDF/B-V uncertainty data. The ENDF/B-V covariance was the *a priori* data used in the GLUCS least

Table 2: Uncertainty of Dosimetry Cross Sections in the ^{235}U Standard Thermal Fission Field

	Dosimetry Reaction	Median Resp. Energy, E_{50} (MeV)	^{235}U Thermal Fission Cross Section			^{352}U Thermal Fission Uncertainty			
			Calc. (mb)	Expt. (mb)	C/E	Spect. Unc. (%)	Xsec. Unc. (%)	Expt. Unc. (%)	C/E Unc. (%)
reactions in Palisades dosimetry									
1	$^{59}Co(n,\gamma)^{60}Co$	1.039	6.118	NA	NA	7.71	4.74	NA	NA
2*	$^{235}U(n,f)FP$	1.642	1216.	1216.	0.9999	4.09	0.319	1.60	4.41
3	$^{237}Np(n,f)FP$	1.987	1330.	1344.	0.9897	4.31	9.34	4.00	11.0
4+	$^{238}U(n,f)FP$	2.638	306.2	309.0	0.9910	4.23	0.535	2.60	4.99
5*	$^{58}Ni(n,p)^{58}Co$	3.970	105.7	108.5	0.9742	4.53	2.44	5.00	7.17
6*	$^{54}Fe(n,p)^{54}Mn$	4.106	80.18	80.46	0.9965	4.71	2.12	2.86	5.90
7	$^{46}Ti(n,p)^{46}Sc$	5.715	10.25	11.60	0.8838	5.41	2.48	3.45	6.87
8*	$^{63}Cu(n,\alpha)^{60}Co$	6.990	0.5211	0.5000	1.042	5.96	2.36	11.0	12.7
other related dosimetry reactions									
9*	$^{93}Nb(n,n')^{93m}Nb$	2.600	140.0	146.4	0.9563	4.14	3.01	3.00	5.93
10*	$^{47}Ti(n,p)^{47}Sc$	3.664	17.95	19.00	0.9449	4.27	3.77	7.40	9.34
11*	$^{59}Co(n,2n)^{58}Co$	12.80	0.2079	0.2020	1.029	10.7	2.91	2.97	11.5
Category I reactions are shaded dark as depicted in this table footer and indicated with a *									
Potential category I reactions are lightly shaded as depicted in this table footer and indicated with a +									

squares analysis (the recommended cross section), so this is not as bad (statistically invalid) as it may sound at first. Since the Palisades analysis used data consistent with the newer GLUCS cross section (the data presented in the SNLRML compilation) and with the smaller $^{46}Ti(n,p)^{46}Sc$ cross section uncertainty, this recommendation should be implemented in future spectrum analyses. This change should not have a significant effect on the least squares spectrum adjustment since the $^{63}Cu(n,\alpha)^{60}Co$ reaction is still present to help fix the high energy part of the spectrum. If anything, this adjustment (attributing a larger uncertainty to the $^{46}Ti(n,p)^{46}Sc$ activities) would place more emphasis on the lower energy 0.85 M/C bias factor due to the influence of the Ni/Fe reactions.

3.4 Fission Dosimeter Measurements

In making their observation on the value of dosimetry measurements, the NRC dismissed the effect of the $^{237}Np(n,f)FP$ and $^{238}U(n,f)FP$ dosimeters stating as their reasons that the number of these dosimeters was small and that these reactions were subject to a large uncertainty. From the Attachment II materials supplied by Palisades, the ^{237}Np dosimeter is used in 1 of 4 surveillance capsules while the ^{238}U dosimeter is used in 2 of 4 surveillance capsules (A240, W290, W290-9, and W110). This is not an insignificant number of measurements if one's attention is restricted to just the surveillance capsule spectrum adjustments - a suggestion made elsewhere in the NRC response (page 9 Reference [SE255]). The ^{238}U dosimeters are used in 3 of 4 Cycle 8 cavity dosimetry sensor sets, 2

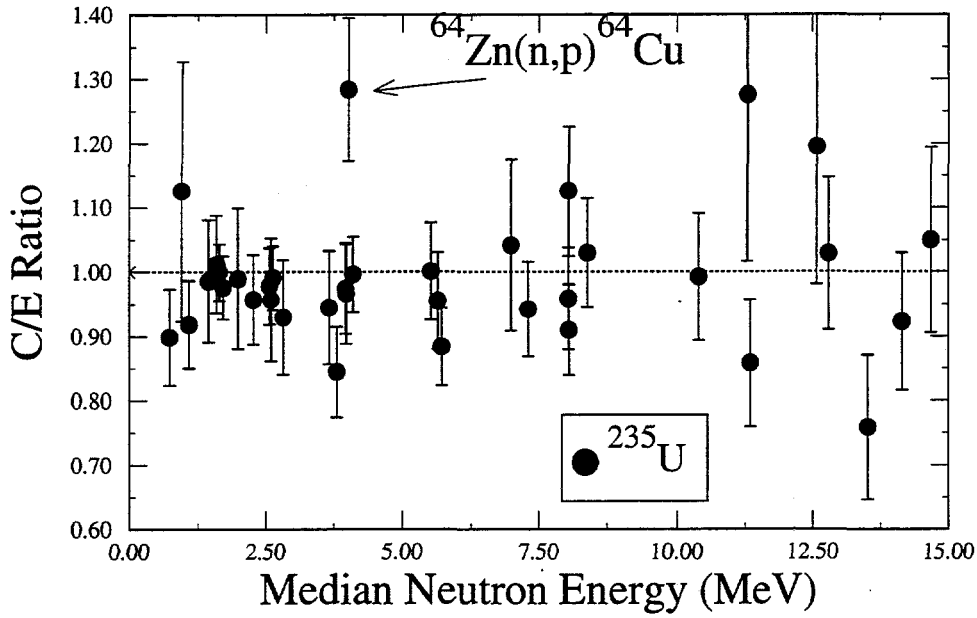

Figure 2: C/E Ratio for ^{235}U Standard Fission Field

Table 3: Comparison of Variation in Dosimetry Cross Sections

Evaluation		Reaction Cross Section (b)		
		$^{54}Fe(n,p)^{54}Mn$	$^{58}Ni(n,p)^{58}Co$	$^{63}Cu(n,\alpha)^{60}Co$
1	ENDF/B-VI	0.280×10^{-1} +/- 2.05%	0.364×10^{-1} +/- 2.34%	0.318×10^{-3} +/- 2.83%
2	GLUCS-93	0.278×10^{-1} +/- 2.00%	0.356×10^{-1} +/- 2.17%	0.321×10^{-3} +/- 2.42%
3	IRDF-90	0.280×10^{-1} +/- 2.00%	0.364×10^{-1} +/- 2.17%	0.318×10^{-3} +/- 2.42%
4	ENDF/V Dosimetry	0.279×10^{-1} +/- 3.34%	0.359×10^{-1} +/- 6.02%	0.355×10^{-3} +/- 5.17%
5	JENDL Dosimetry	0.285×10^{-1} +/- 3.31%	0.364×10^{-1} +/- 6.03%	0.321×10^{-3} +/- 5.30%
Mean (Std. Dev.)		0.279×10^{-1} +/- 0.34%	0.361×10^{-1} +/- 1.03%	0.3266×10^{-3} +/- 4.9%

Table 4: $^{46}Ti(n,p)^{46}Sc$ Cross Section in the ^{252}Cf Standard Fission Field

Experimental		Calculational	
Source	Xsec (mb)	Source	Xsec (mb)
Kirouc, 1973	12.4 (9.7%)	GLUCS-93	12.6 (2.45%)
Alberts, 1975	13.8 (2.17%)	GLUCS-90	12.3 (2.94%)
Dezso, 1977	13.4 (8.21%)	IRDF-82	13.2 (12.6%)
Spiegel, 1978	15.0 (6.67%)	IRDF-90	12.3 (2.45%)
Dezso, 1983	13.6 (8.9%)	JENDL-dos	12.3 (12.6%)
Kimura, 1986	14.04 (4.36%)	E5 Dosimetry	13.2 (12.6%)
Mannhart,1989	14.09 (1.76%)	ENDF/B-VI	13.2 (12.6%)
		Zolatarev (1994)	13.27 (2.39%)

of 6 Cycle 9 cavity sensor sets, and 7 of 7 Cycle 10/11 cavity sensor sets. The ^{237}Np dosimeters are used in 4 of 4 Cycle 8 cavity dosimetry sensor sets, 6 of 6 Cycle 9 cavity sensor sets, and 6 of 7 Cycle 10/11 cavity sensor sets. This does not strike me as a small dosimetry subset that can be dismissed on the basis of the number of measurements. The ^{238}U and ^{237}Np sensors had previously been considered to be a Category I reaction, but recent analysis [Gr97b] suggests that they fail to meet the criteria based on the most recent data. The ^{238}U sensor is very close to a Category I reaction while ^{237}Np has a good C/E but a very large cross section uncertainty component.

3.5 ^{54}Fe(n,p) and ^{58}Ni(n,p) Measurement Uncertainty

The second alternative possibility provided by the NRC for the measurement-to-calculation discrepancy is inaccurate measurements for the ^{54}Fe(n,p) and ^{58}Ni(n,p) dosimeters. No evidence is given to support this conjecture. Since these activity measurements are routinely made at many radiation metrology laboratories without significant problems, since the Palisades measurement procedure appears to have conformed with the ASTM E264 and E263 standard test methods, and since measurements in standard neutron fields have been made with **VERY** small uncertainties [1.34% and 1.30% for ^{54}Fe(n,p) and ^{58}Ni(n,p), respectively, in the ^{252}Cf standard neutron field], there is no obvious reason to suspect the measurements. The ASTM standards report that typical practice can determine these reaction rates with a bias of +/- 3% and a precision of +/- 1%. Since the Palisades uncertainty analysis attributes a 5% uncertainty to these measurements (page 3-15 of Palisades Attachment II) I see no reason to doubt the uncertainty estimate on these measurements.

In the case of the ^{54}Fe(n,p)^{54}Mn reaction, one important potential source of measurement error is the presence of manganese and its action as a contaminant through the ^{55}Mn(n,2n)^{54}Mn reaction. This issue is addressed in the ASTM E263 standard. The Palisades documentation states that they followed ASTM standards and this implies that they used reactor dosimetry-grade iron foils with known iron isotopic composition and known manganese contaminant levels and that they accounted for this contaminant level in their uncertainty analysis.

In the case of the ^{58}Ni(n,p)^{58}Co reaction, one important potential source of measurement error is the burnup of the ^{58}Co through the ^{58}Co(n,γ)^{59}Co reaction or by production from contaminant levels of cobalt through the ^{59}Co(n,2n)^{58}Co reaction. The ASTM E264 standard states that ^{58}Co burnup should be considered when the thermal neutron flux is 3×10^{12} n/(sec-cm^2) or larger. Again since the Palisades dosimetry was conducted in accordance with the ASTM standards they would have accounted for the cobalt contamination in the nickel foils and made corrections, if needed, for the ^{58}Co burnup in the expected thermal neutron flux and included this contribution in setting their measurement uncertainty bounds for this measurement.

3.6 Correlation with Reaction Half-life

One issue about the comparison of the activities for the dosimetry reactions is the different half-lives for the reactions. The $^{58}Ni(n,p)^{58}Co$, $^{54}Fe(n,p)^{54}Mn$, and $^{63}Cu(n,\alpha)^{60}Co$ residual nuclei have half-lives of 70.82 days, 312.12 days, and 1925.1 days, respectively. Since activation levels and decay corrections were made for the dosimetry foil residual products using the monthly reactor power levels, it is unlikely that any time-dependent power fluctuations in the reactor power could play a role in the discrepancy between the measured activities. The NRC response also notes that no trend in the measured M/C ratios appear to be correlated with the half-life of the dosimetry reaction products.

3.7 Summary of Calculated/Measured Reaction Rate Consistency

In summary, the NRC postulated alternatives to accepting the combination of experimental and calculational data used in spectrum adjustments are **MUCH** less credible than an unaccounted bias in the transport calculation.

4. Uncertainty in the ^{235}U Fission Spectrum

Since I have rejected the idea that the $^{54}Fe(n,p)$, $^{58}Ni(n,p)$, and $^{63}Cu(n,\alpha)$ dosimetry cross sections are uncertain enough to explain the 15% observed bias between in-vessel high energy measured reaction rates [M/C = 0.984 for $^{63}Cu(n,\alpha)$] and the low energy reaction rates [M/C = 0.856 for $^{54}Fe(n,p)$ and M/C = 0.8665 for $^{58}Ni(n,p)$], other possible error components should be examined. One possible element is the shape of the ^{235}U fission neutron source spectrum. Uncertainties/errors here would affect the calculation and not the reaction rate measurements. An examination of the bias factors for these reactions in the ^{252}Cf benchmark field shown in Table 1 [M/C = 1.016 and 1.003 for the ^{63}Cu and ^{54}Fe/ ^{58}Ni reactions] completely vindicates the consistency of the dosimetry cross sections in a well-characterized benchmark field. The bias factors for the ^{235}U benchmark field [M/C = 0.96 and 1.015] indicates a 5% bias factor can be attributed to the ^{235}U field. Given the good agreement in the very well characterized ^{252}Cf field, this bias would seem to be attributable to the ^{235}U fission neutron spectrum in this field. These bias factors are in the correct direction to explain the Palisades data [a higher calculated activity for the $^{63}Cu(n,\alpha)$ reaction] - however the bias factors are for a pure unscattered fission benchmark field, not the transported spectrum for which Palisades measurements exist.

It is valuable to try to get a better handle on the energy-dependent uncertainty in the ^{235}U spectrum. It is not easy to find an uncertainty and covariance function which describes the ^{235}U fission spectrum. The ENDF/B-VI files give the best spectrum characterization, which is based on the Madland-Nix formalism. The only source for a covariance matrix which I am aware of is from Reference [Pe85]. Figure 3 shows that the uncertainty in the high energy (> 1 MeV) portion of this neutron spectrum is about 10% with an uncertainty

of about 15% for the portion greater than 10 MeV. When the complete ^{235}U covariance matrix is folded together with the dosimetry cross sections one obtains the 4.7% spectrum-dependent uncertainty component for the $^{54}Fe(n,p)$ and $^{58}Ni(n,p)$ reaction rates and the 6% spectrum-dependent uncertainty component for the $^{63}Cu(n,\alpha)$ reaction rate, as seen in Table 2. One can see from Table 2 that the ^{235}U spectrum contribution to the uncertainty is very important - more important than the cross section contribution to the uncertainty - but it is difficult to quantitatively relate this to the Palisades M/C data.

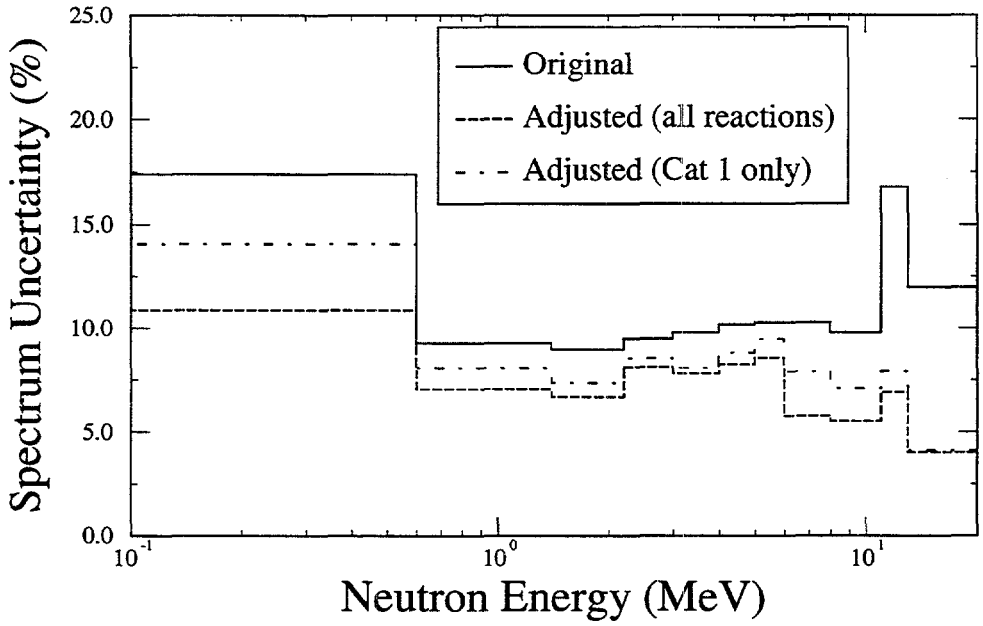

Figure 3: Uncertainty in Prior and Adjusted ^{235}U Standard Fission Spectra

If one performs a least squares analysis on the ^{235}U standard fission benchmark field using all the dosimetry cross sections (and associated uncertainty information) depicted in Figure 2, one can obtain an adjusted ^{235}U fission spectrum. The magnitude of the spectrum adjustment is shown in Figure 4 and the adjusted spectrum uncertainty is shown in Figure 3. One should note that the adjusted ^{235}U fission spectrum has a high energy uncertainty near 7%, a significant decrease from the initial spectrum uncertainty. The next thing noted is that the spectrum adjustment results in a fluence increase from 5-10% for energies above 4 MeV and a decrease by 5% for energies immediately below 4 MeV. This adjustment would (for the pure unscattered ^{235}U fission spectrum) decrease the $^{54}Fe/^{58}Ni$ calculated reaction rates while increasing the ^{63}Cu reaction rate. This is exactly the trend one needs to understand the Palisades M/C data. The M/C data for $^{54}Fe/^{58}Ni$ would increase and the M/C for ^{63}Cu would decrease.

This analysis suggests that the uncertainty in the ^{235}U fission spectrum could play an important role in explaining the observed discrepancy between the calculated and measured reaction rates in the Palisades in-vessel locations. The next step in this analysis should be to use the activity-adjusted ^{235}U fission spectrum as the source term in the 2D discrete ordinates radiation transport calculations. I emphasis that this calculation is recommended just to confirm the importance and direction of change in the calculated activities that is associated with an update in the ^{235}U fission neutron spectrum. It will also serve to validate my conjecture on the importance of the uncertainty in the ^{235}U fission spectra as opposed to the uncertainty in the current state-of-the-art dosimetry cross sections. More work needs to be done with the *a priori* ^{235}U covariance matrix used in the cited work [Gr97b] before a new ^{235}U fission neutron spectrum is recommended for routine applications in radiation transport calculations. A simultaneous spectrum adjustment on the ^{252}Cf and ^{235}U standard benchmark fields would include the effect of the correlated ^{252}Cf adjustment on the dosimetry cross sections and increase the fidelity of the global least squares adjustment of the ^{235}U fission spectrum. This work is underway and will be documented in a future publication.

Some sources [NEA97, reference 85] have ascribed a 7% uncertainty component in the calculation of the >1-MeV fluence to the knowledge of the fission spectrum. This analysis suggests that this 7% discrepancy is in the right direction to help reconcile the Palisades M/C surveillance data.

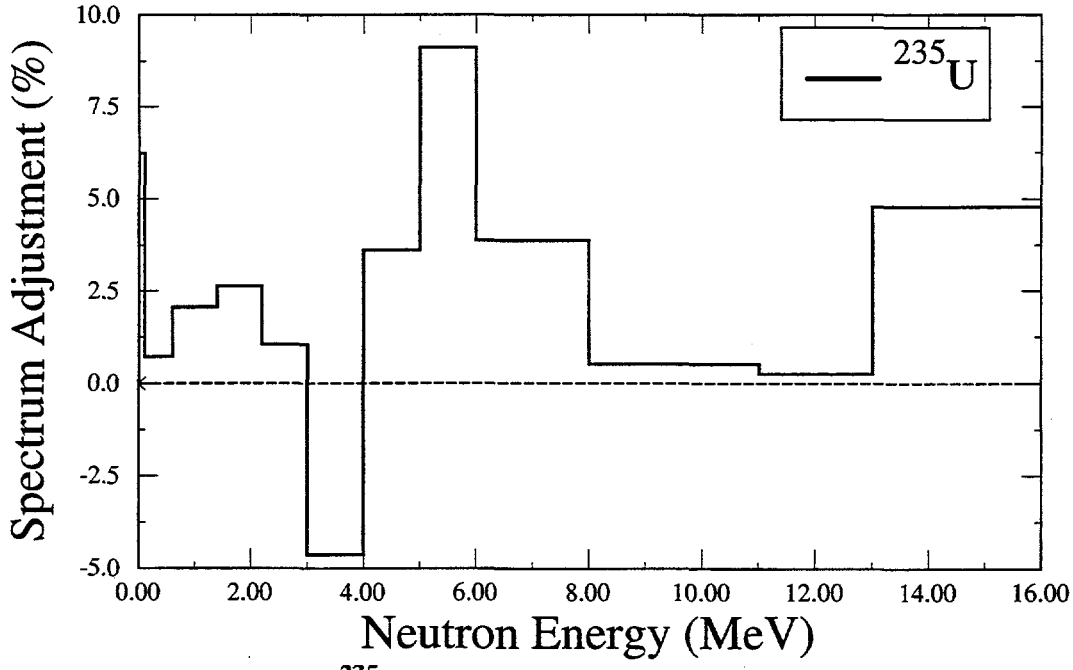

Figure 4: Adjustment of ^{235}U Standard Fission Spectrum

5. FERRET Least Squares Fluence Adjustment

The NRC review [SE255, page 9 section 6.3] states that:

> **"while the adjustment does provide a best fit of the measured data, the dosimeter cross sections, measured reaction rates and calculated spectrum adjustments are made without any physical basis."**

This statement is totally unsupportable as written. The least squares analysis is designed to specifically add the "physical basis" provided by the measured activities to the calculated spectrum. One can request a more careful review of the details of the FERRET least squares methodology, but the general approach is very defensible. The least squares adjustment process does not allow integral data to strongly affect the spectral shape unless the significant discrepancies with the *a priori* radiation transport data are found. One of the pioneers in the least squares adjustment methodology has noted [Pe77c] that

> **"It is clear that through 'integral data' we cannot learn much about the 'differential quantities' unless we have 'strong inconsistencies.' When the integral data are relatively consistent with the differential data, the integral results will not cause our knowledge of the individual differential quantities to be modified."**

The NRC report states that the NRC is presently evaluating the FERRET methodology and will provide a more in-depth report soon. I anxiously await this report to add some substance to the NRC rejection of the methodology.

6. Dispersion in the M/C Factors

The NRC notes that the Palisades data contains several subsets of M/C data which show different biases. I need to review the Palisades data in more detail before I comment on this observation. While I have dismissed the NRC alternate explanations for the pattern they see, the presence of a pattern in the bias factors needs careful consideration. Some of the Palisades responses in Attachment I discuss the variation in their M/C bias factors and make comparisons to that seen at other plants. I need more time to consider this data.

Section 14.1 of this review makes a strong point that the measured reaction rates at the Palisades reactor do not show any dispersion exceeding the Palisades stated measurement uncertainty. Any discussion of the dispersion in measured-to-calculated ratios requires careful study to ensure that **exactly equivalent** modeling techniques and nuclear data were employed in establishing the M/C ratios. I do not have access to the details behind the M/C values reported from other power reactors and can not even attempt to put that data into perspective with the Palisades results.

7. Photofission Correction Factors.

Section 5.0 of the NRC response addresses the photofission contributions to the ^{237}Np and ^{238}U dosimeters. The NRC response raised an important point about the fidelity of the gamma spectrum determination used to support the corrections. The NRC then supported a new analysis of the photofission corrections with increased fidelity for the gamma spectrum. The NRC conclusion was that:

> **"the BUGLE-93 and MATXS12 predictions of the U-238(γ,f) and Np-237(γ,f) reaction rates are in good agreement for both the CPC/W predictions."**

While I am glad to see agreement on this issue, some other ramifications of this correction should have been discussed in more detail in the Palisades NRC submittal. During discussions of this issue with Dr. John Williams (who was involved in the evaluations of the photoneutron corrections to the HFIR dosimetry), Dr. Williams noted that most plants do not consider the photofission corrections - so the question arises whether this correction can affect the basis of the fluence estimate used for the PTS screening criteria? All fission foil data should be corrected for this (if needed) in order to see if the Palisades analysis fits the trends at other plants. Dr. Williams also pointed out that when photofission corrections to the fission foils are important it is likely that photon induced displacements may also need to be considered in assessing the pressure vessel embrittlement.

One issue here is that the Palisades plant probably has a significantly larger photon flux than other plants due to the absence of a thermal shield. Previous analyses [Pe92, NEA97] which I have seen suggest that the photofission correction is about 5% for ^{238}U and 2-3% for ^{237}Np, except for HFIR-type cases. The material provided in the Palisades submittal and the NRC response indicates that CPC/W prediction of the vessel-wall correction is 15% for ^{238}U and 7% for ^{237}Np. The corrections at the Palisades plant are about three times larger than typical, but the ^{238}U/^{237}Np correction ratio is consistent. There is no doubt that this large of a correction factor should be made in the "best estimate" vessel fluence, the question is how to preserve comparisons with measurements at other plants.

Dr. Williams also commented on the uncertainty in this correction. I am not aware of many high fidelity validation or benchmark comparisons of the gamma spectrum on the pressure vessel wall of PWRs. Thus the gamma spectrum, and hence the correction factor, should be assigned a higher uncertainty and this increased uncertainty should be reflected in the least squares analysis. The ASTM standards E-704 and E-705 quote an typical bias of 5% and a precision of 1% for the reaction rate determination of the ^{238}U and ^{237}Np fission reactions. This uncertainty estimate applies to the number of fissions and does not address partitioning of the fissions between neutron-induced reactions and gamma photofission corrections.

The uncertainty in the photofission cross section should also be put on a quantitative basis. A couple of estimates of the photofission cross section have been made in the literature [Ca78, Ve80]. A comparison of these would give some estimate of the uncertainty.

Comparisons of the PCA-PV Blind Test Benchmark Experiment Configuration 4/12, documented in Reference [Sl94a], indicate a C/E of about 0.5 for the calculated and measured integral $0.248 < E_\gamma < 2.731$ MeV gamma-ray fluxes. The gamma-ray energy deposition C/E ratios for the 1/4-T position varied from 1.04 to 1.11. I would suggest, without a totally adequate justification but considering the importance of the higher energy photons to the photofission reactions, that an uncertainty of one half the magnitude of the photofission correction should be added in quadrature to the reaction rate uncertainty. This approach would reflect significant uncertainty in the gamma spectrum flux - which is not too far from the factor of two reported for some other anomalous calculated-to-measured TLD response data I have seen from some research reactors [He97]. Research reactor C/Es for gamma contributions may have reflected problems with the timing for the data collection and the inclusion of contributions from the delayed fission gammas. Some reviews of the gamma spectra in pressure vessel environments [Go97] maintain "gamma-ray spectral calculations possess an uncertainty level no better than 50% (1σ)." Some comparisons of gamma dose at cavity dosimetry locations [Ki94] show good C/E agreement - within 13%. However, this is, again, a comparison of an integrated dose. A comparison of the shape of the energy-dependent cross section for ionizing dose and photofission must be considered before these data are used to justify a lower uncertainty. Since the Palisades documentation quotes counting uncertainties of 5% and decay corrections of 3% for the fission dosimeters, this suggested approach for including the photofission uncertainty would likely result in a reaction rate uncertainty of $[5^2 + 3^2 + (0.5*15)^2]^{1/2} = 9.5\%$ for ^{238}U and $[5^2 + 3^2 + (0.5*6)^2]^{1/2} = 6.6\%$ for ^{237}Np reaction rates.

The spread of M/C data reported in the Westinghouse dosimetry database reflects a significantly larger variation for these fission foil reaction rates than for other activities, but page 3-15 of the Palisades NRC submittal suggests that a reaction rate uncertainty of 5% was used for all sensors. Upon further study of the Palisades/NRC RAI documentation, the Palisades document "Response to Balance of Questions in Attachment 4 to the May 31, 1996 NRC Letter and May 17, 1996, and June 3, 1996 Telecons" section 3.1.2.5 addresses this concern but uses a factor of 25% for the gamma spectrum uncertainty rather than the 50% I would have estimated. This uncertainty contribution is called a "Competing Reaction" contribution. Thus the Palisades approach correctly incorporated a 25% uncertainty in the gamma spectrum. As discussed above I can not justify that my 50% uncertainty is a better estimate than the Palisades 25% uncertainty, but it would be good to test the sensitivity of the FERRET analysis to this change in measurement uncertainty.

8. "Best Estimate" Fluence

A "best estimate" by its very nature involves the consideration of **ALL** available data, both measurements and calculations. The "best estimate" is made by an appropriate combination of the data, so uncertainty estimates on the available data is crucial. The

Palisades methodology has provided a reasonable calculation, reasonable measurement data, and realistic uncertainty measures based on state-of-the-art methods. As such, the data not only should be combined but **MUST** be combined in a statistically valid methodology, i.e. a least squares approach.

A discrepancy between calculation and experiment measures is always disturbing. However, any "best estimate" approach must consider all data in a statistically defensible manner. There is a well researched body of statistical theory that treats the issue of rejection of outlier data [Ro87, Gn72, Ch86]. Any dismissal of the measured data needs to invoke such a statistical approach. To the best of my knowledge, no statistically valid treatment of outlier data would permit the dismissal of the measurement data that I see in the Palisades analysis.

9. Consistency of Calculation and Least Squares Analysis of Experimental Data

The NRC appears to be very concerned about the discrepancies between the calculation and the CPC/W least squares "best estimate" of the neutron fluence. Having many years of experience with both radiation transport calculations and least squares spectrum analysis I am at a loss to understand the basis for their concern. The least squares analysis by CPC/W recommends a bias factor of 0.83, a 17% change. This level of agreement between a measured integral quantity and a calculated integral quantity is consistent with the state-of-the-art in calculational methodology. The least squares approach is generally designed to ensure a statistically valid merging of the experimental reaction rates and the radiation transport calculation. The CPC/W calculation of the fluence is further supported by the AEA Technology Monte Carlo calculation and is generally consistent with the NRC-supported calculation performed by Brookhaven National Laboratory (BNL).

9.1 Tendency of Iron Transmission to be Underestimated by Calculations

The Palisades analysis, which shows that the measured neutron fluence is less than the calculated fluence, is of particular concern since the iron cross section "is known" to underpredict the transmitted neutron fluence. The CPC/W analysis and submittal has suggested that their radiation transported calculated overprediction, which was adjusted down by the least squares adjustment methodology, may be due to the lack of a thermal shield and hence less iron than in typical LWR pressure vessel calculations. An examination of the Winfrith Iron Benchmark supports the CPC/W conjecture.

The Winfrith Iron Benchmark experiment examines the transmission of a fission neutron field through a thick iron shield. The shield consisted of twenty-four 5.08-cm-thick iron plates spaced 6.35 mm apart. The neutron spectrum was measured at four locations using NE-213 detectors placed in slots cut in special iron plates. In addition, activation foil measurements were made at the gaps between the plates. Reference [In95] reports on an analysis of this benchmark experiment and notes:

> **"At 20.32 cm depth in the shield, the broad-group libraries and the self-shielded, VITAMIN-B6 library gave calculated integral fluxes about 30% higher than measured, while the standard-weighted, fine-group libraries (VITAMIN-E and VITAMIN-B6) overpredicted the measurement by about 10%. All libraries underestimated the measured result at greater distances into the shield by an increasing amount. At 101.6 cm into the shield, the concrete-weighted BUGLE-93 library underpredicted the measured integral flux by greater than a factor of 6. Self-shielding and zone-weighting the cross sections reduced this underprediction to about a factor of 2, thus showing the importance of proper processing for deep penetration problems.**

Thus the Palisades results are not anomalous. Very careful benchmark tests, i.e. the Winfrith Iron Benchmark Experiments, also show an **overprediction** of the calculated neutron transmission, relative to the measurements, for small iron thicknesses (~ 20.32-cm). For thick iron transmission (> 50.8-cm), the normal underprediction of the neutron transmission is seen.

We see here, again, a situation where even under the most carefully controlled conditions the *a priori* calculation has severely differed from the measured results. This benchmark experiment underlines the generally accepted position of using measured data whenever possible and only relying on calculations when measurements are not possible - and then to require careful benchmarking in as similar a situation as can be produced and instrumented with diagnostics. Calculations are typically depended upon to provide the systematics in cases where measurements can not be easily performed.

9.2 Benchmark Fields

The C/E values seen in the Palisades analysis are not anomalous nor especially disturbing. A calculational uncertainty of 20% and C/E values that differ from unity by more than 20% are commonly seen even in very carefully controlled benchmark fields.

The Winfrith Iron Benchmark, discussed in the previous section, showed C/E neutron flux values (for the VITAMIN-B6 Fe-self-shielded case) of 1.28 for the 20.32-cm transmission, 0.98 for the 50.8 cm position, and 0.62 for the 101.6 cm position. The activation foils used in the iron benchmark experiment were $^{32}S(n,p)$, $^{103}Rh(n,n')$, and $^{115}In(n,n')$. At the 20.3-cm position the VITAMIN-B6 Fe-self-shielded calculations for these reactions gave C/E values of 1.06, 1.17, and 0.99. At the 50.8-cm position the VITAMIN-B6 standard weighted calculations gave C/E values of 0.86, 0.52, and 0.43. Care must be taken in the interpretation of these C/E values since the cross sections used to calculated the activation were taken from those used for the transport analysis and, **for these reactions**, were not consistent with the recommended cross sections for dosimetry applications. These data, however, certainly suggest that the 20% accuracy for pressure vessel calculations is not an overestimation of the expected calculation-to-measured agreement.

The various detectors behind the 30-cm iron thickness from the CSEWG SDT11 benchmark, when compared with the VITAMIN-B6 calculations, gave C/E values that

ranged from 0.32 to 0.98 [In95]. Strong differences (50%) were often seen between C/E ratios produced from experiments with pure iron (Fe) and stainless steel. This indicates that the cross sections for the other components in stainless steel (nickel, silicon, carbon, chromium, manganese) can have a significant effect on the C/E values.

9.3 Effect of Energy Bin Structure (Fine Group vs. Broad Group)

The Winfrith Water Benchmark Experiment examined the fission neutron transmission through various thicknesses of water. The C/E values for the VITAMIN-B6 fine-group calculations comparing the integral neutron flux varied from 0.83 at 10.16-cm, 0.7 at 25.40-cm thickness, and went back up to 0.78 at a 50.80-cm thickness. Again 20-30% differences in integral metrics [integral flux and $^{32}S(n,p)$ activity] are seen. Here one also notes that when the VITAMIN-B6 fine-group calculations are compared with the related broad-group BUGLE-93 calculations, differences of 10-20% are seen.

When the VITAMIN-B6 C/E ratios are compared to the BUGLE-93 ratios for the SDT11 Benchmark Experiment, some locations show excellent agreement, while others can be off by 50% (the 3-in Bonner ball with Fe at the centerline position).

9.4 Calculated Uncertainty for the International Community

The inputs to Reference [NEA97] from many other countries support the range of a 20% uncertainty in carefully calculated pressure vessel fluences.

Belgium

> The Belgian SCK-CEN and TRACTEBEL EE validated their calculational tools on a range of experimental benchmarks (including the VENUS benchmarks) in 1993 and quote "the global uncertainties of the calculated values are within 20 percent [NEA97]." The SCK-CEN procedure involved the use of the LEPRICON code while TRACTEBEL EE uses MCBEND. It should be noted that these SCK-CEN quotes a 20% uncertainty on the LEPRICON calculation but uses the LEPRICON spectrum adjustment modules to reduce this quoted uncertainty to 4% [NEA97].

Finland

> Reference [NEA97] also quotes the Finland community as stating "For the pressure vessel the corresponding uncertainties are within the range of 20-25 per cent (sic)."

Germany

> SIEMENS/KWU states that "As a result, the uncorrected and unadjusted ratios of calculated and measured fluences only slightly exceed 20 percent."

Japan

Application of the 3D S_N code TORT to the BWR/800 and 1000 MW_e reactors produced "the ratio of calculated-to-measured fluence using Cu, Fe, and Ni detectors at the surveillance position turns out to be 1.7."

At the Japan Materials Testing Reactor (JMTR) at JAERI the fluence is measured using Fe and Co dosimeters. After extensive modeling efforts "the discrepancy between measured and calculated fast fission fluence for this reactor is at +/- 20 per cent (sic) (1.65σ) and at +/- 40% (1.65σ) for thermal neutron fluence."

Korea

The Kori Unit 4 surveillance capsule computational efforts using the BUGLE-93 cross sections and DOT 4.3 result in M/C ratios for dosimetry reactions of:

- $^{54}Fe(n,p)$ 0.7937
- $^{63}Cu(n,\alpha)$ 1.2891
- $^{58}Ni(n,p)$ 0.7486
- $^{59}Co(n,\gamma)$ 0.4529

The calculated-to-measured bias factor used for this Kori Unit 4 reactor was set to 1.23.

Note that these data show a split between the high and low energy dosimeters that is larger than that seen in the Palisades plant and in the same direction. In the future, the current Korean community foresees the use the LEPRICON methodology for an adjustment of the calculated fluence.

Netherlands

An MCNP4A analysis for the HOR research reactor shows that the "agreement between the resulting calculated and measured ex-vessel neutron fluence above 1-MeV is better than 15 per cent and usually even better than 10 per cent."

Sweden

General methods using CASMO and DORT codes produce uncertainties for the fluence greater than 1-MeV of 2-25%.

United Kingdom

Magnox reactor fast fluence C/E values from MCBEND range from 0 to 35%.

United States

The state-of-the-art for U.S. fluence calculation is stated as "Typical calculational uncertainties estimates are between 15-20 per cent (1σ) at the inside of the reactor vessel in the beltline and may be as large as 30 percent in the cavity."

The conclusion drawn in Reference [NEA97] for the reported state-of-the-art in reactor fluence calculations was "the median result appears to fall within 20 percent difference between calculation and measurements."

9.5 BNL Calculated Fluence Uncertainty Estimates

The NRC response to the Palisades submittal supports a BNL fluence calculation which has a BNL-endorsed uncertainty of 14.2%. Even using this value, rather than the more typical 20%, a one sigma deviation of the "best estimate" from the calculation is not typically a serious concern - it occurs 33% of the time for data with a normal distribution. The M/C = 0.83 value is not significantly outside this calculational uncertainty band. This is especially true in light of the previous observation that the ^{235}U spectrum uncertainty probably helps reconcile these data by at least 5-7%.

I would raise some additional questions about the estimation of the uncertainty in the BNL calculations. It is not clear if the uncertainty in the transport cross sections was included in their uncertainty analysis. Their description of the "nuclear data" 7% uncertainty contribution merely states "the nuclear data uncertainty estimate is based on expected data uncertainties." I do not know what terms were considered or how the uncertainty values were estimated. I would expect a larger uncertainty contribution due to the knowledge of the transport cross sections. The Table 2 data indicates that the ^{235}U fission neutron spectrum by itself - before transport uncertainties are introduced - is responsible for a 7% uncertainty in the $^{63}Cu(n,\alpha)$ reaction rate in the neutron spectrum for the ^{235}U fission standard field.

9.6 Consistency of the Palisades Analysis With Other Available Data

The BNL radiation transport calculation appears to have confirmed the fidelity of the Palisades radiation transport methodology. Palisades also went to AEA O'Donnell Inc. and had a Monte Carlo calculation performed with the MCBEND code. This analysis also confirmed the Palisades transport analysis. The AEA work went further. They also used an adjustment methodology to obtain "best estimate" fluence values for the accumulated neutron fluence. These adjusted fluence values, produced with the SENSAK least squares code, were in good agreement with the Palisades FERRET analysis. This seems to indicate that Palisades has not made any gross errors in the application of the least squares methodology.

9.7 Summary of Calculation/Least Squares Consistency

So, the conclusion here is that the Palisades "best estimate" approach is not in serious conflict with the calculated fluence - certainly not in enough conflict to question the CPC/W results without making a definitive statement on what is lacking or in error with their approach.

10. Dosimetry vs. Risk Analysis

The NRC response to the Palisades' least squares methodology suggests that they are not willing to accept a M/C bias factor less than unity. If this is the case, then this is a decision based on factors other than technical dosimetry or spectrum adjustment issues and the NRC position should be clearly stated. If this is a correct statement regarding the NRC position, then their position may be defensible if their arguments involve risk reduction issues. It is important for the planning of future Palisades' activities that the NRC position be properly understood.

Due to issues unrelated to technical dosimetry and spectrum adjustment methods, the NRC may decide that the PTS screening criteria should not use a "best estimate" fluence that is always based on the calculated fluence. Regulatory Guide 1.99 Rev. 2 and ASTM standard E-900, *Standard Guide for Predicting Neutron Radiation Damage to Reactor Vessel Materials*, make it clear that "in the absence of surveillance data for a given reactor (see practice E-185), the use of calculative procedures will be necessary to make the prediction." E-900 also states that "The fluence, '*f*,' is the calculated value of the neutron fluence at the inner surface of the vessel at the location of the postulated defect." The question becomes whether a "calculated value of the neutron fluence" means specifically the radiation transport calculated value, or if it includes a calculative approach, such as the least squares methodology, that results in a "best estimate" neutron fluence. E-900 also states that "When surveillance data for the reactor in question are available, 4.1.1 (Mean Shift at Vessel Inner Surface) may be used to supplement that data and improve its application to the reactor in question." It seems clear that surveillance data should be used to improve the application of the PTS rule. The question then becomes if the surveillance data to be considered are restricted to the determination of the "chemistry factor" or if surveillance data from the dosimetry capsule should also be used to aid in the fluence determination. If the NRC holds that calculated fluence estimates from radiation transport codes always take precedence over a statistical treatment that includes experimental measurements, then there is no advantage (with regard to the application of the PTS screening criteria) to ever having surveillance capsule dosimetry. This would be a sorry state and would not increase my confidence in the accumulated pressure vessel neutron fluence estimates. As a theorist who routinely performs radiation transport calculations (both discrete ordinates and Monte Carlo), I always desire to benchmark my calculation against available measured data. This comparison with actual measurements is not typically easy nor cheap to accomplish, but it should always be encouraged.

The question of how conservative an approach the NRC should take in accepting the accumulated fluence is beyond the scope of this review and beyond the expertise of this reviewer. The Palisades approach uses a "best estimate" fluence. The least squares approach uses all available input data and it produces an uncertainty of the fluence estimate. Should Palisades add a one sigma (~67% confidence) uncertainty to their "best estimate"? Should they add three sigma (~99% confidence) to their estimate? The typical approach to implementing the PTS rule is to use a calculated fluence value from a radiation transport code, not the calculated value plus one or two sigma. The ASTM E-900 and the Regulatory Guide 1.99 appear to support the use of "best estimates" for user input values. The PTS

rule appears to be based on "best estimate" fluence values and the required conservatism on the pressure vessel embrittlement has been built into the screening criteria.

From a dosimetry standpoint, any M/C reaction rate ratio should be permitted just so long as it reflects a "best estimate" derived from a statistically proper combination of input data and associated uncertainty estimates. This position is consistent with the image I have of the Palisades fluence estimation methodology.

A possible NRC position is that a least squares methodology for the fluence estimation is permitted, however, the "best estimate" fluence must employ a sensitivity analysis to relate the neutron spectrum at the location of the surveillance capsule measurements to the neutron spectrum at the location of the critical weld (at the inner wetted surface of the PV) subject to the PTS rule. This would represent a very defensible position and, if this statement reflects the NRC position, then it provides some direction for future Palisades activities. Various approaches to a sensitivity analysis could be employed to respond to this requirement. The most complete response would be to perform a least squares analysis with the LEPRICON [Ma85, Ma86] methodology.

11. Experimental vs. Calculated Neutron Spectrum

The community consensus, as reflected in ASTM standards, encourages the combination of calculated trial spectra with experimental measurements made at the location of interest. The experimental data are considered to be very important. In fact, the ASTM E-1854 "Standard Practice for Ensuring Test Consistency in Neutron-Induced Displacement Damage of Electronic Parts," in addressing the facility requirements for experimenters in research reactor irradiations, states that the

> **"spectrum determination shall be derived with a methodology that gives appropriate weight to experimental measurements. ... A free-field spectrum based solely upon neutron transport calculations is not acceptable."**

In summary, I would give very strong weight to experimental measurements in any spectrum determination. The key question is how to relate the neutron spectrum at the measurement location to the spectrum at the position to be characterized. The Palisades methodology appears to be consistent with the community-consensus approach as detailed in ASTM E-853 *Standard Practice for Analysis and Interpretation of Light-Water Reactor Surveillance Results* and E-944 *Standard Guide for Application of Neutron Spectrum Adjustment Methods in Reactor Surveillance.*

12. Spectrum Adjustment Methodology

I frequently use the SAND-II iterative unfolding code [Gr94] and the LSL-M2 least squares spectrum adjustment code [St85] in spectral determinations. I have an operational version of the STAY'SL code [Pe77a], but do not use it routinely. I have not used the FERRET code, but this code has been properly benchmarked and compared with other least squares approaches [Sc78, Wo81].

There has been much discussion about the use of log-normal distributions (as in FERRET) as opposed to normal distributions [Ti88, Sc78, Wo81]. There are advantages and disadvantages to either approach. There is not an intrinsic problem with the FERRET use of log-normal distributions. "The log-normal distributions provide a suitable way to specify the *a priori* knowledge of a physical quantity that is known to be positive." [Sc78] Care must be taken in applying the proper interpretation of the uncertainty measured when a log-normal distribution is used, that is, the uncertainty refers to the variation in the log-normal variable, but the approach is very sound and has practical value in avoiding negative fluence adjustments.

If one produces bias factors by forming the ratio of a calculated and measured reaction rate, the selection of the reaction to be used can represent an arbitrary or biased selection. The use of a least squares methodology specifically avoids any arbitrary or biased approach to the fluence estimation. As Wootan [Wo81] points out "Subjectivity in the FERRET algorithm does not appear since it has a rigorous mathematical foundation that leads to a unique, most likely, solution and uncertainty."

Various implementations of the least squares methodology exist in codes such as LSL-M2 [St85], FERRET [Sc78], SENSAK, BME-ECN [Sz95a], and STAY'SL [Pe77a]. Although the least squares methodology is employed in classical statistics, the least squares methodology also arises from Bayesian approaches and from the principle of maximum entropy. Codes that were developed from the Bayesian approach to least squares unfolding include MIEKE [No94], ENTROPY [Ma92], MEM [It89], and BASACF [Ti88]. The details of the metric that is optimized varies from code to code. A formulation of the general least squares algorithm can be found in Reference [Sz95b]. Some codes are capable of treating a more general least squares minimization than others and the options to input information on the correlation between input variables differs between codes. In general intercomparisons of these codes have shown that they all produce consistent results when similar input parameters are used. The International Atomic Energy Agency (IAEA) sponsored testing of the consistency of the least squares neutron spectrum adjustment codes in the REAL-80 [Zi84] and REAL-84 [Zi89, Go89] exercises have confirmed this.

The ASTM E-944 standard notes that "the results of any adjustment procedure can be only as reliable as are the input data." A key to a proper spectrum adjustment is proper characterization of the uncertainties and correlations for the input data. The inputs generally consist of an *a priori* neutron spectrum and associated covariance matrix, a set of measured reaction rates and uncertainties, a set in energy-dependent cross section for all the reactions considered and the associated covariance matrix, and the specification of the

correlation between these input values. Reaction rate measurements are routine and have easily determined uncertainty estimates. The reaction rate uncertainties have been confirmed by round robin testing at various laboratories. The correlations between the individual reaction rates are more difficult to determine and require detailed inputs about the radiation metrology laboratory's counting technique. In general, the reaction rates and the cross section uncertainties are well characterized, the problem is the uncertainty and covariance matrix for the input trial spectrum. The Palisades approach to the spectrum input covariance is typical of that used in the community - but it is an issue that needs more discussion. Appendix A presents the mathematical foundations for the least squares approach. The following sections address the details of the implementation of the spectrum adjustment methodology including the *a priori* spectrum covariance matrices, the energy bin structure used in the discrete ordinates radiation transport calculation, the weighting function used to collapse the cross sections into the energy bin structure, and the smoothness of the calculated or adjusted neutron spectra.

12.1 Input Spectrum Covariance Matrix

I think that the Palisades spectrum uncertainty values are reasonable, but they use a spectrum correlation function with a different form than that which I typically employ in my work with the LSL-M2 code. I typically consider the spectrum to be composed of at least three components; a fast fission spectrum, a 1/E scatter component, and a thermal Maxwellian tail. I usually ensure that the fast fission component is not strongly correlated over the breakpoint where the 1/E scatter component matches up with the fast fission component. The fast fission component is strongly correlated within its own energy region, as is the 1/E scattering component. I am concerned that the Palisades strong spectrum correlation extends lower than the energy where this breakpoint occurs for the cavity spectra. This concern is summarized by Perey in Reference [Pe77c] when he states that "It should also be clear now that any structure we have in our input spectrum in energy regions where the evaluations state that the spectrum is fully correlated is reproduced in our solution exactly."

Figure 5 shows the Palisades calculated 47-group spectra for the W290-9 cycle 9 irradiation surveillance capsule position, the ex-vessel 16 degree cycle 9 irradiation dosimetry position, and the critical weld position (first octant equivalent 30 degree position at the reactor vessel clad/base metal interface) from the cycle 9 irradiation. Figure 5 also shows, for comparison purposes, a 640-group representation of the ENDF/B-VI ^{235}U thermal fission neutron spectrum. All of the spectra in Figure 5 are renormalized so that the high energy part of the spectra are comparable. This figure shows that the cavity dosimetry neutron spectrum deviates from the pure fission spectra below about 6 MeV. The Palisades NRC submittal (page 24 of Attachment 1 of Enclosure 1, Consumers Energy Submittal Dated June 12, 1996) indicates that all fluence bins above 5.5 keV have a short range correlation with a range of γ=6 groups and a fairly strong correlation strength of Θ=0.9. I feel that this is too strong a correlation over the region where the pure fission part of the spectrum transitions to the 1/E behavior.

At the same time that I question the baseline spectrum covariance data used for the Palisades trial spectrum, I note that Palisades investigated, in response to RAI issue 3.5, the effect of varying this covariance matrix (page 29 of the above mentioned Attachment 1 of Enclosure 1). Their work, documented in Table 3.4-1, indicates only a ~3% variation (increase) for the fluence greater than 1-MeV, Φ(E>1 MeV), for the surveillance dosimetry position and ~5.6% variation (decrease) for the Φ(E>1 MeV) in the ex-vessel dosimetry spectrum. This investigation of the sensitivity of the input covariance matrices appears to put to rest any concern I had about the effect of the input spectrum covariance matrix unduly biasing the least squares adjusted spectrum.

The Palisades response to the NRC questions on the effect of variations in the uncertainties (RAI 3.6) neglected to address one aspect of the uncertainty used in the FERRET calculation, namely the variation in the uncertainty assigned to the input trial spectrum. The response addressed variation in the input spectrum correlation matrix, the cross section and activation uncertainty values, but not the input spectrum uncertainty. The variation in the spectrum covariance function only addressed the correlation or off-diagonal part of the matrix, not the magnitude of the diagonal elements. If the calculated *a priori* spectrum uncertainty is too large, it allows the activities to have more weight in the adjustment. Although this variation should be investigated, the Palisades spectrum uncertainty allocation is reasonable, in my estimation. The reactor radiation transport and spectrum determination community generally accepts about a 20% variation in calculated spectrum-averaged quantities. The energy-dependent uncertainty assigned to the high energy part of the spectrum in the Palisades analysis, about 30%, is not uncommon when a realistic correlation matrix is used. This observation is based on my experience that the properly propagated uncertainty using the actual correlation matrix with off-diagonal elements is about one half of the simple spectrum-averaged uncertainty obtained using only the diagonal elements.

12.2 Rebinning of Calculated Spectrum

The Palisades NRC submittal indicates that they use the SAND-II spline-fitting procedure to rebin the 47-group calculated spectrum into a 620-group spectrum which is then collapsed into a 53-group FERRET-compatible spectrum. If they used the options available in the normally Radiation Safety Information Computational Center (RSICC) distributed version of the SAND-II code, and Palisades has indicated that they use the normal SAND-II code, then I have sometimes seen a bias introduced in the high energy part of the spectrum due to a coarse input spectrum when differential fluences are positioned at the midpoint energy of the bin. To investigate the potential bias this rebinning may have on the spectrum-averaged cross sections computed by the SAND/FERRET methodology I have used the neutron spectra from the W290-9 surveillance dosimetry location shown in Figure 5 and examined some basic metrics under various rebinning scenarios with the SAND-II code. Figures 6 and 7 show that the various energy bin representations of the spectrum are virtually identical when examined in either linear energy space or logarithmic energy space, as they should be. Table 5 shows the variation in some basic spectrum-averaged metrics produced by various energy-group binning of the same W20-9 initial

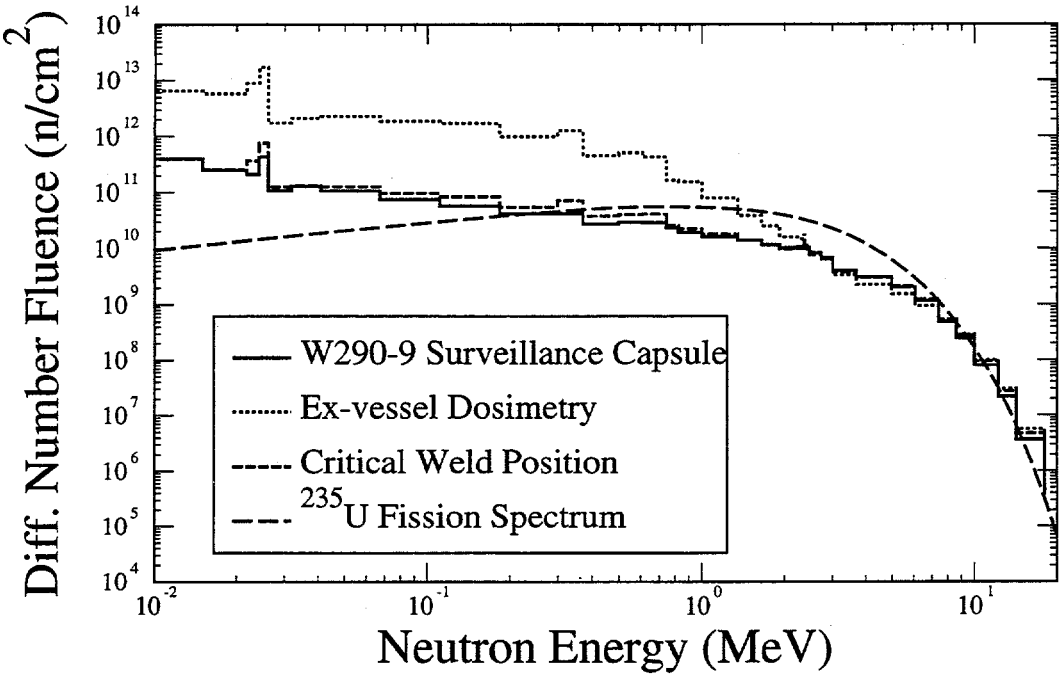

Figure 5: Comparison of Palisades 47-Group Calculated Neutron Spectra with ^{235}U Fission Spectrum

neutron spectrum. The variation in the metrics is seen to be about 1%. This indicates that the energy rebinning is not a source of concern for the Palisades least squares methodology.

Table 5: Effect of Rebinning on Spectrum-Averaged Metrics

Spectrum-Averaged Metric		Neutron Spectrum for W290-9 Location			
		47-Grp. BUGLE Calculation	**640-Grp. Spline Fit of 47-Grp.**	**620-Grp. Palisades Spectrum**	**53-Grp. Palisades Spectrum**
1	Average Energy (MeV)	**0.6843**	**0.6851**	**0.6817**	**0.6866**
2	Φ_{tot}	**1.701×10^{11}**	--	**1.7×10^{11}**	**1.7×10^{11}**
3	$\Phi(E>1\ MeV)/\Phi_{tot}$	**0.2031**	**0.2048**	**0.2035**	**0.2043**
4	$\Phi(E>0.1\ MeV)/\Phi_{tot}$	**0.3724**	**0.3754**	**0.3727**	**0.3727**
5	$^{58}Ni(n,p)^{58}Co$ Xsec. (b)	**0.3618×10^{-1}**	**0.3644×10^{-1}**	**0.3640×10^{-1}**	**0.3635×10^{-1}**
6	$^{54}Fe(n,p)^{54}Mn$ Xsec. (b)	**0.2782×10^{-1}**	**0.2802×10^{-1}**	**0.2800×10^{-1}**	**0.2795×10^{-1}**
7	$^{63}Cu(n,\alpha)^{60}Co$ Xsec. (b)	**0.3139×10^{-3}**	**0.3196×10^{-3}**	**0.3175×10^{-3}**	**0.3149×10^{-3}**

All foldings with cross sections are performed using NJOY94-collapsed cross sections produced from the ENDF/B-VI cross sections

12.3 Spectrum-Collapsed Cross Sections

Another consideration in evaluating the adjustment methodology is the energy bin structure of the response functions. The response function is affected by the weighing function used to collapse the ENDF/B-VI cross section. For fine-group cross sections the effect of the

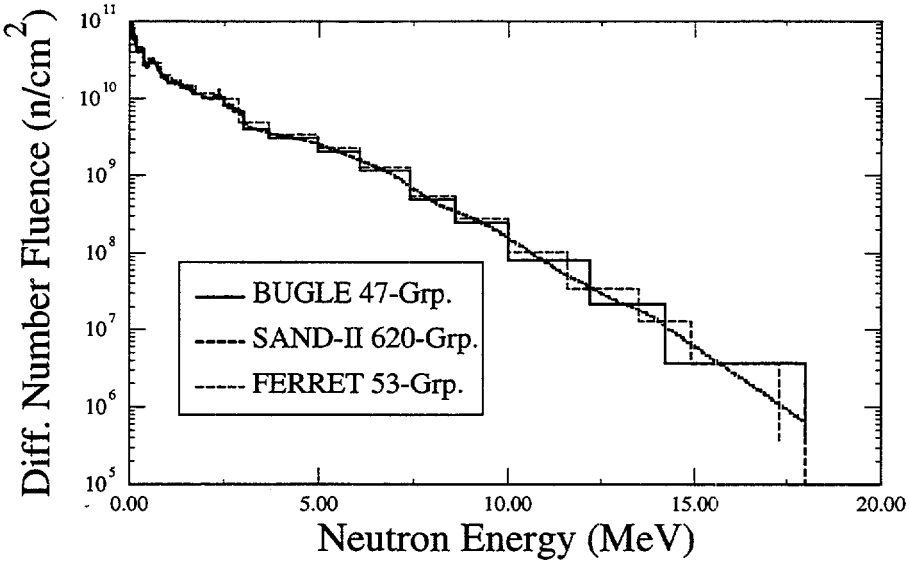

Figure 6: A Linear Energy Comparison of Three Representations of the W290-9 Calculated Spectrum

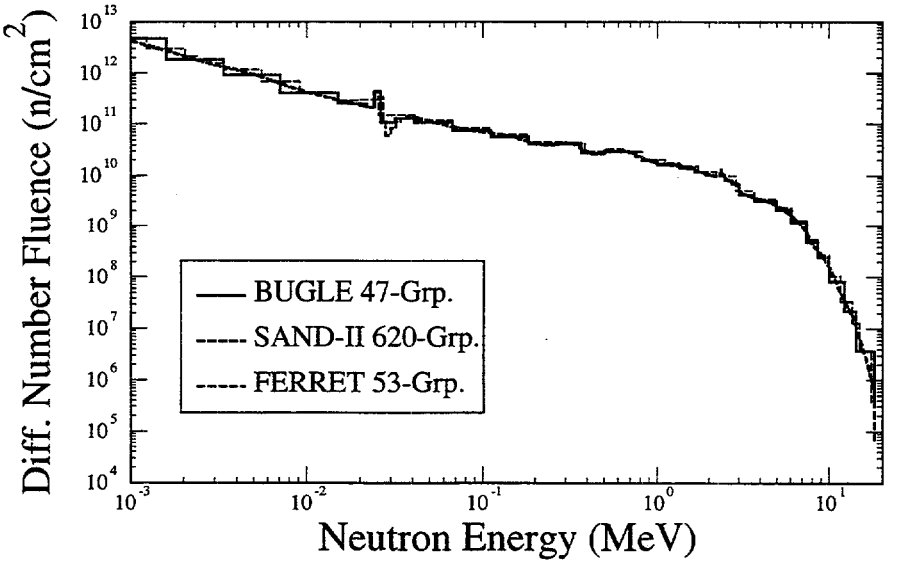

Figure 7: A Logarithmic Energy Comparison of Three Representations of the W290-9 Calculated Spectrum

collapsing function is minimal. For a coarse-group energy structure the effect of this cross section collapsing should be investigated.

The author is currently investigating the effect of various energy bin structures and collapsing weight functions on the spectrum-averaged cross section for dosimetry reactions. For the W290-9 in-vessel surveillance capsule neutron spectrum the effect of the collapsing function appears to be rather small. Data will be reported later to quantify the importance of the collapsing/weighting function.

Although the examinations I have conducted with the W290-9 surveillance capsule neutron spectrum have not shown a strong influence of the weighting function used to collapse the cross sections, work on some previous benchmark has indicated that this can be a concern for deeper penetration spectra. Analysis of the Winfrith Iron Benchmark reported in the BUGLE-93 validation documentation [In95] shows that changing the weighting function from the standard weighting to the iron self-shielded function for the ^{115}In(n,n') and ^{103}Rh(n,n') reactions can result in changes in the C/E ratios for the fine-group VITAMIN-B6 cross sections of 14% and 22%, respectively, at the 20.32-cm location and of 28% and 113%, respectively, at the 35.56-cm location. For these same cases, the ^{32}S(n,p) C/E ratio is only changed by about 3-4%. This suggests that the high energy fluence [> 3-MeV as indicated by the ^{32}S(n,p) reaction] is not sensitive to the cross section collapsing algorithm, but that the low energy fluence [> 0.5-MeV as indicated by the two (n,n') reactions] may be very sensitive to the spectrum used in the cross section collapsing algorithm. The C/E ratios for the neutron flux (from 7.1 keV to 4.72 MeV) from the Winfrith Iron Benchmark indicate that the change in the collapsing function can be 14% and 50% at 20.32-cm and 50.8-cm, respectively. These iron benchmark results leave the influence of the cross section weighting function on the greater than 1-MeV fluence regarded as suspect but not clearly established.

The NESDIP2 Radial Shield and Cavity Experiment [Sl94b] indicates that the 36-keV to 10-MeV neutron fluence is changed by 13.5% when the zone-weighting rather than concrete weighting functions are used to collapse the cross sections in the BUGLE-93 cross section energy grid. In this benchmark, again, the ^{32}S(n,p) C/E ratio shows very little change resulting from the influence of the cross section weighting function, even at deep penetration. The ^{115}In(n,n') and ^{103}Rh(n,n') C/E ratios show significant changes (~11% and 17%, respectively) only at deep penetration (z=91.5-cm, r=0-cm).

Work with the Czech Republic Iron Sphere Benchmark Experiment (NRI) [Ga94] indicates that for this 23-cm sphere leakage experiment using a ^{252}Cf fission neutron source, the calculation underpredicts the high energy leakage, but overpredicts the 1-MeV leakage. The C/E ratios are 0.862, 0.603, 0.503, 1.374, 0.930, and 1.224 for upper energies of 12.2, 5.22, 4.07, 3.01, 2.02, and 1.00 MeV, respectively.

It is my impression that the BUGLE-93 transport cross sections were used in both the Palisades and the BNL radiation transport calculations. The Oak Ridge work on BUGLE-

96 [Sl94a] concludes that "the original BUGLE-93 library Fe data called '1/4-T weighted' is not shielded appropriately for RPV fluence calculations. The new Fe data in the BUGLE-93 library called 'CS-weighted' and 'SS-weighted' Fe is recommended." This observation leads me to wonder which BUGLE-93 Fe cross section was used in the Palisades fluence analysis. This sensitivity to cross section processing details also leads me to be suspicious of any transport calculations which are not directly supported by calculated reaction rate measurements.

12.4 Smoothness of Calculated/Adjusted Neutron Spectra

From my experience with spectrum determination, using iterative and least squares methods as well as Monte Carlo calculations, I have found that it is very helpful to examine the differential number and differential energy spectrum representations for the presence of artificial structures that are artifacts of the calculational methodology. Figure 5 showed the differential number representation of the various calculated spectra from the dosimetry positions. The only feature of note in this figure is the 25-keV transmission window that is well known to result from a notch in the iron cross section and, as such, is not an artifact of the spectrum determination process.

Figure 8 shows the differential energy representations of the same spectra. Note that the curves in this figure are arbitrarily normalized so that the high energy parts of the spectra overlap. There are no obvious artifacts in the spectral representations that would indicate a problem with the calculated spectrum determination. The ex-vessel calculated neutron spectrum exhibits a change in behavior below about 3-MeV. The cause of this change in behavior is not clear to the author, but the calculated neutron spectra are smooth enough so as not to raise any overriding concern about the fidelity of the calculation. The differential energy representation shows that the surveillance capsule calculated neutron spectrum is nearly identical to the calculated spectrum at the critical weld position. However, one can see very significant shape changes between the spectral shape at the ex-vessel dosimetry location and that at the critical weld. This is a matter of concern that will be addressed in Section 14.

To be consistent with this analysis, the FERRET adjusted spectrum should be subjected to the same inspection. Figure 9 shows the differential energy representation of the W290-9 53-group FERRET adjusted spectrum in logarithmic energy space. Again no unusual artifacts are seen. The FERRET adjusted spectrum is practically indistinguishable from the calculated spectrum when viewed in logarithmic energy space. Some difference is seen near the 25-keV transmission window in iron. The BUGLE calculated spectrum has a more well defined transmission peak, partly due to the fact that the BUGLE energy structure was designed to address this transmission window. A transmission window near 2.5-MeV is also seen in the calculated spectrum. This window is not seen in the adjusted spectrum, but this could, again, be attributed to the energy bin structure. The exact cause of this 2.5-MeV window is not know to the author, but the transmission corresponds to a very small energy bin in the BUGLE cross sections that was presumably placed in the energy bin structure to accommodate some feature of the reactor pressure vessel cross sections.

Figure 10 shows the same neutron spectra in linear energy space. The difference between the calculated and FERRET-adjusted spectrum is still small in this figure. The difference is seen between about 3-MeV and 1-MeV. This adjustment behavior is consistent with the least squares methodology. The *a priori* neutron spectrum can only be adjusted in regions where there are reaction rate data to force an adjustment. To resolve the discrepancy between the $^{64}Cu(n,\alpha)$ and $^{58}Ni(n,p)$ & $^{54}Fe(n,p)$ reactions, the spectrum adjustment is made below the $^{64}Cu(n,\alpha)$ threshold and only extends through the $^{58}Ni(n,p)$ & $^{54}Fe(n,p)$ thresholds in so far as is demanded by the stiffness of the spectrum correlation function. One can also see from the figure that the difference between the transport spectrum and the least squares adjusted spectrum is small relative to the radiation transport modification on the ^{235}U source fission neutron spectrum.

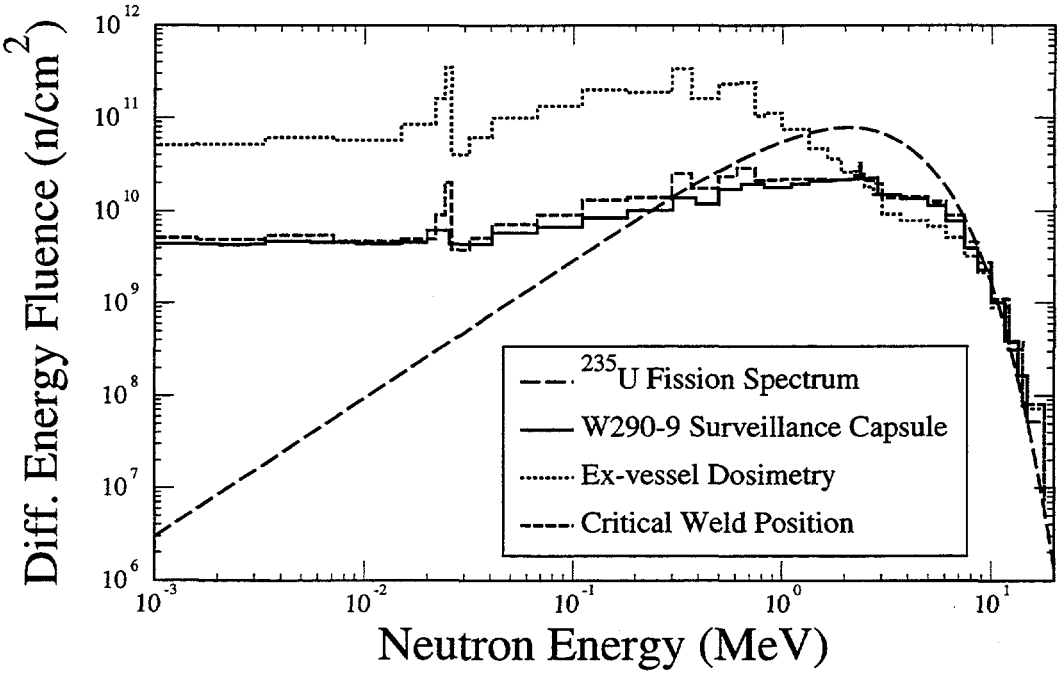

Figure 8: Differential Energy Representation of the Neutron Environment at the Calculated Dosimetry Positions

13. Location of Surveillance Dosimetry and the Limiting Weld

The surveillance capsule dosimetry is the closest measurement one has to the environment at the limiting weld - so these data should be used. But one should confirm the legitimacy of this approach by showing that the calculated spectra at these locations are very similar in shape. Figure 5 shows that the neutron spectra at the surveillance capsule position and at the inner wetted surface of the critical weld for the pressure vessel are virtually identical.

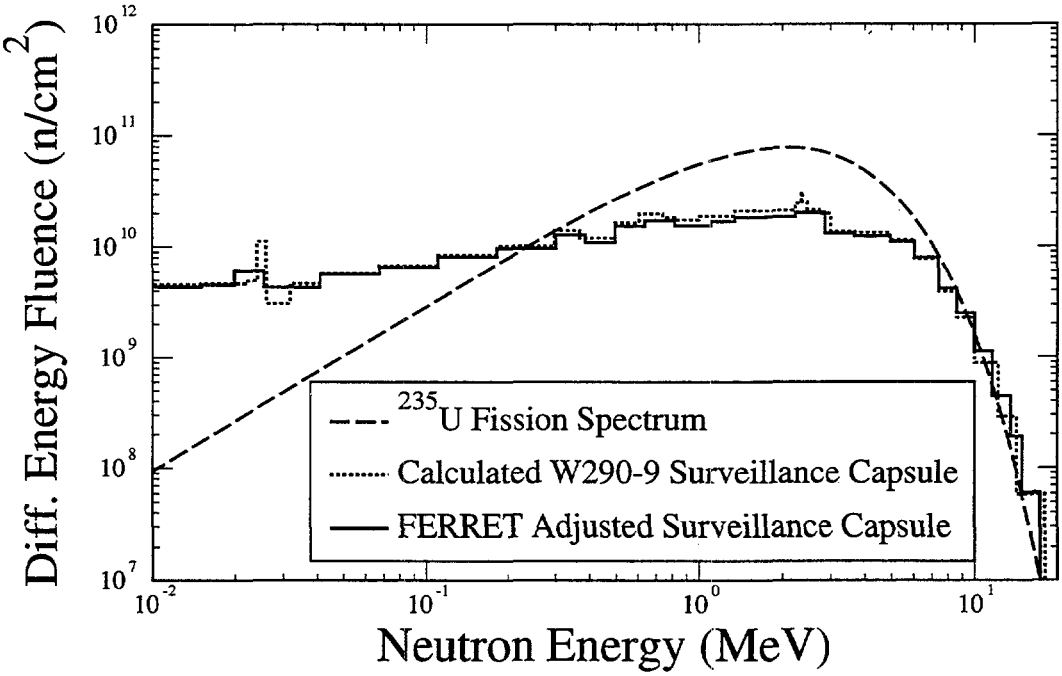

Figure 9: Logarithmic Differential Energy Representation of FERRET-Adjusted Neutron Environment at the Surveillance Capsule Location

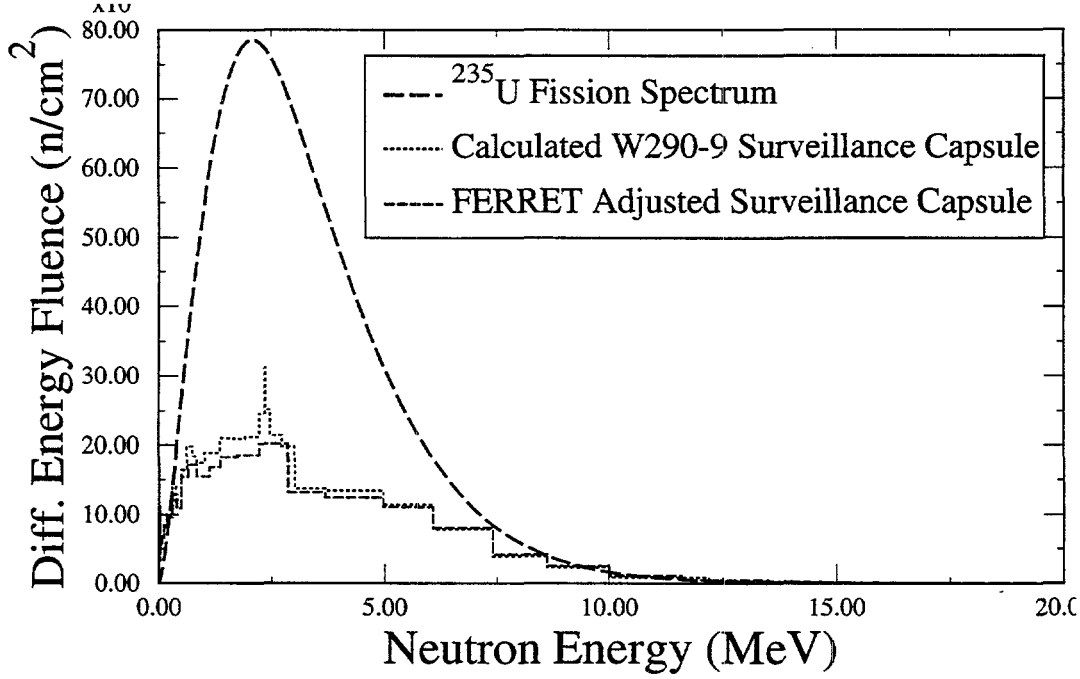

Figure 10: Linear Differential Energy Representation of FERRET-Adjusted Neutron Environment at the Surveillance Capsule Location

The agreement is so exact that one could easily dismiss the need for any further sensitivity analyses to confirm the equivalence of using an adjusted spectrum **at the surveillance location** to represent the actual critical weld neutron spectrum.

One piece of data in the Palisades' submittal does raise some concern about this equivalence of spectra. The Tables 4.1-5 thru 4.1-15 on page 4-11 thru 4-21 compare the azimuthal variation in the neutron spectrum. These tables show a 13% variation in the $\phi(E>0.1)/\phi(E>1.0)$ metric at 20 degrees - the location of the surveillance capsule. This possible variation between the spectra at the surveillance capsule and at the critical weld is a concern. A variation in the clad-base metal fluence ratios (greater than 0.1 MeV divided by greater than 1-MeV) at the azimuthal position of the surveillance capsule raises a question about the deviation of the neutron spectrum induced by the presence of the surveillance capsule. If the spectra are not very close in shape, then it is legitimate to request that a statistical correlation be established between the two calculated spectra with a sensitivity analysis. I am not sure how to reconcile this deviation in the azimuthal symmetry with the good agreement between the calculated spectra at the surveillance capsule and that at the critical weld, as depicted in Figure 5.

14. In-vessel and Ex-vessel Bias Factors

The Palisades methodology appears to involve calculating a bias factor at all surveillance capsules and at the ex-vessel cavity dosimetry locations and averaging the bias factors to get a "best estimate" for the bias factor at the location of the critical weld. The NRC brings up a very valid concern when they question the weight given the cavity dosimetry bias factor. The Palisades approach of considering all the dosimetry is only valid if one can establish a strong correlation between the neutron spectrum and flux at the dosimetry locations and at the critical weld locations. This correlation was not substantiated in the Palisades supplied material.

Figures 5 and 8 show plots in differential number and energy space of the in-vessel and ex-vessel calculated spectra as well as the calculated neutron spectrum at the critical weld location. These plots agree with the trend I have seen in other sources [He93]. Significant spectral shape differences are seen between the in-vessel and ex-vessel spectral shapes. One can argue that the calculated spectrum at the critical weld location is virtually identical to that for the surveillance capsule, and thus is strongly correlated. But this argument can not be extended to include the ex-vessel cavity dosimetry.

The use of the cavity dosimetry bias factors requires that Palisades establish a correlation between the spectrum at the critical weld and at the cavity dosimetry location. One can do this with adjoint discrete ordinates radiation transport calculations or with the perturbation feature in the MCNP Monte Carlo code. This sensitivity study does not have to be as detailed as that provided by the LEPRICON code. Several packages exist that will assist in a sensitivity study that varies dimensions and cross sections. Packages to consider include FORSS [Lu81], SUSD [Fu88], SENSIT-2D [Em82], and SWANLAKE [Ba73].

In the absence of this sensitivity analysis to correlate the two spectra (and hence the bias factors) I suggest that Palisades only use the bias factors from the surveillance capsule locations. The consistency of the bias factor at the surveillance capsule positions needs to be examined. An examination of the Palisades Table 7-1.1 on page 7-3 suggests that this approach might change the average "best estimate" bias factor from 0.831 +/- 0.067 to 0.8345 +/- 0.013. This is not a significant change to the Palisades request, but it avoids some difficult questions about the application of the cavity dosimetry data. The only drawback associated with this approach is that it reduces the dataset of bias factors to four values.

14.1 Consistency of Spectrum Adjustments for Capsule Positions

An inspection of the bias factors and the reaction rate ratios for the surveillance capsule dosimetry data provided in the Palisades distributed material (Section 5: Evaluation of Surveillance Capsule Dosimetry) provides insight into the consistency of the surveillance capsule data. Consistency in these data is a requirement if one is to have confidence in the Palisades least squares adjustment methodology. Table 6 shows the FERRET least squares adjusted bias factors and the high energy to low energy ratios of the reaction rate data. The table shows excellent consistency (~2%) in the adjustment factor for the fluence greater than 1-MeV produced by the FERRET least squares methodology but the standard deviation in the measured reaction rate data appears to contradict all previous comments about the consistency of the measured data. An inspection of Table 6 shows that the reaction rate ratio discrepancy is restricted to the A240 capsule data. Closer inspection of the Palisades discussion of the surveillance capsule dosimetry reveals while most dosimetry data were read by Westinghouse using the procedures detailed in the submittal, radiometric counting for the A240 capsule data was performed by the Battelle Memorial Institute and, in this case, "the measured specific activities were not reported." Instead, the "Capsule A240 reaction rates were developed directly from the derived neutron flux and spectrum-averaged reaction cross sections reported in Reference 4," a citation by Perrin in report BCL-585-12 dated March 13 1979. These data suggest that the developed "measured" data reported in the Section 5 data for capsule A240 are not correct. It may be that the neutron flux used to develop the "measured" reaction rate data incorporated the M/C adjustment. Palisades should sort out this discrepancy in the NRC-submitted material. If the discrepancy can not be resolved, then the NRC is justified in questioning the consistency of the measured surveillance capsule data. If the A240 capsule measured data are ignored (this is not an arbitrary decision, the rationale for this decision was detailed in the previous sentences) then the reaction rate ratios are very consistent (within the reported dosimetry uncertainty values of ~5%).

A previous recommendation was made to only consider spectrum adjustment factors based on the measured dosimetry at the surveillance capsule location, and not, in the absence of a sensitivity analysis, at the ex-vessel cavity dosimetry locations. It is valid to inspect the consistency of the ex-vessel cavity dosimetry consistency in evaluating the fidelity of the Palisades reaction rate measurements. Table 7 shows the consistency of the ex-vessel cavity dosimetry reaction rate ratios. Clear differences are seen between the dosimetry for

capsules at the core midplane and at the core bottom. This is not surprising and fits with the expectations from the radiation transport calculations. The Cycle 10/11 Capsule S $^{58}Ni(n,p)$ reaction rate is very anomalous, deviating by over 10 sigma. I suspect that the data provided has a typographical error. An impartial statistical treatment of outliers will support dismissing this point from the analysis of data consistency, but I suggest that Palisades investigate the cause of the data discrepancy for this reaction/capsule. When the Capsule S data are ignored the dosimetry measurement data are seen to be very consistent. The expected midplane standard deviation is about 2.6%. This is consistent with the guidance provided by the ASTM standards and is significantly less than the 5% assumed in the Palisades analysis. The standard deviations for the core bottom data are also consistent with expectations. The observed 6-7% standard deviation is larger than the 5% Palisades uncertainty value for the reaction rate data, but this not disturbing when one considers that the core bottom dataset consisted of only four elements.

It is very important in making statements on the consistency of experimental reaction rate measurements that one does not include uncertainties from other sources than the measurements. In the above analysis I examined ratios of high and low energy activation reactions in order to eliminate the sensitivity to the actual source irradiation time and to the exact location of the dosimetry capsule. I wanted to isolate the uncertainty contributions which arise uniquely from the foil measurement technique. This is also why I separated the core bottom dosimetry locations from the core midplane results. If one looks at ratios of C/M values rather than ratios of activities, then one can infer **nothing** about the consistency of the experimental dosimetry measurements. The variations in the calculational model details and in the vintage of the transport cross sections far outweigh the variation in the actual reaction rate measurement process. The other sources of uncertainty that affect the application of the resulting reaction rate data, such as irradiation time and location of the dosimetry capsule, should be considered only when one attempts to use the fluence at the dosimetry location to infer the fluence at the critical weld position. These uncertainty sources should not be confused with the reaction rate uncertainty.

To further check the consistency of the spectrum adjustment at the surveillance capsule locations, I recommend that Palisades select one position and use FERRET to produce an adjusted spectrum, then use this adjusted spectrum (with the adjusted covariance matrix) as the trial function in the adjustment of the spectra for the other surveillance capsule positions. If the FERRET least squares adjustment was valid and the deviation from the calculated DORT spectrum represents a systematic cross section problem in the radiation transport calculation, then the subsequent FERRET adjustments should result in very small additional adjustments.

Note that this recommended approach to an excursion FERRET calculation is not entirely justified from a statistical standpoint since the reaction rate measurements at the surveillance capsule positions are strongly correlated (for a given reaction) and influence the adjusted spectrum. The second adjustment fails to account for the correlation between the reaction rates and the new trial spectrum. Thus I do **NOT** suggest that this approach replace the normal FERRET operation. I only suggest the application of this approach to

Table 6: Consistency of the FERRET Adjustment at the Surveillance Capsule Position

Surveillance Capsule		FERRET Φ(E>1-MeV) Adjustment	Unadjusted Reaction Rate Ratio	
			$^{58}Ni(n,p)/^{63}Cu(n,\alpha)$	$^{54}Fe(n,p)/^{63}Cu(n,\alpha)$
1.	A240 cycle 2, 1/78	0.855	140.64	112.27
2.	W290 cycle 5, 8/83	0.842	106.32	81.05
3.	W110 cycle 10, 6/93	0.827	100.70	74.83
4.	W290 cycle 9	0.817	102.60	79.21
Standard Deviation of Data (all data)		2.0%	16.76%	19.75
Standard Deviation of Data (capsules 2, 3, and 4)		1.52%	2.77%	4.08%

Table 7: Consistency of the FERRET Adjustment at the Ex-vessel Cavity Dosimetry Positions

Ex-vessel Cavity Dosimetry Location		Unadjusted Reaction Rate Ratio	
		$^{58}Ni(n,p)/^{63}Cu(n,\alpha)$	$^{54}Fe(n,p)/^{63}Cu(n,\alpha)$
1.	Cycle 8, Capsule B	106.56	76.02
2.	Cycle 8, Capsule D	103.99	74.56
3.*	Cycle 8, Capsule E (bottom)	129.15	87.94
4.	Cycle 8, Capsule G	99.64	72.33
5.	Cycle 9, Capsule A	99.73	73.02
6.*	Cycle 9, Capsule C (bottom)	125.66	87.43
7.	Cycle 9, Capsule J	102.69	72.66
8.	Cycle 9, Capsule K	101.16	70.74
9.*	Cycle 9, Capsule L (bottom)	117.75	79.88
10.	Cycle 9, Capsule N	100.0	70.64
11.	Cycle 10/11, Capsule O	96.73	69.62
12.	Cycle 10/11, Capsule P	101.11	70.66
13.*	Cycle 10/11, Capsule Q (bottom)	112.21	75.65
14.	Cycle 10/11, Capsule R	98.18	71.31
15.*	Cycle 10/11, Capsule S	185.54	67.47
16.	Cycle 10/11, Capsule T	103.51	73.78
17.	Cycle 10/11, Capsule U	101.34	71.43
Standard Deviation of Core Mid-plane Data (all except Capsule S)		2.65%	2.6%
Standard Deviation of Core Bottom Data		6.3%	7.2%
The light shading corresponds to a core bottom position and is indicated with a *			
The dark shading corresponds to the Capsule S dosimetry which is suspected of a typographical error and is indicated with a *			

test the consistency of the spectrum adjustment at the surveillance capsule positions. When this step is performed, Palisades should report the M/C values for the reaction rates. A minimal deviation in the M/C from unity would be expected if the spectrum adjustment is consistent.

15. Conclusion

The NRC evaluation of the Palisades accumulated fluence methodology appears to reject the experimental reaction rate measurements since they conflict with the radiation transport calculations. In reality, when proper consideration is given to the uncertainty in the measurements and calculations, there is no true discrepancy. The NRC approach is to reject the measurements since the M/C ratios for the high energy reactions [$^{63}Cu(n,\alpha)^{60}Co$] conflict with the low energy reactions [$^{58}Ni(n,p)^{58}Co$ and $^{54}Fe(n,p)^{54}Mn$]. In truth, the variation in the M/C ratios can be easily ascribed to the uncertainty in the calculated reaction rates. The measured reaction rates are among the best and lowest uncertainty data available to support decisions on accumulated fluence. The use of the experimental data is beyond reproach; however, care must be taken in how the reaction rates are employed to make fluence estimates. Palisades does not and should not simply take ratios of measured and calculated reaction rates to make fluence estimates. This approach would be totally indefensible and the NRC would be correct in labeling any conclusion arbitrary. The Palisades approach, however, employes a rigorous least squares methodology that includes inputs from all available sources along with the associated uncertainty and covariance data. All of this information, not an arbitrary subset, is used in the Palisades approach to produce an accumulated fluence estimate. The methodology also provides an uncertainty for estimates of the least squares fluence.

In summary, the Palisades fluence estimate and approach are valid, defensible, and conform to the community consensus approaches as incorporated into the ASTM set of standards.

16. References

[Ba73] D. E. Bartine, et al., SWANLAKE, A Computer Code Utilizing ANISN Radiation Transport Calculations for Cross-Section Sensitivity Analysis, Oak Ridge National Laboratory, Oak Ridge, TN, report ORNL/TM-3809, 1973.

[Ca78] J. T. Caldwell, E. J. Dowdy, B. L. Berman, R. A. Alvarez, P. Meyer, Photonuclear Measurements on Fissionable Isotopes Using Mono-energetic Photons, Los Alamos National Laboratory, report LA-UR 76-161J, 1978.

[Ch86] S. Chatterjee, A. S. Hadi, "Influential Observations, High Leverage Points, and Outliers in Linear Regression," Statistical Science, Vol. 1, pp. 379-416, 1986.

[Dr77] J. B. Dragt, J. W. M. Dekker, H. Gruppelaar, A. J. Janssen, "Methods of Adjustment and Error Evaluation of Neutron Capture Cross Sections:

Application to Fission Product Nuclides," Nuclear Science and Engineering, Vol. 62, pp. 117-129, 1977.

[Em82] M. J. Embrechts, SENSIT-2D: A Two-Dimensional Cross-Section Sensitivity and Uncertainty Analysis Code, Los Alamos National Laboratory, Los Alamos, NM, report LA9515-MS, 1981.

[Fu88] K. Furta, Y. Oka, S. Kondo, SUSD: A Computer Code for Cross-Section Sensitivity and Uncertainty Analysis Including Secondary Neutron Energy and Angular Distributions, Oak Ridge National Laboratory, Oak Ridge, TN, report ORNL/TR-88/18, November 1988.

[Ga94] I. C. Gauld, H. McIlwain, G. R. Penner, "AECL Experience With Processing and Testing ENDF/B-VI For Shielding Applications," presentation to the Cross Section Evaluation Working Group meeting at Oak Ridge Tennessee on October 26, 1994 and published in the meeting minutes.

[Gn72] R. Gnanadesikan, J. R. Kettenring, "Robust Estimates, Residuals, and Outlier Detection with Multiresponse Data," Biometrics, Vol. 28, pp. 81-124, March 1972.

[Go89a] V. Goulo, "Role of Covariances in Reactor Dosimetry," Reactor Dosimetry: Methods, Applications, and Standardization, ASTM STP 1001, H. Farrar, E. P. Lippincott, Eds., American Society for Testing and Materials, Philadelphia, pp. 434-438, 1989.

[Go89b] R. Gold, "Neutron Fluence Determination For Light Water Reactor Pressure Vessels," Reactor Dosimetry, ASTM STP 1228, Harry Farrar IV, E. P.Lippincott, J. G. Williams, D. W. Vehar Eds., American Society for Testing and Materials, Philadelphia, 1994, pp. 104-113.

[Go97] R. Gold, "A Challenge to the International Reactor Dosimetry Community: Quantify Gamma-ray Spectra," Reactor Dosimetry, Proceedings of the 9th ASTM-EWGRD International Symposium, eds. H. Abderrahim, P. D'hondt, B. Osmera, World Scientific, September 1997.

[Gr93] P. J. Griffin, J. Kelly, T. F. Luera, J. VanDenburg, SNL RML Recommended Dosimetry Cross Section Compendium, Sandia National Laboratories, Albuquerque, NM, report SAND92-0094, November 1993.

[Gr94] P. J. Griffin, J. G. Kelly, J. W. VanDenburg, User's Manual for SNL-SAND-II Code, Sandia National Laboratories, Albuquerque, NM, report SAND93-3957, April 1994.

[Gr96] P. J. Griffin, "Comparison of Uncertainty Metrics for Calculated Dosimetry Activities," American Nuclear Society (ANS) Radiation Protection & Shielding Topical Meeting held in North falmouth, Massachusetts on April 21-25, 1996, Volume 1 of the proceedings, pp. 27-35.

[Gr97a] P. J. Griffin, "Comparison of Calculated and Experimental Dosimetry Activities for Benchmark Neutron Fields," Reactor Dosimetry, Proceedings of the 9th ASTM-EWGRD International Symposium, eds. H. Abderrahim, P. D'hondt, B. Osmera, World Scientific, September 1997.

[Gr97b] P. J. Griffin, J. G. Williams, "Least Squares Analysis of Fission Neutron Standard Fields," IEEE Transactions on Nuclear Science, Vol. 44, No. 6, December 1997, pp. 2071-2078.

[He93] J. L. Helm, Reactor Vessel Irradiation Damage: Absorbed Dose Estimation, Electric Power Research Institute, report EP 89-21, 1993.

[He97] C. R. Heimbach, "Gamma-ray Leakage From a Critical Assembly," Reactor Dosimetry, Proceedings of the 9th ASTM-EWGRD International Symposium, eds. H. Abderrahim, P. D'hondt, B. Osmera, World Scientific, September 1997.

[In95] D. Ingersoll, R. E. White, et al., Production and Testing of the VITAMIN-B6 Fine-Group and BUGLE-93 Broad-Group Neutron/Photon Cross-Section Libraries Derived from ENDF/B-VI Nuclear Data, Oak Ridge National Laboratory, report ORNL-6795, also NUREG/CR-6214, January 1995.

[Ke89] J. G. Kelly, "Neutron Spectrum Adjustment with SAND-II Using Arbitrary Trial Functions," Reactor Dosimetry: methods, Applications, and Standardization, ASTM STP 1001, Harry Farrar IV and E. P. Lippincott, Eds., American Society for Testing and Materials, Philadelphia, pp. 460-468, 1989.

[Ki94] S. Q. King, D. M. Gilliam, "Characterization of the Gamma Field in the B&W Owners Group Cavity Dosimetry Benchmark Experiment," Reactor Dosimetry, Proceedings of the Eighth ASTM-Euratom Symposium on Reactor Dosimetry, held in Vail, Colorado, 29 August - 3 September 1993, ASTM STP 1228, 1994, pp. 447-455.

[Lu81] J. L. Lucius, C. R. Weisbin, J. H. Marable, J. D. Drischler, R. Q. Wright, J. E. White, A User's Manual for FORSS Sensitivity and Uncertainty Analysis Code System, Oak Ridge National Laboratory, Oak Ridge, TN, report ORNL-5316 (ENDF-291), January 1981.

[Ma71] B. R. Martin, Statistics for Physicists, Academic Press, London, 1971.

[Ma85] R. E. Maerker, B. L. Broadhead, J. Wagschal, "Theory of a New Unfolding Procedure in Pressurized Water Reactor Pressure Vessel Dosimetry and Development of an Associated Data Base," Nuclear Science and Engineering, Vol. 91, pp. 369-392, 1985.

[Ma86] R. E. Maerker, B. L. Broadhead, B. A. Worley, M. L. Williams, J. Wagschal, "Application of the LEPRICON Unfolding Procedure to the Arkansas Nuclear One-Unit 1 Reactor," Nuclear Science and Engineering, Vol. 93, pp. 137-170, 1986.

[Ma89] M. Matzke, "Unfolding and Radiation Damage Predictions with and without *a priori* Information," Reactor Dosimetry: Methods, Applications, and Standardization, ASTM STP 1001, H. Farrar, E. P. Lippincott, Eds., American Society for Testing and Materials, Philadelphia, pp. 425-433, 1989.

[Ma92] P. Marinkovic, S. Avdic, M. Pesic, N. Zavaljevski, "The Effect of the Neutron Spectra Unfolding Method on the Fast Neutron Dose Determination," Nuclear Instruments and Methods in Physics Research, Vol. A321, pp. 333-335, 1992.

[NEA97] Computing Radiation Dose to Reactor Pressure Vessel and Internals: State-of-the-Art Report, Nuclear Energy Agency, Organization for Economic Co-operation and Development, report NEA/NSC/DOC(96)5, 1997.

[No94] H. Nolthenius, Neutron Spectrum Adjustment and the NMF-90, report ECN-I-94-zxz, April 1994.

[Pe77a] F. G. Perey, Least-Squares Dosimetry Unfolding: The Program STAY'SL, Oak Ridge National Laboratory, Oak Ridge, TN, report ORNL/TM-6062 (ENDF-254), October 1977.

[Pe77b] F. G. Perey, "Uncertainty Analysis of Dosimetry Spectrum Unfolding," Second ASTM-EURATOM Symposium on Reactor Dosimetry: Dosimetry Methods for Fuels, Cladding, and Structual Materials, October 977.

[Pe77c] F. G. Perey, "Spectrum Unfolding by the Least-Squares Method," IAEA Technical Committee Meeting on Current Status of Neutron Spectrum Unfolding, Oak Ridge, TN, October 10-12, 1977.

[Pe78] F. G. Perey, Contributions to Few-Channel Spectrum Unfolding, Oak Ridge National Laboratory, Oak Ridge, TN, report ORNL/TM-6267 (ENDF-259), February 1978.

[Pe92] L. Petrusha, "Photofission Effects in B&W 177-FA Reactor Vessel Surveillance Capsule Dosimeters," Proceedings of the Seventh ASTM-EURATOM Symposium on Reactor Dosimetry, held in Strasbourg, France, 27-31 August 1990, Kluwer Academic Publishers, 1992, pp. 537-545.

[Ro87] P. J. Rousseeuw, A. M. Leroy, Robust Regression and Outlier Detection, John Wiley & Sons, New York, New York, 1987.

[Sc78] F. Schmittroth, J. A. Rawlins, "Dosimeter Based Adjustments of Fast Neutron Spectra," paper delivered to the American Nuclear Society, June 18-23, 1978, San Diego, California and reported in report HETL-SA-1480, Hanford Engineering Development Laboratory.

[SE255] Safety Evaluation by the Office of Nuclear Reactor Regulation Palisades: Pressure Vessel Fluence Reevaluation Consumers Company Docket No. 50-255, Nuclear Regulatory Commission, Washington D.C., 1997.

[Sh89] D. Shalitin, J. J. Wagschal, Y. Yeivin, "A Contribution to the Theory of Reactor Pressure Vessel Dosimetry," Reactor Dosimetry: Methods, Applications, and Standardization, ASTM STP 1001, H. Farrar, E. P. Lippincott, Eds., American Society for Testing and Materials, Philadelphia, pp. 399-404, 1989.

[Sl94a] C. Slater, "The Pool Critical Assembly (PCA) 'Blind Test' Benchmark," presentation to the Cross Section Evaluation Working Group meeting at Oak Ridge Tennessee on October 26, 1994 and published in the meeting minutes.

[Sl94b] C. Slater, "The NRESDIP2 Radial Shield and Cavity Experiment," presentation to the Cross Section Evaluation Working Group meeting at Oak Ridge Tennessee on October 26, 1994 and published in the meeting minutes.

[Sm91] D. L. Smith, Probability, Statistics, and Data Uncertainties in Nuclear Science and Technology, American Nuclear Society, Lagrange Park, Illinois, 1991.

[Sm93] D. L. Smith, A Least-Squares Computational Tool Kit, Argonne National Laboratory, Argonne, Illinois, report ANL/NDM-128, April 1993.

[St85] F. W. Stallman, LSL-M2: A Computer Program for Least-Square Logarithmic Adjustment of Neutron Spectra, Nuclear Regulatory Commission, Washington D.C., report NUREG/CR-4349, 1985.

[Sz95a] E. J. Szondi, H. J. Nolthenius, User's Guide to the Cross Section Processing Code X333 (Version 95-1), Institute of Nuclear Techniques, Technical University of Budapest, report BME-NTI 222/95, May 1995.

[Sz95b] E. J. Szondi, H. J. Nolthenius, E. M. Zsolnay, User's Guide to the Neutron Spectrum Adjustment Code STAYNL (Version 95-1), Institute of Nuclear Techniques, Technical University of Budapest, report BME-NTI 223/95, May 1995.

[Ti88] M. Tichy, "Bayesian Approach to Neutron Spectrum Adjustment," Nuclear Instruments and Methods in Physics Research, Vol. A267, pp. 502-508, 1988.

[Ve80] V. V. Verbinski, C. G. Cassapakis, W. K., Hagan, G. L. Simmons, "Photofission Corrections in Neutron Dosimetry for Reactor Pressure Vessel Lifetime Studies," Nuclear Science and Engineering, Vol. 75, pp. 159-166, 1980.

[Vl77] M. Vlasov, IAEA Consultants' Meeting on Integral Cross Section Measurements in Standard Fields, Summary Report, Conclusions and Recommendations, IAEA, Vienna, Report INDC(NDS)-81/L+Dos., 1977.

[Wo81] D. W. Wootan, F. Schmittroth, Comparison of SAND-II and FERRET, Hanford Engineering Development Laboratory, report HETL-TC-1589, January 1981.

[Zi79] W. L. Zijp, Proceedings of the Advisory Group Meeting on Nuclear Data for Reactor Dosimetry, IAEA, Vienna, Report ECN-78-163, pp. 187-219, May 1979.

[Zi84] W. L. Zijp, E. M. Zsolnay, H. J. Nolthenius, E. J. Szondi, G. C. H. M. Verhaag, "Intercomparison of Predicted Displacement Rates Based on Neutron Spectrum Adjustments (REAL-80 Exercise)," Nuclear Technology, Vol. 67, November 1984.

[Zi89] W. L. Zijp, E. M. Zsolnay, H. J. Nolthenius, E. J. Szondi, "On the Problems Encountered in Activation Spectrometry and Subsequent Radiation Damage Predictions," Reactor Dosimetry: Methods, Applications, and Standardization, ASTM STP 1001, H. Farrar, E. P. Lippincott, Eds., American Society for Testing and Materials, Philadelphia, pp. 415-424, 1989.

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APPENDIX A

The Mathematical Foundations of the Least Squares Methodology

Introduction

It is inconceivable to me that anyone would reject a least squares approach to a parameter estimation and attempt to justify this position on a scientific and technical basis. This is like someone rejecting the statistical treatment of measured data. Of course it is not uncommon for people to attempt to misuse statistical analyses. Thus, the approach I have taken to this review, and the approach the NRC should take to the Palisades submittal, is to carefully and rigorously evaluate the input data and the correlations between the parameters. A rejection of the least squares approach to the PV fluence estimation can not be made on technical grounds but the input parameters used in the least squares analysis should be subjected to careful scrutiny and the sensitivity of the results to the input parameters should be well understood.

In light of the strong statement made in the previous paragraph, it is probably a good idea to provide a brief synopsis of the least squares approach, its statistical roots, and how it is employed in codes such as FERRET. The following sections present a foundation for the least squares adjustment process and are based on presentations found in References [Dr77, Ma71, Ma89, Pe77a, Pe77b, Pe78, Sh89, Sm91, Sm93, Sz95b]

Notation

To aid in the presentation of the least squares formalism, it is good to introduce a uniform mathematical notation. Let θ_i represent a range of parameters, where i is an index variable which takes on values from 0 to N, which we wish to estimate. Let η_{ij} represent the j^{th} measurement of the parameter θ_i. Several parameters, θ_i, are of interest in the estimation process. These parameters include the reaction rates, the spectrum fluence values, and the dosimetry cross sections. Let a_i represent the reaction rates, where the reaction index i goes from 1 to m_a. A bold symbol **A** will be used to represent the vector formed by the reaction rates. Thus, the reaction rate vector is notated as:

$$A = [a_i]_{m_a} \tag{1}$$

Let ϕ_i represent the energy-dependent fluence values with the energy index i going from 1 to m_E. The vector of fluence values is then

$$\Phi = [\phi_i]_{m_E} \tag{2}$$

The cross section values for the j^{th} energy of the i^{th} reaction are notated as Σ_{ij}. The cross section matrix has dimension $m_\Sigma = m_a \times m_E$ and is notated as:

$$S = [\Sigma_{ij}]_{m_a m_E} \tag{3}$$

Let

$$S_i = [\Sigma_{ij}]_{m_E} \tag{4}$$

indicate the one dimensional vector of energy-dependent cross section values for reaction i.

Each parameter has a corresponding uncertainty and may be correlated with other parameters. We can characterized the uncertainty by a relative covariance matrix. Let $\mathbf{M}_\theta$ be the relative covariance matrix for parameters θ. Thus the relative covariance for the reactions rates is given by $\mathbf{M}_a$, the relative covariance for the group fluence rates is given by $\mathbf{M}_\phi$, and the relative covariance for the cross sections is given by $\mathbf{M}_\Sigma$. The symbol $\mathbf{0}$ is used to represent a matrix where all the matrix elements are zero.

The symbol Θ is used to describe the generic column vector of parameters θ_i that are being estimated. If the parameters under study concern reaction rates, fluence rates, and cross sections, then the column vector Θ has dimension $(m_a+m_\phi+m_\Sigma)x1$ and can be written as a vector composed of vectors, or

$$\Theta = \begin{bmatrix} A \\ \Phi \\ S \end{bmatrix} \tag{5}$$

The relative covariance matrix for Θ is notated as $\mathbf{M}_\theta$ and its matrix elements are notated as $c^m{}_{\theta ij}$.

Let the transpose of a matrix be notated by a superscript "T". Thus the transpose of a matrix $\mathbf{Q}$ is notated as $\mathbf{Q}^T$. The inverse of a matrix is indicated by a superscript "-1". Thus the inverse of a matrix $\mathbf{Q}$ is notated as $\mathbf{Q}^{-1}$. We denote a diagonal matrix built up from a vector with an overline. Thus a matrix $\overline{\mathbf{A}}$ is made up from the reaction rate vector with elements $\overline{a}_{ii} = a_i$ and $\overline{a}_{ij} = 0$ for $i \neq j$. Matrix multiplication is denoted by a bullet ($\bullet$). Thus the matrix equation $\mathbf{A} = \mathbf{B} \bullet \mathbf{D}$ implies that

$$a_{ij} = \sum_k b_{ik} d_{kj} \tag{6}$$

The covariance matrix for parameters Φ is notated as $\mathbf{N}_\theta$ and its matrix elements are notated as $n_{\theta ij}$ or as $\sigma^\theta{}_{ij}$. The covariance matrix is related to the relative covariance matrix by the relationship

$$N_\theta = \overline{\Theta} \bullet M_\theta \bullet \overline{\Theta} \tag{7}$$

If the reaction rates, fluence rates, and cross sections are uncorrelated, then this covariance matrix can also be written as a matrix of the covariance matrix for the individual parameter types, or

$$M_\theta = \begin{bmatrix} M_a & 0 & 0 \\ 0 & M_\phi & 0 \\ 0 & 0 & M_\Sigma \end{bmatrix} \quad (8)$$

Iterative Approach

Given the notation developed in the previous section, the physics of the dosimetry measurements gives us the mathematical relationship:

$$A = S' \bullet \Phi \quad (9)$$

Here **A** is a (m_a x 1) column vector of measured reaction rates, Φ is a (m_Ex1) column vector of neutron fluence rates, and **S'** is a m_a x m_E matrix of cross sections. Given a measured set (vector) of m_a reaction rates, $\mathbf{A}^m$, the goal of spectrum unfolding approaches is to determine the fluence vector Φ. If m_E=m_a, then the solution is uniquely defined by taking the inverse of **S'**. Thus

$$\Phi = S'^{-1} \bullet A^m \quad (10)$$

If m_E<m_a, then the system of equations is overdetermined and a general unique solution may not exist. In the typical spectrum unfolding/adjustment case m_E>m_a and the problem is underdetermined.

In an iterative spectrum unfold one introduces a trial spectrum $\Phi^{(0)}$ and calculates a set of reaction rates $\mathbf{A}^{(0)}$ from the equation

$$A^{(0)} = S' \bullet \Phi^{(0)} \quad (11)$$

Based on the difference between $\mathbf{A}^m$ and $\mathbf{A}^{(0)}$, an algorithm is used to determine a better approximation of Φ. The better approximation is denoted as $\Phi^{(1)}$. The procedure is repeated "n" times until

$$A^m \cong S' \bullet \Phi^{(n)} \quad (12)$$

The SAND-II, SPECTRA, and CRYSTAL BALL codes are examples of this type of iterative unfolding code. The differences in these codes are generally due to differences in the algorithms used to improve the approximation $\Phi^{(i)}$.

Least Squares Approach

The iterative approach presented in the previous section is generally not free of subjective evaluation because we are asking too much from too little data. Some approaches [Ke89]

use a smoothness criterion in order to obtain a consistent user-independent "unfolded" neutron spectrum. Perey states [Pe77b] "The ultimate user usually does not care much for such an answer unless we can prove that the method of calculation has not introduced uncertainties which are comparable or at worse even greater than those we give him." It was this criticism of the iterative spectrum determination algorithms that led to the application of the least squares approach to the spectrum determination problem. The least squares approach provides "a formulation of the dosimetry problem which is slightly different mathematically from the usual one, but admits an exact solution [Pe77b]." The "exact unique" solution comes from changing the question slightly and asking what is the "most likely" value of the neutron spectrum and its uncertainty. The iterative approach asks the question "What is the neutron spectrum?" The least squares approach asks "what is the most likely solution?" As one of the pioneers in the area, F. Perey [Pe77b], states "The mathematical difference between the two formulations is so great that there is a unique and well known solution to one and to my knowledge no satisfactory one to the other." Here Perey rejects the iterative unfold process as not satisfactory while embracing the least squares approach.

Single Variable Least Squares

The least squares approach was first proposed by Gauss when he was a schoolboy. The initial formulation for a single variable, θ, was to find the "most likely" value of θ, given "n" measurements (η_1, η_2, η_3, ... η_n) with uncorrelated errors (σ_1, σ_2, σ_3, ... σ_n), that satisfied the equation

$$\chi^2 = \sum_{i=1,n} \left[\frac{(\eta_i - \theta)^2}{\sigma_i^2} \right] = minimum \qquad \textbf{(13)}$$

This is the typical least squares expression taught to every high school physics student even today.

Generalized Least Squares Spectrum Adjustment

This single variable least squares method can be generalized to treat a set of parameters θ_i. There exists measurable metrics y_j where $y_j=f_j(\Theta)$ with current (reaction rate) measurements and *a priori* (radiation transport calculations) estimates y^o_j and associated covariance values $\sigma^{y(\theta)}$. The least squares formulations calls for solving the matrix equation:

$$\chi^2 = (y^o - f(\Theta))^T \bullet N_{y(\theta)}^{-1} \bullet (y^o - f(\Theta)) = minimum \qquad \textbf{(14)}$$

If the number of parameters is equal to 1 and the data errors are uncorrelated, and $f(\theta)=\theta$, then $y^o_i = \eta_i$, $n^{y(\theta)}{}_{ii}=\sigma_i$, $n^{y(\theta)}{}_{ij}=0$ for $i \neq j$, and Equation 14 reduces to Equation 10. In the case where $f(\theta)$ is nonlinear in the function of θ, the least squares method often linearizes the approach using a Taylor series in the parameters. A nonlinear least squares approach

can also be used. In a nonlinear least squares method one iterates to find the design function, **G**. More details on the **G** matrix are provided later in this section as the details of the solution of Equation 14 are developed.

When Equation 14 is applies to the least squares adjustment with measured activities A^o, *a priori* energy dependent fluence rates from radiation transport calculations ϕ^o, and *a priori* energy dependent cross sections S^o, the equation becomes

$$\chi^2 = \begin{bmatrix} \Phi^{\,o} - \Phi \\ S^{\,o} - S \\ A^o - A \end{bmatrix}^T \bullet \begin{bmatrix} N_{\phi o} & 0 & 0 \\ 0 & N_{\sigma o} & 0 \\ 0 & 0 & N_{am} \end{bmatrix}^{-1} \bullet \begin{bmatrix} \Phi^{\,o} - \Phi \\ S^{\,o} - S \\ A^o - A \end{bmatrix} = minimum \qquad \textbf{(15)}$$

In this equation we have assumed that there are no correlations between the reaction rates, the fluence rate values, and the cross sections. $\mathbf{N}_{\theta o}$ represents the covariance of the *a priori* fluence rate. $\mathbf{N}_{\sigma o}$ represents the covariance of the *a priori* cross sections. $\mathbf{N}_{am}$ represents the covariance of the measured activities.

We introduce a parameter vector **P** composed of the input parameters for which we have a *priori* information.

$$P = \begin{bmatrix} \Theta \\ S \end{bmatrix} \qquad \textbf{(16)}$$

In the case of the activities, we have measured data and a relationship between the activities and the other parameters, i.e. the cross sections and the fluence rates.

The least squares equation can then be written

$$\chi^2 = \begin{bmatrix} P^{\,o} - P \\ A^o - A \end{bmatrix}^T \bullet \begin{bmatrix} N_{po} & 0 \\ 0 & N_{am} \end{bmatrix}^{-1} \bullet \begin{bmatrix} P^{\,o} - P \\ A^o - A \end{bmatrix} = minimum \qquad \textbf{(17)}$$

In this equation $\mathbf{P}^o$ and $\mathbf{N}_{po}$ are defined from the input *a priori* values for Φ, **S**, $\mathbf{N}_{\phi o}$, and $\mathbf{N}_{\sigma o}$, and **A** is calculated from **P**.

Let $\mathbf{A}^c$ represents the activities calculated from **P**, the solution of Equation 17, that is, from the adjusted cross sections and fluence rate values. Let $\mathbf{N}_{ac}$ represent the covariance of these calculated activities. Then the solution to Equation 17, the value of P' that minimizes Equation 17, is given by

$$P' = P^o + N_{po} \bullet G^T \bullet (N_{ac} + N_{am})^{-1} \bullet (A^o - A^c) \quad \textbf{(18)}$$

where **G** has dimension m_a x [m_E + (m_a x m_E)] and is given by

$$G = \begin{bmatrix} S_1^T \Theta^T & 0 & 0 & \dots & 0 \\ S_2^T & 0 & \Theta^T & 0 & \dots & 0 \\ S_3^T & 0 & 0 & \Theta^T & \dots & 0 \\ S_4^T & 0 & 0 & 0 & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \Theta^T \end{bmatrix} \quad \textbf{(19)}$$

$\mathbf{S}_i^T$ is an energy-dependent row vector (the transpose of the column vector) of the cross sections for the i^{th} reaction and has dimension m_E. Θ^T is the m_E dimensional row vector of the energy-dependent neutron flux values. The matrix $(\mathbf{N}_{ac}+\mathbf{N}_{am})^{-1}$ is called the weight matrix. The solution in Equation 18 exists only if this weight matrix is nonsingular. A singular weight matrix is not common so this is not generally a concern. References [Sm91, Pe77a, Pe77b, Sz95b] provide additional details on the expressions for the minimum χ^2 and the adjusted covariance matrices.

Conclusions on Least Squares Spectrum Adjustment

"The least-squares solution for the joint density function $\overline{P}$ is often said to be 'best' or 'most likely' by virtue of the 'minimum variance theorem' which guarantees that it minimizes the variance of any linear combination of the parameters [Pe77c]". If the errors in the observations are normally distributed, then the method of least squares gives the same results as the method of maximum likelihood. The maximum likelihood estimators are consistent and have a distribution that tends to normality for large samples. Furthermore, they have minimum variance in the limit of large samples [Ma71]. The solution to Equation 14 is "most likely" by virtue of the fact that it minimizes the χ^2 function. It is also unbiased and satisfies a minimum variance theorem [Pe77b]. There is little doubt that the least squares approach has a rigorous mathematical foundation. It can in no way be labeled "arbitrary." "The idea of 'very best solution' has implicit in it the fact that we have used to obtain it all observations which were ever made, for whatever purpose, related to the σ_{ij}'s an ϕ_j's of this problem and that these observations are exploited to the fullest extent of our current knowledge [Pe77c]" (emphasis in original). "The least squares method removes any concern we have about biases in the algorithm since it is an unbiased algorithm, [Pe77b]".

Any question about the least squares methodology would have to focus on the reliability and sensitivity of the *a priori* input data. "How realistic and credible is our solution will therefore depend upon how realistic and credible are our estimates of the covariance

matrices $\mathbf{N}_a$, $\mathbf{N}_\Sigma$, and $\mathbf{N}_\phi$" [Pe77b]. Section 12.2 of this review addresses the input covariance matrices in more detail. Perey notes [Pe77b] that one potential problem with this formulation is that the group structure has to be fine enough not to make a serious approximation in the use of Equation 9 to calculate the reaction rates. This issue is addressed in more detail and shown not to be an issue in Section 12.3 of this review.

Perey summaries the status of the least squares spectrum adjustment when he says [Pe77b]

> **"The method of least squares, with its better theoretical foundation and by making explicit the assumptions upon which the solution is based, has the potential for generating much more credible answers than we currently obtain. ... Since this concept allows us to guarantee more likely answers than we currently get, even when we have a poor idea of what the covariance matrices are, immediate benefits can be obtained using the method of least squares."**

And from Reference [Pe77c], the

> **"least-squares method does provide the best complete solution, with uncertainties, to the problem as it is understood."**

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