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CONTENTS

ABSTRACT v

I. INTRODUCTION. 1

II. BASIC LIBRARY FORMAT. 3

III. GROUP STRUCTURE 6

IV. CHOICE OF INTEGRAL EXPERIMENTS. 7

V. ACCURACY OF THE INTEGRAL EXPERIMENTS. 11

VI. CROSS SECTIONS TO BE ADJUSTED 11

VII. INTEGRAL PARAMETER CROSS SECTION SENSITIVITIES. 18

VIII. CALCULATIONAL METHODOLOGY 19

IX. METHODS BIAS AND UNCERTAINTIES. 20

A. Determination of Calculational Biases and Associated Uncertainties. 20

B. Procedure for Formally Including Methods Biases and Uncertainties in the Adjustment Process 39

CONCLUSIONS. 45

ACKNOWLEDGMENTS. 46

REFERENCES 47

APPENDIX I 53

APPENDIX II. 55

ABSTRACT

The present work proposes a specific plan of cross section library adjustment for fast reactor core physics analysis using information from fast reactor and dosimetry integral experiments and from differential data evaluations. This detailed exposition of the proposed approach is intended mainly to elicit review and criticism from scientists and engineers in the research, development, and design fields. This major attempt to develop useful adjusted libraries is based on the established benchmark integral data, accurate and well documented analysis techniques, sensitivities, and quantified uncertainties for nuclear data, integral experiment measurements, and calculational methodology. The adjustments to be obtained using these specifications are intended to produce an overall improvement in the least-squares sense in the quality of the data libraries, so that calculations of other similar systems using the adjusted data base with any credible method will produce results without much data-related bias. The adjustments obtained should provide specific recommendations to the data evaluation program to be weighed in the light of newer measurements, and also a vehicle for observing how the evaluation process is converging.

This report specifies the calculational methodology to be used, the integral experiments to be employed initially, and the methods and integral experiment biases and uncertainties to be used. The sources of sensitivity coefficients, as well as the cross sections to be adjusted, are detailed. The formulae for sensitivity coefficients for fission spectral parameters are developed. A mathematical formulation of the least-square adjustment problem is given including biases and uncertainties in methods.

I. INTRODUCTION

The present work proposes a plan of cross section adjustment for fast reactor core physics analysis using information from fast reactor and dosimetry integral experiments and from differential data measurements and evaluations. The detailed exposition of the proposed approach is intended mainly for review and criticism from integral experimentalists, from basic data evaluators, from methods analysts and from reactor designers. In summary, this is our first major attempt in the development of adjusted libraries using well documented nominal values, sensitivities, and uncertainties. The adjustments are intended to produce an overall improvement (in a least-squares sense) in the quality of the data libraries rather than an empirical fitting which improves only nominal estimates of reactor performance parameters using a particular calculational procedure. We do not expect, however, that any specific cross section parameter need necessarily be closer to its true value, because of the generally broad resolution with which integral experiments are measures of nuclear data. We begin with consideration of the more conventional ^{239}Pu and ^{235}U systems since considerable information from both differential and integral measurements is readily available. The extension to alternative breeder systems will be made pending completion of relevant fast reactor integral experiments and analysis.

Data adjustments are widely used in the framework of many leading Fast Breeder Programs[1,2,3,4] and were originated from techniques proposed as early as 1964[5] and since then widely improved.[6] At first, only core related adjustments were performed, but in view of the claimed performance of such techniques in the improvement of the prediction ability for reference design parameters, shielding related data have recently been considered for adjustment.[7,8] Since the original papers in this field, many improvements have been introduced including the use of generalized perturbation theory for sensitivity calculations,[9] comprehensive statistical formulation with allowance for uncertainty correlations,[10] transport methods for sensitivity analysis,[11,12] interactive techniques for on-line adjustments[13] and the development of a procedure for basic parameter adjustment.[14,15]

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There has always been a debate on the "quality" of the adjusted data and their applicability with respect both to their performance when used by a reactor designer and to their possible utilization by basic data evaluators as supplementary sources of information. At least three questions have to be answered for a systematic discussion of this problem:

(a) Which integral measurements are used, and what are the associated covariance matrices?

(b) Which differential data uncertainties are introduced in the adjustment, and, in particular, what correlations are used?

(c) Which calculational method is employed, and how is its uncertainty factored into the analysis?

Various answers have been proposed for each of these questions. In particular, for (a) there have been two opposing philosophies (1) the inclusion of a very large number of integral measurements including mockup designs[2], and (2) a more cautious use of integral measurements emphasizing the "clean" ones.[1,6] With regard to (b), the need for reliable covariance matrices has long been stressed but only recently have evaluated covariance files become available.[16,17] Consideration of the last point (c), an assessment of the calculational method uncertainty, is an attempt to make data adjustments as independent of the calculational tools as possible, increasing thereby the range of utilization. No systematic nuclear data adjustment incorporating evaluated methods uncertainties was known to the authors at the time of this writing.* Moreover, much of the earlier adjustment work was not intended to lead to more accurate microscopic data, even though many of the adjustments have been compared, in detail, with reliable evaluations.

The present work is a proposed plan for core-related data adjustment, with emphasis on clean benchmark integral experiments and with the important introduction of recently developed covariance files, including those for methods uncertainties. (All results obtained in the adjustment effort will have to be examined in the light of the allowable interpretation of least-squares solutions.) These input files lead to a covariance matrix of the

*However, Ref. 15 contains the type of information indicative of that to be developed, hopefully more comprehensively, as part of this study.

adjusted cross sections which, in turn, can be propagated (using sensitivity coefficients) to compute data uncertainties in performance parameters of systems to be designed. The *a posteriori* uncertainties provide a measure of confidence in the cross section adjustment recommendations provided to the evaluation community.

II. BASIC LIBRARY FORMAT

The self-shielding factor method[18], based on a representation of the self-shielded cross section as a product of an infinitely dilute group cross section and a self-shielding factor, is well-suited (but not necessary) for the adjustment procedure. Within this formalism, one may apply the adjustment to the infinitely dilute group cross section leaving to a later iteration the verification of the underlying hypothesis that the variations in self-shielding factors are small compared to the infinite dilution cross section variations. Since f-factors are ratios of cross sections, they tend to be less sensitive than the multi-group cross section to a variation in some resonance parameter. In practice, the following hypothesis is suggested [using the notation of Ref. (19)].

$$\delta\sigma_G^{x,z} \tilde{=} \delta\sigma_G^{x,\infty} f_G^{x,z} \qquad (1)$$

with respect to cross sections, σ, of type x, group G, in zone z (or ∞ dilution) and self-shielding factors (f).

Greenspan et al[20] have shown that the sensitivity of the group capture cross section to variations in the capture width is primarily through the infinitely dilute cross section (above 2 keV in ^{238}U, the contribution through the f-factor channel is smaller than 1%). The situation with regard to the impact of variations in the neutron width on changes to the group capture cross section is less clear. In the resolved energy range, the highest sensitivities of group capture cross sections to the neutron width is for the predominantly capture resonances ($\Gamma_\gamma > \Gamma_n$), wherein the f-factor channel is also negligible. However, for the scattering ($\Gamma_n > \Gamma_\gamma$) resonances in the resolved energy range, the spectral fine structure effects of Γ_n on the capture cross section (through the f-factor channel) were shown to be significant (sensitivities of $\sim$ - 0.2). This effect became less

important as the energy increased (e.g., the unresolved energy range). In a similar vein, increases in the background cross section lead to a relative flattening of the energy dependence of the total cross section causing a reduction in the resonance self-shielding and a corresponding increase in the group capture cross section. In this case, the only mechanism for including this phenomena into the adjustment procedure would be through the f-factor "channel." However, as above, this effect was observed to be important only for the predominantly scattering resonances.

In the unresolved energy range, the relative importance of the f-factor "channel" diminished. Greenspan et al[20] "found that the $P_{\gamma\gamma}$ (sensitivities of variations in the capture width to the group capture cross section) approach unity and they result essentially from the direct effects (impact on the infinitely dilute cross section). The $P_{\gamma n}$ (sensitivities of variations in the neutron width on the group capture cross section) are pretty small with Spectral Fine Structure Effects (SFSE) playing the major role. ....In summary, even though SFSE are generally significantly lower for the unresolved resonances than for the resolved ones, errors of the order of 10% might be expected in certain problems due to the neglect of SFSE in the unresolved energy range."

There is currently a lack of information for comparison of the effect of the total number of scattering versus capture resonances, for the analysis of propagating the group sensitivities to resonance parameters with the sensitivities of some desired result with respect to the group constants, or the assessment of the impact of the relative uncertainties and correlations of Γ_n and Γ_γ. Primarily because of the simplicity of dealing exclusively with the infinitely dilute cross section, we will continue to utilize Eq. (1) for our initial work, but we propose to study in detail the need for including the f-factor "channel" within our adjustment procedure.

For the first iteration of our adjusted libraries, only the inclusion of integral information related to eigenvalue and reaction rates is proposed. This is because, at this time, documented uncertainty information related to integral parameters such as central worths, Doppler, etc., is currently limited, as is quantified information regarding uncertainties due to analytical approximations (biases and covariances) made in computing

these parameters. Incorporation of these integral measurements at a later time is expected, and this may necessitate the expansion of Eq. (1) to include the variation in the shielding factors. Finally, since the resulting analysis scheme must predict properties such as sodium voiding, etc., the first adjusted libraries are not likely to completely eliminate the need for bias factors. It is expected, however, that these bias factors will be reduced considerably, at least for those parameters for which we have added pertinent integral information (e.g., breeding ratio, and integral parameters with similar nuclear data sensitivities), and that the remaining bias factors (e.g., for calculation of voiding, for extra methods problems in engineering mockup criticals, etc.) will then provide the target for successive improvements to the analysis scheme.

The specific proposal then is to perform the adjustments on the infinitely dilute cross sections (at least for the first round of testing) modifying the ISOTXS file[21] accordingly. The sensitivity profiles may then be interpreted as $(dR/R)/(d\sigma_G^{X,\infty}/\sigma_G^{X,\infty})$. The new set of infinitely dilute cross sections would then be folded with the "old" f-factors providing new self-shielded cross sections for use in analysis. The updated library would be available in ANISN format[22] in accordance with the requirements of the FORSS system.[23]

The only way in which the adjusted $\sigma_G^{X,\infty}$ then influences the self-shielding factor calculation is through their impact on the calculation of σ_o, the background cross section/absorber atom. For any new calculation, the adjusted $\sigma_G^{X,\infty}$ and the old f should be used as a first approximation, which may very often be satisfactory. If one chose to use an MC^2-2 type approach[24] for cross section generation (not done in this work), the adjustment procedure could be applied to a "reference" composition library (σ_{ref}), and any other composition library ($\sigma_G^{X,Z}$) could be related to that one by means of coefficients of the type

$$\sigma_G^{X,Z} = \sigma_{ref}\, f_G^{X,Z} \quad . \tag{2}$$

The hypothesis, as before, is that as a first approximation, no adjustment would be applied to $f_G^{X,Z}$.

III. GROUP STRUCTURE

Since the adjustment procedure is independent of the energy structure adopted, the latter is chosen according to (1) the needs of the potential designer of a reference system and (2) the needs of the evaluator to get credible information from the adjustment which might be used as part of the evaluation process. A broad group (∿10 groups) scheme seems appropriate for an adjustment that is intended to provide feedback to an evaluation or cross section measurement program since cross section measurements are often made over a broad energy range. A more detailed group scheme, of the order of 30 groups, would be consistent with the current design methodology and critical experiment analysis.

In particular, we propose that adjustments be performed in a 13-energy-group structure (see Table I) which includes all energy boundaries above 454 eV used at ANL in their 12-group unit lethargy structure for sensitivity studies. We have subdivided the single group from 67 keV to 183 keV into two equal lethargy groups with a boundary at 111 keV (∿100 keV is a natural boundary between different types of differential experimental techniques).

Table I. Broad Energy Group Structure for Data Adjustment Studies

Group	Energy Range
1	10.000 MeV - 17.333 MeV
2	3.679 - 10.000
3	1.353 - 3.679
4	0.498 - 1.353
5	0.183 - 0.498
6	0.111 - 0.183
7	0.067 - 0.111
8	24.79 keV - 67.38 keV
9	9.119 - 24.79
10	3.355 - 9.119
11	1.234 - 3.355
12	0.454 - 1.234
13	Thermal - 0.454

We've also added a group above 10 MeV for problems related to shielding, threshold reactions, etc., although we expect these problems will require different energy group structures. Finally, the two energy groups below 454 eV were combined into one. The resulting group structure is compatible with the 126-energy-group structure[25] in use at ORNL and is of approximately the same size as group structures (six-group[26], ten-group[12], etc.) employed in the past. A parallel adjustment in a 26-energy-group structure (see Table II), a subset of the 50-energy-group structure[27] (from 10 MeV to 22 eV presently in use at Westinghouse and General Electric, should provide a tool directly applicable by the designer.

IV. CHOICE OF INTEGRAL EXPERIMENTS

There has been intense discussion, for some time now, regarding the appropriateness of including specific types of integral experiment results in any adjustment procedure. Least-squares procedures, as manifested in codes such as AMARA[28] and UNCOVER[29], have been used (particularly in the United Kingdom[1]) in connection with the so-called "clean experiments." These were carefully designed measurements of reaction rates and critical mass. In particular, the type of experiments included in the adjustment of the FGL5 set[1] is listed below:

(a) k_{eff} values of uranium- and plutonium-fueled critical assemblies.
(b) k_∞ measured in null-reactivity test zones.
(c) Bucklings measured in the central regions of critical assemblies.
(d) Central reaction rate ratios. Fission rates in ^{238}U, ^{239}Pu and ^{240}Pu, and capture in ^{238}U, relative to fission in ^{235}U.
(e) Spectrum measurements at the center of assemblies.
(f) Small sample reactivity perturbation measurements relative to a standard sample (^{235}U or ^{239}Pu).

In an adjustment procedure designed to provide nuclear data, it appears desirable to avoid complicated design-oriented integral experiments (such as the ZPPR-5 experiments for core disassembly simulation[30]) and those integral experiments whose calculational uncertainties are less understood.

Table II. The 26-Energy-Group Structure Proposed for Adjusted Libraries Useful for Design and Integral Experiment Analysis (Based on Half-Lethargy Intervals)

Group	Upper Energy (eV)
1	1.73330E 07
2	1.00000E 07
3	6.06530E 06
4	3.67880E 06
5	2.23130E 06
6	1.35340E 06
7	8.20850E 05
8	4.97870E 05
9	3.01970E 05
10	1.83160E 05
11	1.11090E 05
12	6.73790E 04
13	4.08680E 04
14	2.47880E 04
15	1.50340E 04
16	9.11880E 03
17	5.53080E 03
18	3.35460E 03
19	2.03470E 03
20	1.23410E 03
21	7.48520E 02
22	4.54000E 02
23	2.75360E 02
24	1.67020E 02
25	1.01300E 02
26	6.14420E 01

There are a number of experiments available which measure the effect of voiding and small sample reactivity worths. These experiments have been used to establish bias factors for calculated safety parameters but are not routinely applied in the sense of data testing. Scattering material worths are difficult to properly compute, representing a cancellation of comparable size positive and negative terms. Central worth measurements of fissile materials are probably reliable, but the well-known C/E discrepancy[31] leads us to propose introduction of this experimental data in a second separate step (after experience with eigenvalue and reaction rates) in which the analysis of central worths can be isolated. Inclusion of these worth measurements will permit the study of different types of data (e.g., β_{eff}) with different sensitivities and independently measured parameters.

The following information will be used in our first adjustments: k_{eff}, and measured ratios of central reaction rates including the ratio of captures in ^{238}U to fissions in $^{235}U[^{28}c/^{25}f]$, fissions in ^{238}U to fissions in $^{235}U[^{28}f/^{25}f]$, and fissions in ^{239}Pu to fissions in $^{235}U[^{49}f/^{25}f]$; alternatively, the same reactions relative to $^{239}Pu(n,f)$ instead of $^{235}U(n,f)$ may be used, as appropriate. Additional reaction rates (and/or ratios), for other important reactions are available from measurements in clean dosimetry fields. These include $^{238}U(n,f)$, $^{235}U(n,f)$, $^{56}Fe(n,p)$, $^{27}Al(n,\alpha)$, $^{239}Pu/^{235}U$ and $^{238}U/^{235}U$ fission ratios.

The facilities in which many of the above measurements were made include critical experiments of interest to the designer of a demonstration size reactor as well as those of interest to the designer of a large commercial power plant. The ZPR-6/7[32] and ZPR-6/6A[32] represent spectra characteristic of large, dilute mixed oxide assemblies. The ZPR-3/48[33] and ZPR-9/31[34] are similar but are carbide rather than oxide experiments. Additional experiments for adjustment could include the GODIVA[35] and JEZEBEL[35] assemblies which have larger sensitivities to high energy data. It has already been pointed out[26] that the principal fission cross sections in these assemblies are highly correlated (^{239}Pu fission cross section is often measured relative to ^{235}U) and that the primary slowing down mechanism is inelastic scattering. Hence, correlations across materials, reactions,

inelastic levels, and energy are expected to be important. (If the correlations are not taken into account, the assemblies should be omitted from the adjustment. The sensitivity of the adjustments to different estimates of the fissile inelastic covariance files will be tested.)

Several of the dosimetry benchmark experiments are very useful for fast reactor cross section adjustment. These experiments are performed in clean, one-dimensional geometry and in configurations quite different than the Argonne critical experiments (stacked platelets) discussed above. The ^{252}Cf free field[36,37] is a spectrum governed by the spontaneous fission neutron spectrum of ^{252}Cf and, as such, is probably the best characterized field of those under consideration. The Intermediate Energy Standard Neutron Field (ISNF)[38] is a fast neutron spectrum resulting from the slowing down of ^{235}U thermal fission spectrum neutrons in carbon, the lower energy region being tailored by the use of a boron shell.

The set of experiments described above were chosen because of the status of documentation, availability of quantified uncertainty information, degree of confidence in the measurements, sensitivities of the measurements to specific cross section data, and the accuracy with which it is perceived that the measurements can be computed. As such, the set of measurements satisfying these multiple needs is currently relatively small (~25). We fully expect this situation to improve in the future with the potential addition of multiple measurements performed in ZPPR-9[39], STF[40], PROTEUS[41], GCFR critical[42], ZPR-9 carbide and oxide zones[34,43,44], ZEBRA-8[45], CFRMF[46], EBR-II[47], and others.

Before the "final" adjustment is made, a close inspection of all the sensitivity profiles will be necessary. If, for example, near equality exists between the profiles of the same integral parameter in two different assemblies with substantially different calculation/experiment ratios, the standard deviations of the integral measurements as well as the calculational procedure should be re-examined. The inspection of sensitivity profiles can also give guidance concerning the range of applicability of the adjusted data, as was done[48] for ZPR-6/7 and CRBR. Cross sections developed from this adjustment procedure will be tested by comparison against integral results from assemblies not specifically included in the adjustment such

as ZPPR-2[35], ZPR-3/56B[35] and ZPR-3/11.[35]

V. ACCURACY OF THE INTEGRAL EXPERIMENTS

It is of vital importance to assign reasonable uncertainties and correlations to the integral experimental data, a task which has only recently been formally undertaken. Our first-round adjustments are expected to rely heavily upon these preliminary estimates, which will clearly be improved with future iteration. However, even these files do include some estimates of correlations for measurements of different parameters for the same assembly, for the same parameter measured in different assemblies, and for different parameters measured in different assemblies.

Table III presents estimated standard deviations and a correlation matrix for 14 of the integral experiments we propose to include in our adjustment. This data was taken from the recent work of Collins and Lineberry.[49] Table IV presents some of the components of the ZPR-9/31 reaction rate uncertainties given in Table III to illustrate the type of effects under consideration. Table V presents typical results[49] for the calculation/experiment comparisons of these experiments based upon ENDF/B-4 data. These results are intended to be indicative of the type of agreement which is currently obtained for the "same" quantities derived from integral measurements and calculated using differential data evaluations. The adjustments to be employed herein will be based upon calculated results from ENDF/B-5 data with a specified calculational procedure described in later sections of this report.

Much of the pertinent uncertainty data for the ^{252}Cf and ISNF field measurements, with which we propose to begin this study, is provided in Table VI. Various researchers[38,50-52] are evaluating or plan to re-evaluate the covariance matrices for the dosimetry spectral indices and reaction ratios.

VI. CROSS SECTIONS TO BE ADJUSTED

The calculation of the integral parameters will be made using ENDF/B-5 for all materials of interest. However, it is only necessary to include

Table III. Covariance Matrices for Integral Experiment Results Selected from CSEWG Benchmarks (Collins and Lineberry[49])

	Experiment	Std. Dev. (%)	Correlation Matrix													
	ZPR-3/48		1	2	3	4	5	6	7	8	9	10	11	12	13	14
1	k	0.10	1	0	0	0	0	0	0	0	0	0	0	0	0	0
2	$^{28}c/^{25}f$	4.4		1	0.53	0	0.30	0	0	0.26	0	0.01	0	0	0	0
3	$^{28}f/^{25}f$	4.6			1	0	0	0.19	0	0	0.18	0	0	0	0	0
	ZPR-6/6A															
4	k	0.10				1	0	0	0	0	0	0	0	0	0	0
5	$^{28}c/^{25}f$	2.7					1	0.26	0	0.38	0	-0.35	0	0.15	0	-0.15
6	$^{28}f/^{25}f$	2.8						1	0	0	0.48	-0.23	0	0	0.37	-0.26
	ZPR-6/7															
7	k	0.10							1	0	0	0	0	0	0	0
8	$^{28}c/^{49}f$	2.3								1	0.24	0.40	0	0.21	0.12	0.13
9	$^{28}f/^{49}f$	2.9									1	0.34	0	0.04	0.57	0.24
10	$^{25}f/^{49}f$	2.1										1	0	0.05	0.24	0.53
	ZPR-9/31															
11	k	0.10											1	0	0	0
12	$^{28}c/^{49}f$	2.3												1	0.17	0.19
13	$^{28}f/^{49}f$	2.6													1	0.46
14	$^{25}f/^{49}f$	2.4														1

Note that measurements of criticality in the various configurations are assumed to be uncorrelated with each other and with reaction rates measured in the same or different assemblies.

Table IV. Estimated 1σ Uncertainties (%) for Reaction Rate Measurements in ZPR-9/31

		^{25}f	^{28}f	^{28}c	^{49}f
I.	Counting Statistics: Activation Foils and Fission Chambers				
	Random: Statistics	1.1	1.1	1.3	0.8
	Geometry and Zero Extrapolation of Fission Counters				
	^{235}U Counter	0.4			
	^{238}U Counter		0.4		
	^{239}Pu Counter				0.4
	Composition Uncertainty		0.3		
II.	Calibration of Foils with Chambers				
	Mass ^{235}U in F.C.	1.2			
	Mass ^{238}U in F.C.		1.2		
	Mass ^{239}Pu in F.C.			1.4	1.4
	Alpha Calibration $^{28}c/^{49}f$ Using ^{243}Am			1.0	
III.	Cell Averaging Uncertainty				
	Surface Foil/Plate Average				
	Plate Average from Foil Measurements:				
	^{235}U Foils:	0.4			
	^{239}Pu Foils:				0.4
	^{238}U Foils: Fuel Plate Capture			0.5	
	: ^{238}U Plate Capture			0.8	
	: Fuel Plate Fission		0.9		
	: ^{238}U Plate Fission		0.6		

Note: Entries in the same row except for the random statistics are correlated.

Table V. Calculation/Measurement Comparisons Based Upon Version 4 Cross Sections*

No.	Experiment	Measured Value	Experiment[a] Uncertainty (%)	Y_{Exp}[b]
	ZPR-3/48			
1	k	1.000	0.10	0.991
2	$^{28}c/^{25}f$	0.1370	4.4	0.926†
3	$^{28}f/^{25}f$	0.03260	4.6	0.990†
	ZPR-6/6A			
4	k	1.000	0.10	0.985
5	$^{28}c/^{25}f$	0.1378	2.7	1.028
6	$^{28}f/^{25}f$	0.02388	2.8	0.937
	ZPR-6/7			
7	k	1.000	0.10	0.984
8	$^{28}c/^{49}f$	0.1422	2.3	1.072
9	$^{28}f/^{49}f$	0.02422	2.9	0.968
10	$^{25}f/^{49}f$	1.071	2.1	1.036
	ZPR-9/31			
11	k	1.000	0.10	0.989
12	$^{28}c/^{49}f$	0.1230	2.3	1.066
13	$^{28}f/^{49}f$	0.0300	2.6	0.960
14	$^{25}f/^{49}f$	1.036	2.4	0.978

*Appendix II provides more detail regarding the source for the numbers shown in the columns "Measured Value" and "Y_{exp}".

†These results are currently being re-evaluated, per telephone conversation with P. J. Collins on 4/2/79.

[a]This column does not include uncertainties in either the calculation or bias.

[b]Y_{exp} = (Calculation + Bias)/Experiment where bias designates known corrections (e.g., homogeneous to heterogeneous, one-dimensional to two-dimensional, etc.) to give calculation pertinent to actual experiment.

Table VI. Estimated Uncertainties and Correlations for Dosimetry Benchmark Experiments for Fast Reactor Cross Section Adjustment

No.	Experiment	Measured Value	Rel. Std. Dev. %	^{252}Cf Field			ISNF	
				1	2	3	4	5
1	^{25}f	1.205 barns	2.1	1	0.38	0.43	0.30	0.44
2	^{28}f/^{25}f	0.2644	1.1		1	0.13	0.69	0.11
3	^{49}f/^{25}f	1.500	1.3			1	0.23	0.95
4	^{28}f/^{25}f	0.0920	0.62				1	0.23
5	^{49}f/^{25}f	1.155	1.3					1

Remarks:

1. The derivation of the matrix relies on Refs. (37) and (38) and on additional information extracted from the original Laboratory notebooks by D. M. Gilliam (NBS). A reevaluation of the error analysis was performed at ORNL-EPD by R. E. Maerker and J. J. Wagschal.

2. Only experiment 1 is an absolute measurement – all others are ratio measurements. The same experimental technique was used in all these experiments, and the major contributor to the uncertainties is the mass assay uncertainty.

3. The values of experiments 4 and 5 were derived by combining the different experimental values in Ref. (38) taking all correlations into account.

in an adjustment procedure those cross sections with significant sensitivities (considering the associated uncertainties) for any of the integral parameters of interest. Covariance files will also be taken from ENDF/B-5[16] supplemented by existing data[17] where data from Version 5 is not available and where the differences between the Version 4 and Version 5 files are insignificant with respect to the characterization of the differential covariance files.

At this time, the cross sections to be adjusted are listed below:

Cross Sections* Included in the Adjustment Procedure

C(n,n), C(n,n′)

O(n,n), O(n,n′)

Na(n,n), Na(n,n′), Na(n,γ)

Fe(n,n), Fe(n,n′), Fe(n,γ)

Ni(n,γ)

Cr(n,γ)

^{235}U(n,f), ^{235}U(n,γ), ^{235}U($\bar{\nu}$), ^{235}U(χ), ^{235}U(n,n′), ^{235}U(n,n)

^{238}U(n,f), ^{238}U(n,γ), ^{238}U($\bar{\nu}$), ^{238}U(n,n′), ^{238}U(χ), ^{238}U(n,n)

^{239}Pu(n,f), ^{239}Pu(n,γ), ^{239}Pu($\bar{\nu}$), ^{239}Pu(χ), ^{239}Pu(n,n′), ^{239}Pu(n,n)

^{240}Pu(n,f), ^{240}Pu(n,γ), ^{240}Pu($\bar{\nu}$)

^{241}Pu(n,f), ^{241}Pu($\bar{\nu}$)

*Note that secondary angular distribution data have not yet been considered.

This list is meant to be generally inclusive and contains cross sections with marginally significant sensitivities. If, based on our initial results, we find these cross sections to have had no significant adjustment, they will be removed from later iterations. What differentiation we have between the structural material capture cross sections may be provided by direct tests of the Fe cross section in a dosimetry field. Since the dominant part of the ^{238}U inelastic in mixed oxide systems is channeled through the discrete levels, we do not include uncertainty in the inelastic spectral shape. We have only approximate covariance files for ^{235}U(n,n′) and ^{239}Pu(n,n This is a very difficult file to evaluate because of the presence of fission. As we have noted earlier, a covariance file for the total neutron emission spectrum (fission plus inelastic) would still be quite valuable in this

regard. The sensitivity of the adjustments to different estimates of the fissile inelastic covariance files will be tested.

Each reaction is characterized by a covariance matrix (26x26)* and correlations exist, of course, across energy range and reaction type. Not all energy groups will require adjustment (e.g., below $^{238}U(n,f)$ threshold, etc.). In past studies,[12] preliminary files for fission, capture, and $\bar{\nu}$ of the principal heavy nuclides, and elastic and non-elastic for Na, Fe, and O were developed by evaluators at ORNL. In later studies,[53] these files were supplemented with a fission spectrum temperature variance and covariance information for ten groupings of inelastic levels for ^{238}U inelastic scattering. In all of these cases, we would hope to replace these files with the differential covariance data from the ENDF/B-5, if at all feasible.

It is important to note that ENDF/B-5 is the first release which contains substantial differential covariance information. These files should represent a significant improvement over our earlier files[17] since they will, for the most part, be evaluated by the expert who is also the evaluator of the material cross sections of interest. The Version 5 files should also significantly extend the scope (in terms of number of materials and reactions) of our existing covariance files. However, our existing files[17] were developed using similar techniques and have already been used in application[12]; thus, they are roughly of the same "quality" and are not likely to contain "gross blunders," at least for the important reactions. This is not necessarily true of the emerging ENDF/B-5 files which are being developed using a variety of dissimilar techniques and which may likely vary in credibility. It is the purpose of the CSEWG Phase I and II review processes to provide a minimum level of screening of the proposed files and to eliminate most of the major inconsistencies.[16] If we find that:

(1) similar adjustments are obtained using the ENDF/B-5 and our current covariance files (i.e., the adjustments are insensitive to detailed features of covariance shape and magnitude),

(2) the input data are adequately consistent and the adjustments are in accord with our experience and expectations, or at least are not in violation of good sense,

*A (13x13) covariance matrix is also to be used for the information feedback to the measurement program.

(3) inclusion or deletion of any specific integral parameter measurement does not markedly change the result, and

(4) calculated predictions of performance parameters of a broad range of systems not included in the adjustment are improved using the adjusted data,

then the current level of covariance estimation (both differential and integral) may be adequate for integral parameter prediction and for specific recommendations back to the evaluation process (assuming methods bias and uncertainty are also specified--see below). The ongoing data testing program causes a problem for systematic adjustment procedures in that some of the same integral experiments have already been taken into account in the ENDF/B evaluations in a way that is difficult to quantify. To date, we do not have an explicit way to handle this problem when "raw" evaluations are not available.

The CSEWG Fast Reactor Data Testing Subcommittee reports that sensitivity information and recommendations for evaluation are adequate in multigroup form (i.e., recommended changes are proposed over broad intervals rather than for specific cross section parameters). The specific recommendation developed from systematic adjustments of data using CSEWG benchmarks would be an appropriate starting point for consideration of evaluation updates for subsequent versions. Such recommendations would have to be weighed against newer differential and integral data measured and the effects of any improvements in methods in the interim period. In this weighing process, it is important that one recognize the explicit uncertainties and correlations that will be attached to the adjusted cross section parameters. Also, sensitivity coefficients will be scanned to show what parameters, known to be important elsewhere, are not "tested" by the integral experiments. Finally, an updated adjustment made with the additional data would be the tool by which one could observe whether the evaluation process is indeed converging.

VII. INTEGRAL PARAMETER CROSS SECTION SENSITIVITIES

The adjustment process requires sensitivity data for the integral experiments of Table III and VI of Section V, for the cross sections

discussed in Section VI, in the group structure of Tables I and II. Essentially all of these sensitivity coefficients, based upon calculations using ENDF/B-4, have been generated[51-54] and are available from RSIC.[55] These profiles will be used directly under the assumption that the sensitivity profiles are relatively stable with respect to small cross section changes. However, some additional data is undoubtedly required. For example, sensitivities of the fission ratio (^{28}f/^{49}f) to the parameters of the functional representation of the fission spectrum will have to be generated since they have not been previously computed (see Appendix I). More generally, where the form of the data presented has changed markedly from Version 4 to Version 5 (e.g., Maxwellian fission spectrum to energy-dependent Watt spectrum; evaporation spectrum for continuum to inelastic pseudo discrete-inelastic scattering, etc.), new sensitivities will have to be generated. This is clearly the case for the fission spectrum of the fertile and fissile materials and for the inelastic scattering representation of ^{238}U. These sensitivities for as-built critical experiments contain no k-reset[53] as would the sensitivities for a design model. (The concepts about which sensitivities, k constrained or unconstrained, should be used as part of the adjustment procedure will be reviewed.)

VIII. CALCULATIONAL METHODOLOGY

Pseudo-composition independent multi-group neutron cross section data will be generated from ENDF/B-5 in a fine (~174 energy groups) multi-group structure using the MINX code.[56] Infinitely dilute cross sections and Bondarenko factors will be input to the Bonami-II code[57] whereby the cross sections will be self-shielded and space energy collapsed. Transport calculations will then be performed using the ANISN code[22] and specifications provided in the CSEWG benchmark book[35] [including appropriate corrections for dimensionality (1D→2D), order of scattering ($P_3 \rightarrow P_\infty$), etc.]. An updated version of the PUFF code[58] will be used to generate multi-group covariance matrices. Where additional sensitivities need be computed, the JULIET module[23] of the FORSS system will be applied.

The computed performance parameters for the critical experiments will be analyzed in detail, and an attempt will be made to assess both the calculational bias and the residual uncertainty (see Section IX). Relevant

information will include numerical experiments wherein key calculational parameters (e.g., group structure, weighting function, space mesh, etc.) will be varied. Moreover, independent calculations of the same parameters made by other participating CSEWG laboratories, will be available as part of the ENDF/B-5 data testing process.

IX. METHODS BIAS AND UNCERTAINTIES

Data adjustment procedures are usually employed in connection with a well specified ensemble of calculational tools. These procedures continue to be used[1-4] in predicting values of design parameters, but no claim is made for "better" cross sections or "unique" adjustments since the adjustments computed presumably included hidden biases due to methods approximations. In an attempt to cope with this difficulty, and thereby improve the quality of the adjustments to the differential data as well as the integral data, we have begun to separate and quantify the biases and uncertainties associated with the calculational approximation. These biases and uncertainties must still clearly be associated with the calculational procedure described in earlier sections. The discussion of this subject is divided below into two parts:

- Determination of calculational methods biases (extrapolation to best estimate predictions) and associated uncertainties
- Procedure for formally including methods bias and uncertainties in the adjustment process

Each of these is described below in turn.

A. Determination of Calculational Biases and Associated Uncertainties

The quantitative assessment of calculational biases and associated uncertainties is an extremely difficult and important subject. Some recent work in this regard is that of McKnight and Collins[59], who have provided preliminary estimates of the homogeneous-to-heterogeneous, streaming, diffusion-to-transport, spherical-to-cylindrical, and cylindrical-to-3-D X-Y-Z corrections (and estimated uncertainties) for the eigenvalue and reaction rates of ZPR-6/7 as part of the clarification of the CSEWG fast reactor benchmark specifications. They are in the process of evaluating

this information for all of the integral parameters to be employed ultimately in our adjustment procedure. Other relevant information pertaining to processing methods uncertainties is contained in minutes[60] of the Processing Methods Testing Subcommittee of the Code Evaluation Working Group, and other work pertaining to cross section comparison of different processing codes.[61,62,63]

For the "free field" dosimetry benchmark measurements, the flux is just the relevant fission spectrum and only small (~1.5%±0.7%) transport corrections (e.g., multiple scattering) have been made.[37] The flux spectra are folded with infinitely dilute group constants obtained by processing the ENDF/B data into multi-group form. As we shall see below, infinitely dilute group constants can be processed with uncertainties estimated to be smaller than 0.1% (provided a data base is exactly specified). Associated uncertainties in flux spectra due to source shape, nuclear data, methods, etc. have been evaluated.[52] For the critical experiments, the situation is considerably more complex. The experimental facility is modelled and reduced for user convenience to a one-dimensional representation with appropriate correction factors. These correction factors can have significant uncertainty associated with them. Similarly, the requirements for cross section processing are more severe. The cross sections must be self-shielded since the flux is computed in bulk, heterogeneous media with implicit approximations regarding the flux shape. It has been known for some time that the approximations associated with obtaining appropriately shielded group constants can be significant.[62] Thus, in the discussion below, estimated biases and correction factors pertaining to the reduction of the experiment to a suitable one-dimensional model are considered first. Next, the biases and uncertainties associated with the transport calculation of the neutron flux are considered. Finally, the uncertainties associated with shielded group cross section generation are estimated. All corrections from the actual experimental configuration to the benchmark model are taken from the ANL work[59] and are clearly separated from the computation of the benchmark model which is performed with the calculational methodology described in this report. In general, we report biases and uncertainties only for eigenvalue and the selected reaction rate ratio experiments to be analyzed. The biases are most often

experiment-dependent, but the uncertainties in the biases are assumed constant for all of the critical assemblies (i.e., the uncertainties associated with modelling parameters for ZPR-6/7 are assumed common to ZPR-6/6A, ZPR-9/31, and ZPR-3/48). The contribution to response uncertainties due to uncertainties in the computation of sensitivity coefficients are assumed to be negligible (~1% in fission and capture sensitivities) based upon comparisons[54] of fast reactor sensitivities computed at ANL and ORNL. (It may also be noted that sensitivity coefficients will always be multiplied by cross section differences; thus, uncertainties in sensitivity coefficients will tend to second-order corrections $[(S+\Delta S)(\Delta\sigma)]$).

1. Reduction of the Experimental Configuration to a Suitable One-Dimensional Model

The procedure involved in this modelling activity involves several steps. First, the actual three-dimensional heterogeneous configuration is reduced, usually to two-dimensional cylindrical geometry, by volume weighting various constituents in each of the zones. Equivalent heterogeneous cross sections are determined by space-energy collapsing the computed flux spectrum obtained for representative cells (platelet configurations in drawers). At this stage, a streaming correction is determined since the heterogeneous cross section set determined in the previous step does not properly account for leakage effects (as the moderator in each drawer lines up, planar streaming paths are created). A new set of homogeneous cross sections is determined for the two-dimensional model (i.e., neglecting the actual spatial fine structure), and a homogeneous/heterogeneous eigenvalue bias correction is determined. Next, using the homogeneous cross section set, a one-dimensional model is constructed by performing a boundary search with the eigenvalue presumed to be that which was obtained for the two-dimensional model using homogeneous cross sections. Bias factors for the reaction rate ratio between the one- and two-dimensional models are determined by difference. It should also be noted that the capability now exists at Argonne National Laboratory to model each drawer and platelet for the entire reactor individually for those problems where these correction factors are highly uncertain. Finally, a correction is

estimated for the non-normal unit cell used only in the ZPR-6/7 measurements. This correction accounts for the subdivision of the Pu-U-Mo fuel plate into two halves to permit the placing of a foil between them. Each half is canned in steel resulting in an excess of structural material relative to the other drawers. The U assembly ZPR-6/6A didn't require such canning (no Pu), and different experimental techniques to relate the fission rate measured outside the plate to that at its central position were used for the other Pu assemblies.

Hence to summarize, the following includes estimates of corrections and uncertainties pertaining to eigenvalue and central reaction rate ratios for (a) modelling the three-dimensional geometry in two-dimensions, (b) streaming between drawers, (c) homogeneous-to-heterogeneous corrections, (d) modelling the two-dimensional geometry in one-dimension, and (e) corrections for the non-normal ZPR-6/7 unit cell. Biases as defined in this paper are added to or multiplied into the computed model value before final comparison to integral experiment results.

a. Modelling the three-dimensional experimental configuration in two-dimensions. The bias factors associated with this correction have been determined by McKnight and Collins[59] to be negligible (i.e., 1.000±0.0003 for both eigenvalue and central reaction rate ratios) as applied to ZPR-6/7. The correction is typical of results found when comparing R-Z and X-Y-Z diffusion theory. The fact that the bias factor approaches unity merely reflects the large size of the ZPR-6/7 (and ZPR-6/6A, ZPR-3/48, and ZPR-9/31) assembly; thus, details of modelling the exterior boundary are expected to have little impact for eigenvalue and central reaction rate ratios. For the purpose of this work, the three-dimensional to two-dimensional modelling bias factors will be assumed as unity, and their uncertainties will be neglected for each of the four ANL critical assemblies.

b. Bias factors and uncertainties pertaining to streaming between drawers. The bias factors were determined directly by constructing (in addition to the reference "heterogeneous" cross section set) a new cross section set which contained directionally-dependent diffusion coefficients[64-66] derived using the Benoist method applied to the unit cell. The result of whole reactor calculations, with and without inclusion of

the leakage effect, was used to determine the bias factor. The uncertainty in the streaming bias for reactivity was estimated from the difference in results obtained using equivalent approaches for the determination of the directionally-dependent diffusion coefficient, i.e., the Benoist and the Gelbard methods.

The bias factors will be assumed to apply to each of the four ANL critical assemblies based upon the fact that they have comparable fuel and coolant volume fractions. We will assume uncertainties in the same parameter in different assemblies are fully correlated, but uncertainties in different integral parameters are uncorrelated. (No data currently exists regarding the magnitude of the correlations.) This assumption will be tested by investigating "trial" correlations to see whether their impact could be significant.

Table VII. Bias Factors and Uncertainties Pertaining to Plate Streaming in ZPR-6/7

ZPR-6/7 Parameter	Streaming Bias	Estimated Uncertainty in Bias Factor (1σ)
k	-0.0030 (A)*	± 0.0003
$^{28}c/^{49}f$	0.9985 (M)	± 0.0005
$^{28}f/^{49}f$	1.0036 (M)	± 0.0012
$^{25}f/^{49}f$	0.9989 (M)	± 0.0004

*A (additive)
M (multiplicative)

c. Bias factors and uncertainties pertaining to the use of a homogeneous instead of a heterogeneous model. Since the reference benchmark model is actually a homogeneous model, bias factors were determined by comparing results of whole reactor R-Z calculations using the reference space energy self-shielded cross sections (representing the actual heterogeneous drawer configuration) and cross sections deduced for the two-dimensional homogeneous model. The bias factors are significant and are assembly-dependent. We list in Table VIII the bias factors for ZPR-6/7; similar factors for the other three critical assemblies can be found in the

benchmark book.[35] The uncertainties in the bias factors are perceived to arise mainly from approximations in generating cross sections for the unit cell. Thus, the quoted uncertainties were obtained by comparing results of homogeneous/heterogeneous bias factors computed for the unit cell with deterministic and point Monte Carlo methods. Little information exists, as before, regarding the correlation of the uncertainties. Hence, as before, only uncertainties in the same parameter in different assemblies will be (fully) correlated.

Table VIII. Bias Factors and Uncertainties Pertaining to the Determination of the Homogeneous/ Heterogeneous Correction in ZPR-6/7

ZPR-6/7 Parameter	Homogeneous/Heterogeneous Bias Factor	Estimated Uncertainty in Bias Factor (1σ)
k	+0.0166 (A)	± 0.002
$^{28}c/^{49}f$	0.9775 (M)	± 0.003
$^{28}f/^{49}f$	1.0095 (M)	± 0.005
$^{25}f/^{49}f$	1.0189 (M)	± 0.002

d. Bias factors and uncertainties for modelling the ZPR-6/7 two-dimensional cylindrical geometry as a one-dimensional sphere. The calculation was performed with an outer boundary search to preserve the eigenvalue obtained for the two-dimensional cylindrical geometry case using homogeneous cross sections. Hence, the bias factor for k was constrained to be unity. The impact on the other parameters is listed below in Table IX.

Table IX. Bias Factors and Uncertainties for Modelling the ZPR-6/7 Two-Dimensional Cylindrical Geometry as a One-Dimensional Sphere

ZPR-6/7 Parameter	2-D to 1-D Bias Factor	Estimated Uncertainty in Bias Factor (1σ)
k	1.0000 (M)*	± 0.0003
$^{28}c/^{49}f$	1.0007 (M)	± 0.0002
$^{28}f/^{49}f$	1.0013 (M)	± 0.0004
$^{25}f/^{49}f$	1.0000 (M)	± 0.0002

*M (multiplicative)

These bias factors are small enough such that we propose to apply the bias factor (to each of the four critical assemblies) and neglect entirely the uncertainty associated with them.

e. Bias factor and uncertainty associated with ZPR-6/7 corrections from non-normal experimental to normal unit cell. Reaction rates in ZPR-6/7 were measured using foils placed between two "half-thickness" Pu-U-Mo fuel plates whereas the normal unit cell contained one 1/4" thick plate. Thus the experimental loading had approximately 33% less Pu-Mo, 15% less ^{238}U and 7.5% more stainless steel than the reference unit cell. Current experiments for plutonium systems use foils outside the cladding of the normal fuel plates and make use of subsidiary experiments to determine the "plate average" experimental values. Corrections for reaction rates in the ZPR-6/7 experimental unit cells (estimated by calculations for the two heterogeneous cells) are as follows in Table X.

Table X. Bias Factors and Uncertainties Associated with the Non-Normality of the ZPR-6/7 Unit Cell

ZPR-6/7 Parameter	Bias Factor	Estimated Uncertainty in Bias Factor (1σ)
$^{28}c/^{49}f$	1.0029 (M)*	± 0.001
$^{28}f/^{49}f$	0.9673 (M)	± 0.011
$^{25}f/^{49}f$	0.9879 (M)	± 0.003

*M (multiplicative)

The uncertainties in the bias factor were assumed to be approximately 1/3 of the difference between the bias factor and unity; this bias factor and uncertainty applies only to ZPR-6/7.

2. Approximations made in performing the transport calculation (for a given set of multi-group cross sections

a. Corrections to better approximate higher order transport theory.

The calculations will be performed using transport theory with S_8P_3 approximation. Thus, there is no bias to be applied to correct from diffusion theory to S_8P_3. There are, however, biases to be associated with going from S_8P_3 to $S_\infty P_\infty$. These are considered here to be negligible and this will be verified during data testing.

The mesh spacing for the benchmark calculation has been recommended as part of the CSEWG specifications. During the course of the data testing, we will verify that introduction of a finer radial mesh does not have any significant impact on the computed results.

3. Biases and uncertainties associated with the generation of self-shielded cross sections in the one-dimensional model

Recent comparative studies of the Large Core Code Evaluation Working Group have shown[67] that "broad few-group cross sections can yield excellent agreement with fine-group ones, provided the cross sections are generated in sufficient detail. Very good agreement was found between the homogeneous cross sections processed by General Electric using MINX/TDOWN-III and by Argonne National Laboratory using MC^2-2/SDX." With regard to eigenvalue and reaction rates, the same type of agreement was observed as part of the Processing Methods Testing activity of the Code Evaluation Working Group.[60] We attempt below to quantify the results of this experience and establish what is meant by "good agreement" based upon our experience in Processing Methods Testing and CSEWG Data Testing.

a. Uncertainties in processed group constants. Tables XI-XIV illustrate the flux averaged multi-group cross section percent difference between cross sections computed by ANL and ORNL for the principal materials in a mixed oxide LMFBR composition (i.e., the ZPR-6/7 infinite media problem of the Processing Methods Testing Subcommittee). The percent differences are tabulated relative to the ANL values and are indicative of the differences in processed group constants obtained using independent techniques based upon the same data base (ENDF/B-4). Also listed is the percentage of the flux in each of the broad energy regions for which different cross section representations are provided.

Table XI. Observed Differences in $^{239}Pu(n,f)$ Multi-Group Constants Obtained Using Different Processing Strategies for Fast Breeder Mixed Oxide Systems

Energy Region	$^{239}Pu(n,f)$ % Flux	Multi-Group Cross Section % Difference (Rel. to ANL)
Resolved (1 eV-301 eV)	0.2	-2.48
Unresolved (301 eV-25 keV)	23.3	0.73
Smooth (25 keV-20 MeV)	76.5	0.004

Comments

Smooth Energy Region: Max % Dif., 0.03%; some sign cancellation

Unresolved Energy Region: Max % Dif., ~1.5%, ORNL almost consistently higher

Resolved Energy Region: Max % Dif., ~12.5% (below 50 eV)

Table XII. Observed Differences in $^{238}U(n,\gamma)$ Multi-Group Constants Obtained Using Different Processing Strategies for Fast Breeder Mixed Oxide Systems

Energy Region	$^{238}U(n,\gamma)$ % Flux	Multi-Group Cross Section % Difference (Rel. to ANL)
Resolved (1 eV-4 keV)	5.7	-0.50
Unresolved (4 keV-45 keV)	25.1	0.07
Smooth (45 keV-20 MeV)	69.2	0.098

Comments

Smooth Energy Region: Max % Dif., 0.32%; some sign cancellation

Unresolved Energy Region: Max % Dif., 0.50%; significant sign cancellation

Resolved Energy Region: Max % Dif. (above 500 eV max dif. is 2%, below differences are >50%)

Table XIII. Observed Differences in $^{238}U(n,f)$ Multi-Group Constants Obtained Using Different Processing Strategies for Fast Breeder Mixed Oxide Systems

	$^{238}U(n,f)$	
Energy Region	% Flux	Multi-Group Cross Section % Difference (Rel. to ANL)
Subthreshold (50 keV-500 keV)	48.8	0.042
Smooth (500 keV-20 MeV)	20.5	-0.015

Comments

Subthreshold Energy Region: Max % Dif., 1.7%; cross section negligible

Smooth Energy Region: Max % Dif., 0.4%; some sign cancellation but differences by group essentially negligible

Table XIV. Observed Differences in $^{235}U(n,f)$ Multi-Group Constants Obtained Using Different Processing Strategies for Fast Breeder Mixed Oxide Systems

	$^{235}U(n,f)$	
Energy Region	% Flux	Multi-Group Cross Section % Difference (Rel. to ANL)
Resolved (1 eV-82 eV)	0.0	2.3
Unresolved (82 eV-25 keV)	23.5	0.37
Smooth (25 keV-20 MeV)	76.5	0.02

Comments

Smooth Energy Region: Max % Dif., 0.12%; some sign cancellation

Unresolved Energy Region: Max % Dif. above 500 eV, ~1.1%; ORNL consistently higher

Resolved Energy Region: Max % Dif., ~3%; lots of cancellation, flux negligible

The variation in the group-to-group matrix scattering elements is considerably larger. For materials such as Fe, Na, and O, the predominant scattering species, an uncertainty of 40% is considered realistic. It is essential to note, however, that this uncertainty is highly anti-correlated between within-group ($\sigma_{g\to g}$) and out-of-group ($\sigma_{g\to g'}$) transfers since the uncertainty in the total scattering cross section is relatively small. The bulk of the uncertainty in transfer matrix elements arise from the lack of knowledge of the detailed flux spectrum near the bottom of an energy group. In particular, the treatment of resonances of other materials (other than the material for which the transfer matrix element is being computed) is highly approximate. There is no correlation assumed between out-of-group transfers for different energy groups since the location of material resonances relative to one group boundary has little to do with the resonance structure near another group boundary. The estimated uncertainty is given in Table XV.

Table XV. Estimated Covariance for the Computation of Multi-Group Transfer Matrices

Group Transfer Matrix Elements	Estimated Rel. Std. Dev. (%)
In-group	40
Out-scatter	40
Cor ($\sigma_{g\to g}$, $\sigma_{g\to g'}$) $\simeq -1$	(total scattering cross section well-known)
Cor ($\sigma_{g\to g'}$, $\sigma_{h\to h'}$) $\simeq 0$	(removal from bottom of group, uncorrelated between successive groups)

The correlations between in-scatter and out-scatter results in large compensating effects. For example, increasing all out-scatter cross sections by 1%, and decreasing within-group scattering by the same absolute amount results in an eigenvalue change of 0.01%, which represents the cancellation of two terms of opposite sign whose magnitude is of the order of 2.5%.

Finally, our comparisons of fission spectra indicate that there is up to a 0.6% difference in fission fraction/group between different processing methods due to whether one computes a composition-dependent spectrum, takes the spectrum to be that of the principle fissioning species, allows for incident energy dependent-spectra, etc.

Combining the data of Tables XI-XV with the discussion above, accounting for the fact that there has been some cancellation in taking weighted averaged multi-group differences, and in factoring in our experience with other comparative calculations, we arrive at the evaluated processing methods uncertainty indicated in Table XVI. The correlation matrix is assumed to be represented as fully correlated within the resolved, unresolved, and smooth energy regions and uncorrelated between each of these regions. This has yet to be justified. (It is also intended to be fully correlated across isotopes for each type of energy region.) This is largely based upon the different processing algorithms used in each of the energy ranges. These global estimates for uncertainty in self-shielded cross sections obviously consist of the combination of several effects including resonance reconstruction, linearization, Doppler broadening, unresolved energy region processing, assumed flux spectrum, energy group structure, groupwise numerical averaging and space energy collapse. There is some data on each of these parts separately, but it is sparse and not well documented.

Using the data in Table XVI along with available sensitivity coefficients, we have tried to propagate the estimated uncertainties in the group constants to uncertainties in the relevant integral parameters. This resulted in variances in eigenvalue, central $^{28}c/^{49}f$, and central $^{28}f/^{49}f$ of 0.43%, 0.9% and 0.8% respectively for ZPR-6/7. The $^{25}f/^{49}f$ uncertainty was not determined explicitly since it will surely be comparable to, and probably less than, the uncertainty for $^{28}c/^{49}f$. Tables XVII-XXII indicate the sensitivities and uncertainties for each of the integral parameters. These uncertainties will be assumed to be common to each of the four ANL critical experiments. There is clearly a correlation between integral parameters of different types (as well as full correlation between the same parameter in different assemblies), and this will be determined by folding the processing method uncertainties with sensitivities for the different parameters. A similar analysis is required for results from the ISNF facility.

Table XVI. Evaluated Processing Methods Uncertainties for Fast Breeder Mixed Oxide Systems

Energy Region	Rel. Std. Dev. (%)
$^{239}Pu(n,f)$	
Resolved (1 eV-301 eV)	2.5
Unresolved (301 eV-25 keV)	1.3
Smooth (25 keV-20 MeV)	0.1
$^{238}U(n,\gamma)$	
Resolved (1 eV-4 keV)	3.0
Unresolved (4 keV-45 keV)	0.8
Smooth (45 keV-20 MeV)	0.2
$^{238}U(n,f)$	
Subthreshold (50 keV-500 keV)	0.1
Smooth (500 keV-20 MeV)	0.1
Group Transfer Matrices	40.0
$Cor\ (\sigma_{g\to g'}, \sigma_{g\to g'}) \simeq -1$	
$Cor\ (\sigma_{g\to g'}, \sigma_{h\to h'}) \simeq 0$	
Fission Spectrum Source Shape	0.6

Table XVII. Sensitivities and Estimated Multi-Group Cross Section Processing Uncertainties for the Eigenvalue of Typical Mixed Oxide Systems

Cross Section	Energy Region	Sensitivity	Estimated Std. Dev. (%)	Product (cols. 4 and 5) ($\Delta k/k$ %)
^{49}f	Resolved (1 eV-301 eV)	0.002	2.5	0.005
^{28}c	Resolved (1 eV-4 keV)	-0.072	3.0	-0.216
			Fully Correlated Subtotal	-0.21
^{49}f	Unresolved (301 eV-25 keV)	0.172	1.3	0.223
^{28}c	Unresolved (4 keV-45 keV)	-0.091	0.8	-0.072
			Fully Correlated Subtotal	0.15
^{49}f	Smooth (25 keV-20 MeV)	0.424	0.1	0.042
^{28}c	Smooth (45 keV-20 MeV)	-0.080	0.2	-0.016
^{28}f	Smooth (500 keV-20 MeV)	0.079	0.1	0.008
			Fully Correlated Subtotal	0.03

Table XVIII. Summary of Estimated Eigenvalue Variance Due to Processing Method Uncertainties ($\%^2$)

Resolved Energy Region (^{49}f, ^{28}c)	$(-0.21)^2$
Unresolved Energy Region (^{49}f, ^{28}c)	$(0.15)^2$
Smooth Energy Region (^{49}f, ^{28}c, ^{28}f)	$(-0.03)^2$
Total Group Cross Section Variance =	0.067
Group-to-Group Matrix Variance* =	0.080
Fission Spectrum Source Shape* =	0.040
Total Estimated Variance =	0.187
Total Eigenvalue Std. Dev. =	0.43%

*The numerical value utilized in this table is derived from experience in Processing Methods Testing.[60]

Table XIX. Sensitivities and Estimated Multi-Group Cross Section Processing Uncertainties for the Central $^{28}c/^{49}f$ Ratio of Typical Mixed Oxide Sysems

Cross Section	Energy Region	Sensitivity	Estimated Std. Dev.	Product (Cols. 4 and 5) ($\Delta R/R$ %)
^{49}f	Resolved (1 eV-301 eV)	-0.004	2.5	-0.01
^{28}c	Resolved (1 eV-4 keV)	0.283	3.0	0.85
			Fully Correlated Subtotal	.84
^{49}f	Unresolved (301 eV-25 keV)	-0.315	1.3	-0.41
^{28}c	Unresolved (4 keV-45 keV)	0.337	0.8	0.27
			Fully Correlated Subtotal	-0.14
^{49}f	Smooth (25 keV-20 MeV)	-0.753	0.1	-0.075
^{28}c	Smooth (45 keV-20 MeV)	0.270	0.2	-0.054
^{28}f	Smooth (500 keV-20 MeV)	0.0046	0.1	0.004
			Fully Correlated Subtotal	-0.017

Table XX. Central $^{28}c/^{49}f$ Estimated Variance Due to Processing Method Uncertainties ($\%^2$)

Resolved Energy Region (^{49}f, ^{28}c)	$(0.84)^2$
Unresolved Energy Region (^{49}f, ^{28}c)	$(-0.14)^2$
Smooth Energy Region (^{49}f, ^{28}c, ^{28}f)	$(-0.02)^2$
Total Estimated Variance	= 0.72
Total Estimated Std. Dev.	= 0.9%

(Impact of fission spectrum source and group-to-group matrices assumed negligible)

Table XXI. Sensitivities and Estimated Multi-Group Cross Section Processing Uncertainties for the Central $^{28}f/^{49}f$ Ratio of Typical Mixed Oxide Systems

Cross Section	Energy Region	Sensitivity	Estimated Std. Dev.	Product (cols. 4 and 5) ($\Delta R/R$ %)
^{49}f	Resolved (1 eV-301 eV)	-0.003	2.5	-0.0075
^{28}c	Resolved (1 eV-4 keV)	0.082	3.0	0.246
			Fully Correlated Subtotal	0.24
^{49}f	Unresolved (301 eV-25 keV)	-0.213	1.3	-0.277
^{28}c	Unresolved (4 keV-45 keV)	0.101	0.8	0.080
			Fully Correlated Subtotal	-0.20
^{49}f	Smooth (25 keV-20 MeV)	-0.556	0.1	-0.056
^{28}c	Smooth (45 keV-20 MeV)	0.081	0.2	0.016
^{28}f	Smooth (500 keV-20 MeV)	0.969	0.1	0.097
			Fully Correlated Subtotal	0.057

Table XXII. Central $^{28}f/^{49}f$ Estimated Variance Due to Processing Method Uncertainties ($\%^2$)

Resolved Energy Region (^{49}f, ^{28}c)	$(0.24)^2$
Unresolved Energy Region (^{49}f, ^{28}c)	$(-0.20)^2$
Smooth Energy Region (^{49}f, ^{28}c, ^{28}f)	$(0.57)^2$
Total Estimated Cross Section Variance	= 0.10
Group-to-Group Matrix Variance	= 0.16
Fission Spectrum Source Shape	= 0.36
Total Estimated Variance	= 0.62
Total $^{28}f/^{49}f$ Std. Dev.	= 0.80%

B. Procedure for Formally Including Methods Biases and Uncertainties in the Adjustment Process

Conceptually, our data adjustment may be viewed as a calculation with input data A and output data B. The input A consists of the following:

(A1) Evaluated infinitely dilute group cross sections and related nuclear data parameters (as from current ENDF files and described in preceding Section VI). There are M such parameters, the m'th being σ_m, where m represents a specific material, group, and reaction, etc.

(A2) Experimentally-based evaluated values of benchmark integral quantities. There are N such integral measurements, the n'th being I_n.

(A3) Calculated values I_n^c of these benchmark integral quantities using the appropriately self-shielded group cross sections corresponding to the infinitely dilute cross sections of (A1) above, and with the biases (A5) described earlier in this section (IX.A).

(A4) Absolute sensitivity coefficients S_{nm} which are the derivatives of the calculated values of the integral quantities in (A3) with respect to the infinitely dilute group cross sections in (A1) (NxM matrix).

(A5) A set of K individual biases (the k'th is b_k) as discussed in the first part of this section (IX.A), and a prescription in the form of an (NxK) matrix β_{nk} for applying these biases to obtain corrected values of the calculated integral quantities.

(A6) Covariances B_σ associated with infinitely dilute cross sections and nuclear data in (A1) (MxM matrix),

(A7) Covariances B_I associated with the experimental values of the benchmark integral quantities in (A2) (NxN matrix),

(A8) Covariances B_b associated with the biases (A5) of the benchmark integral experiments due to calculational approximations and modelling assumptions and assuming no contribution from the cross section uncertainties (KxK matrix).

The corresponding output from this data adjustment will be the following:

(B1) An adjusted set of values σ_m' for the infinitely dilute group cross sections (and other nuclear data parameters).

(B2) An adjusted set of values I_n' for the benchmark integral quantities,

(B3) An adjusted set of individual biases b_k' corresponding to each correction as discussed in the first part of this section.

(B4) A covariance matrix associated with the above three sets (B1-B3) of adjusted values.

(B5) A number of quantities (such as χ^2 per degree of freedom) useful for evaluating the quality of the adjustment.

The following comments are in order:

1. Covariances associated with the sensitivity coefficients are not part of the input, but are assumed to be sufficiently small that the sensitivities may be regarded as fixed. In other words, we assume there are no uncertainties in the sensitivity coefficients.
2. In principal, there may be correlations between the input data (A1), (A2), and (A3) so that one should use a single covariance matrix instead of the three in (A6), (A7), and (A8). However, we have no such correlational data at the present. Our treatment allows such correlations if they are known.
3. Many previous adjustment schemes disregarded methods uncertainties and hence required no input (A8) and gave no output (B3).
4. The evaluated infinitely dilute group cross sections (A1) will be based on the ENDF/B-5 nuclear data files.
5. In (A3) the calculated values I_n^c of the benchmark integral experiments are assumed to include all of the known corrections, i.e., the individual biases (A5) as presented above in the first part of this section.
6. The calculated values of the integral quantities are given by

$$I^c = F_0(\sigma) + \beta b \qquad (3)$$

where $F_o(\sigma)$ is the basic calculation which depends on the model and calculational techniques and approximations, and where b is a bias vector which corrects various aspects of the basic calculation. The matrix β apportions the various bias contributions to the appropriate integral quantities, and elements of this matrix typically are 0 or 1. In the case where there is one bias for each integral experiment, β is a unit matrix.

The adjusted values are related by

$$I' = F_o(\sigma') + \beta b' \quad . \tag{4}$$

Assuming linearity we express this in terms of sensitivity coefficients

$$I' = I^C + S\Delta\sigma + \beta\Delta b \tag{5}$$

where

$$\Delta\sigma = \sigma' - \sigma \tag{6}$$

and

$$\Delta b = b' - b \quad . \tag{7}$$

We can express Eq. (5) in matrix form by

$$[-1, \beta, S] \begin{bmatrix} I'-I^C \\ b'-b \\ \sigma'-\sigma \end{bmatrix} = 0 \tag{8}$$

which, in terms of the notation which follows, can be expressed as

$$A(x'-x^C) = 0 \quad . \tag{9}$$

The mathematics of adjustment without methods uncertainties has been developed in Refs. (4) and (12). Adjustment with methods uncertainties included was developed in Ref. (68). The following forms of the equations are equivalent to the results of Ref. (68) but are more convenient. The principal results are as follows:

$$x' = x_{exp} + P\,(x_c - x_{exp}) \tag{10}$$

where x_{exp} is a vector of combined integral experiments (A2), individual biases (A8), and evaluated infinitely dilute group cross sections (A1),

$$x_{exp} = \begin{bmatrix} I_1 \\ \vdots \\ I_N \\ b_1 \\ \vdots \\ b_K \\ \sigma_1 \\ \vdots \\ \sigma_M \end{bmatrix}, \tag{11}$$

and x^c is a similar vector with calculated values (which have the unadjusted methods biases already added on) for the integral quantities (A3) replacing the experimental values, i.e.,

$$x^c = \begin{bmatrix} I_1^c \\ \vdots \\ I_N^c \\ b_1 \\ \vdots \\ b_K \\ \sigma_1 \\ \vdots \\ \sigma_M \end{bmatrix}, \tag{12}$$

and x' is the vector of adjusted values for the integral experiments (B2), the adjusted individual biases (B3), and adjusted infinitely dilute cross sections (B1), i.e.,

$$x' = \begin{bmatrix} I'_1 \\ \vdots \\ I'_N \\ b'_1 \\ \vdots \\ b'_K \\ \sigma'_1 \\ \vdots \\ \sigma'_M \end{bmatrix} . \tag{13}$$

The (N+K+M)x(N+K+M) matrix P is given by

$$P = B_{exp}\, \delta^T G^{-1} \delta \tag{14}$$

where (N+K+M)x(N+K+M) matrix B_{exp} is the covariance matrix corresponding to the experimental values of the integral quantities (A2), the biases (A5), and the evaluated cross sections (A1), i.e.,

$$B_{exp} = \begin{bmatrix} B_I & 0 & 0 \\ 0 & B_b & 0 \\ 0 & 0 & B_\sigma \end{bmatrix} . \tag{15}$$

Actually, if correlations are known between integral measurements and evaluated group cross sections, the covariances instead of the zeros may be put into B_{exp}.

δ is an Nx(N+K+M) matrix formed by the negative of the NxN unit matrix, the matrix β which relates the biases to the calculated integral values, and the sensitivity matrix S of (A4). Superscript T indicates the transpose.

$$\delta = [-1, \beta, S] . \tag{16}$$

The corresponding constraint on an output adjusted x' is given by

$$\delta\Delta x = -\Delta I + \beta\Delta b + S\Delta\sigma = 0 \quad . \tag{17}$$

The NxN matrix G is formed from δ and B_{exp}

$$G = \delta B_{exp}\delta^T \quad . \tag{18}$$

The principal contribution to the adjusted covariance matrix B' is given by

$$B' = B_{exp} - PB_{exp} \quad . \tag{19}$$

The value of chi-square, which is the minimum of the least squares objective function, may be evaluated by the following expression:

$$\chi^2 = (x^c - x_{exp})^T \delta^T G^{-1} \delta (x^c - x_{exp}) \quad . \tag{20}$$

CONCLUSIONS

The present work proposes a specific plan of cross section adjustment for fast reactor core physics analysis using information from fast reactor and dosimetry integral experiments and from differential data measurements and evaluations. Through an integration of results from various disciplines, which is required for the success of such a procedure, we have been able to obtain the variety of information necessary for a credible and useful analysis. The output adjusted library and covariance estimates will be used to estimate nominal parameter values with uncertainties for related reactor designs with a reduced dependence upon data-related bias factors. The adjustments themselves should provide specific recommendations to nuclear data evaluation programs.

As part of this work, specific recommendations for library format, group structure, cross sections to be adjusted, sources of differential data covariance, sources of sensitivities, calculational methodology, choice of integral experiments, sources of integral experiment covariances, and calculational "methods" uncertainties were deduced. In particular, the systematic formulation of methods biases and uncertainties, as well as their incorporation within the adjustment methodology, were determined. The information from the systematic combination of differential and integral data is equivalent to that sought in testing the adequacy of evaluated nuclear data sets. Finally, the adjustment process will provide us with a more global view of analysis by forcing us to openly recognize and quantify what we are doing.

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APPENDIX I

Sensitivity Coefficients of Performance Parameters with Respect to Fission Spectrum Parameters

Summary:

Since the sensitivity expressions for the parameters of the fission spectrum have not been described explicitly in our earlier work, the resulting formulas are described briefly below. We assume that fission neutrons are born isotropically in the laboratory system and that parameters describing the merging spectrum depend upon incident energy (E') through a linear functional dependence on J parameters θ_j as follows:

$$\theta_j(E', a_1, a_2) = a_{1j} + a_{2j}E' \qquad j = 1,j \quad . \tag{I.1}$$

The application of sensitivity theory leads to the following sensitivity of response R (depending on the forward but not the adjoint flux) with respect to a^F_{ij}, the i^{th} parameter in the j^{th} term of the incident energy dependence of fissile nuclide F:

$$\frac{\partial R/R}{\partial a^F_{ij}/a^F_{ij}} = \int dE \int dE' \left[\frac{\partial R}{\partial \chi^F(E,E')} \frac{\chi^F(E,E')}{R}\right] \alpha^F_j(E,E') \beta^F_{ij}(E') \tag{I.2}$$

$$+ \frac{1}{k_{eff}} \int d\underline{r} \int dE \frac{\Gamma^*}{R} \int dE' \, (\nu\Sigma_f)^F \phi_0 \chi^F \alpha^F_j \beta^F_{ij}$$

where

$$\alpha^F_j \equiv \frac{\theta^F_j}{\chi^F} \frac{\partial \chi^F}{\partial \theta^F_j}$$

and

$$\beta^F_{ij} \equiv \frac{a^R_{ij}}{\theta^F_j} \frac{\partial \theta^F_j}{\partial a^F_{ij}} \quad .$$

The quantity in square brackets in the first integral on the right of Eq. (I.2) represents the contribution to the relative sensitivity of R with respect to χ due only to the explicit mathematical dependence of R on χ.

Γ^* is the relative generalized adjoint for response R (averaged over solid angle) and ϕ_0 is the forward flux (integrated over solid angle). For a Maxwellian type spectrum, there is but one parameter θ(J=1). In this representation,

$$\chi = \sqrt{\frac{4E}{\pi\theta^3}}\, e^{-E/\theta} \tag{I.3}$$

and

$$\alpha = E/\theta - 3/2 \quad . \tag{I.4}$$

For a Watt type spectrum there are two parameters, θ_1 and θ_2.

$$\chi = \sqrt{\frac{4\theta_2}{\pi\theta_1^3}}\, \exp(-\theta_1/4\theta_2 - E/\theta_1)\, \sinh((E/\theta_2)^{1/2}) \tag{I.5}$$

and

$$\alpha_1 = E/\theta_1 - \theta_1/4\theta_2 - 3/2 \tag{I.6}$$

$$\alpha_2 = \frac{1}{2} + \frac{\theta_1}{4\theta_2} - \frac{1}{2}\,(E/\theta_2)^{1/2} \coth\,((E/\theta_2)^{1/2}) \quad . \tag{I.7}$$

Using the notation of Ref. (19), and assuming no direct effect contribution [no first term in Eq. (I.2)], the multi-group expression for the sensitivity of of R is:

$$\frac{\partial R/R}{\partial a_{ij}^F/a_{ij}^F} = \frac{1}{k_{eff}} \sum_Z d_{FZ} \sum_{I\in IZONE(Z)} V_I \left\{ \Big/ \sum_{G=1}^{NOG} (\nu\sigma_f)^Z_{FG} \right. \tag{I.8}$$

$$\left. \times \sum_{G'=1}^{NOG} \frac{\Gamma^o_{IG'}}{R}\, \chi^F_{G'G}\, \alpha^{Fj}_{G'G}\, \beta^{iFj}_{GG'} \right\} \quad .$$

Typical calculations assume that χ and α are independent of incident energy. In this case, there is only one relevant a_f and the corresponding β_f is unity.

APPENDIX II

Sources of Information for Numbers Appearing in Table V

Measured Values:

1. For experiments 1-5 and 7, the source is R. D. McKnight, "Benchmark Testing Using ENDF/B Versions III and IV," *Nucl. Sci. Eng.* 62(2): 309 (1977). See also R. D. McKnight, "Benchmark Testing Using ENDF/B Versions III and IV," ZPR-TM-214, Argonne National Laboratory (September 5, 1975).

2. For experiments 6 and 8-10, the data in Ref. (1) has been revised by P. J. Collins and D. N. Olsen, Argonne National Laboratory, Idaho, due to reweighting of calibration techniques which were originally given equal weight, also some revision to the original uncertainties.

3. For experiments 11-13, the source is R. D. McKnight, "Benchmark Specifications in CSEWG Format for ZPR-9 Assembly 31, the Advanced Fuels Program Carbide Benchmark Critical Assembly," ZPR-TM-281, Argonne National Laboratory (June 13, 1977).

4. For experiment 14, the source is private communication, J. A. Morman, Argonne National Laboratory, to P. J. Collins, Argonne National Laboratory, Idaho (January 1979).

Calculations:

1. For integral parameters 1-10, the source is R. D. McKnight, "Benchmark Testing Using ENDF/B Versions III and IV," *Nucl. Sci. Eng.* 62(2): 309 (1977). See also R. D. McKnight, "Benchmark Testing Using ENDF/B Versions III and IV," ZPR-TM-214, Argonne National Laboratory (September 5, 1975).

2. For integral parameters 11-14, the source is R. D. McKnight, "Benchmark Specifications in CSEWG Format for ZPR-9 Assembly 31, the Advanced Fuels Program Carbide Benchmark Critical Assembly," ZPR-TM-281, Argonne National Laboratory (June 13, 1977).

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