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Integral Data Evaluation of Stainless Steel, 239Pu, 240Pu, and H₂O for Homogeneous **Plutonium Systems**

U. P. Jenquin J. K. Thompson T. J. Trapp D. A. Kottwitz

August 1979

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INTEGRAL DATA EVALUATION OF STAINLESS STEEL, ²³⁹Pu, ²⁴⁰Pu, and H₂O FOR HOMOGENEOUS PLUTONIUM SYSTEMS

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August 1979

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EXECUTIVE SUMMARY

Theory-experiment correlations of plutonium-fueled systems using ENDF/B cross-section data have usually resulted in calculated neutron multiplication values which are several percent higher than measured values. The discrepancies could be due to cross-section data, theoretical methods, and/or interpretation of the experiment. We have performed neutronics analyses of homogeneous plutonium critical experiments to determine where some of the cross sections may be deficient. New thermal cross-section data (0-3 eV) were generated for 239 Pu and 240 Pu capture, fission, and neutrons per fission. Two scattering kernels for hydrogen bound in water were also generated. Calculated values of $k_{\rm eff}$ using this new data were compared with corresponding values using ENDF/B-IV data.

The results indicate that the ²⁴⁰Pu resonance data is sufficiently well known for hydrogen-moderated plutonium systems. The data in the vicinity of the 0.3 eV ²³⁹Pu resonance and the hydrogen-bound-in-water kernel were found to be very important in determining the multiplication of plutonium systems. As a result, it is recommended that additional cross-section measurements be made for ²³⁹Pu to determine this data more accurately. Also, the two scattering kernels generated for this project should be refined and a more thorough evaluation of neutron scattering in water needs to be made utilizing experimental data and theoretical models currently available.

In systems using stainless steel as structural and/or neutron control, a large fraction of the neutron absorptions occur in the stainless steel. Therefore, the cross-section data for the components of stainless steel must be known quite accurately. Analyses of several systems containing stainless steel indicate that the uncertainty in calculated values of k_{eff} is small using current estimates of the uncertainties in the cross sections. Experiments more appropriate for the evaluation of stainless-steel data should be performed.

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INTRODUCTION

Neutronics analyses of systems containing plutonium have demonstrated the need to improve the calculational methods and/or the cross-section data. For some plutonium systems the theory-experiment correlation has been very had; outside of the range one would expect due to estimated uncertainties in methods and data. For other plutonium systems the theory-experiment correlation is much better than one would expect considering the uncertainties in methods and data.

In an attempt to improve the neutronics analysis of plutonium systems, the Nuclear Regulatory Commission (NRC) commissioned Battelle, Pacific Northwest Laboratory (PNL) to define where the neutron cross sections for the isotopes of plutonium on ENDF/B-IV can be improved. NRC's main interest was in application to criticality safety analysis of shipping spent light water reactor (LWR) fuels. Since stainless steel is used structurally in shipping casks and is a good neutron poison, NRC also requested an assessment of the adequacy of ENDF/B-IV data for the constituents of stainless steel.

The first task of the project was to define a set of integral benchmark experiments.⁽¹⁾ These have been documented in NUREG/CR-210 (Benchmark Experiments to Test Plutonium and Stainless Steel Cross Sections). In this report we assess the accuracy of ENDF/B-IV plutonium and stainless steel cross sections. A selected portion of the benchmarks in NUREG/CR-210 were used in the analyses.

CALCULATIONAL MODEL

The principal calculational tools consist of the NITAWL, XSDRNPM, and KENO-IV codes⁽²⁾ and a 25-group cross section set which was collapsed from a 218-group ENDF/B-IV set⁽³⁾ generated by Oak Ridge National Laboratory (ORNL). The 25-group structure is given in Table 1. This calculational model is what GRNL had been using for criticality safety analyses at the time we initiated our calculations. Our version of NITAWL performs a NIT⁽⁴⁾ calculation down to 3.05 eV. Recently ORNL has gone to a NIT calculation down to 0.5 eV. They have also added 2 groups at high energies and reprocessed some of the cross sections: These differences lead to minor changes in calculated reactivity value but have a negligible impact on relative differences. Hence, small changes in the methods do not affect our conclusions.

XSDRNPM was used to calculate the systems amenable to one-dimensional analysis. For the remaining systems KENO-IV was used. Comparisons between ENDF/B-IV cross sections and alternate data sets were done only for the systems calculated with XSDRNPM. The differences are of the order (or smaller) of the uncertainty in the KENO-IV results, hence it is not possible to draw conclusions for the more complicated systems.

The plutonium benchmarks used in the correlations are summarized in Table 2. A wide range of H/Pu atom ratios is covered. The 240 Pu content also covers a wide range; however, it would have been desirable to have more systems with a high 240 Pu content (>20%). A more detailed description of the benchmarks is given in Reference 1.

Two pair of benchmarks were used to test stainless steel cross sections. A comparison between the two systems gives information on the stainless steel cross sections. Benchmarks 15a and 15b (see Table 2) are homogeneous reflected plutonium systems. The stainless steel wall is thicker in Benchmark 15b. The reactivity effect due to the extra stainless steel is compensated by a slight change in the solution composition. The other pair of benchmarks used for stainless steel evaluation consist of lattices fueled with UO₂. The same fuel is used in each benchmark. Benchmark 42b has aluminum clad while 42a has stainless steel clad. The difference in reactivity is compensated by a change in the number of fuel rods required for criticality.

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Six of the homogeneous plutonium benchmarks (those with an asterisk in Table 2) were selected to be reanalyzed with alternate data in an attempt to determine the sensitivity of the results to different evaluations of the data. The reanalysis was accomplished by substituting each set of alternate data for the ENDF/B-IV data, one set at a time.

IMPROVED DATA

The data identified to have the greatest effect in calculating plutoniumfueled thermal systems consists of: ²³⁹Pu capture, fission, and neutron production; ²⁴⁰Pu capture due to the 1 eV resonance; and the thermal scattering cross section for water. The source of the alternate data sets is decribed below.

ALTERNATE NUCLEAR DATA FOR 239Pu AND 240Pu BELOW 3 eV

Alternate evaluations for ²³⁹Pu and ²⁴⁰Pu below 3 eV were taken from preliminary studies in which selected differential experimental nuclear data for these isotopes were fitted with a non-linear parameter estimation technique.⁽⁵⁾ After briefly reviewing the formalism, the results of the investigations for each isotope will be discussed.

Theoretical Formalism

The evaluation technique is essentially nonlinear-weighted least-squares fitting. As such its range of validity is restricted by the two implicit assumptions on the statistical nature of the data inherent to all least-squares analysis, viz:

- . The data are not subject to significant systematic bias $(\hat{\mu} = \mu)$
- . All data are samples from a common population (σ^2 is a constant)

One further caveat concerning least-squares analysis is that a single flyer (datum "distant" from theory) can induce non-trivial local perturbations of the theory. If the data to be fitted do not meet the assumptions or exhibit flyers, the model used to describe the data must be formulated in such a way as to compensate for these deficiencies.

Unfortunately, experimental nuclear data may fail on all counts. Systematic bias may be induced by normalization errors or energy-scale errors. It is not uncommon for flyers to be present. Finally, due to differences in reporting by different experimenters, uncertainty measures, if they are reported at all, may reflect total uncertainties or only certain components of

the total uncertainty. Hence, data from different experiments may exhibit widely disparate variances.

To minimize the effects of systematic bias, each data set is allowed three experimental parameters to adjust the normalization and energy-scale for those data within that data set. These parameters are not required, but if they are present, they are treated on a par with the theory parameters. An internal weight-adjustment scheme may be used to down-weight flyers and to balance the variances between data sets to satisfy the common population assumption. However, taking such liberties with reported data is not to be taken lightly, for it introduces a new set of complications. First, it forces one to work with an implicit relation between measurement and theory rather than the more common case of an explicit theory. Second, data which were in principle originally statistically independent are now correlated, and correlation introduces complexity in any statistical analysis. The first complication is one of mechanical detail. The second complication is actually an illusion. If the experimental parameters are statistically significant, the original data in fact were not statistically independent for they exhibit a common systematic bias. Indeed, the correlation is shifted from the measurement-space to the parameter-space, leaving the data essentially statistically independent. Furthermore, since the correlation effects are now contained in the parameter-space, a modest sophistication of the residuals analysis yields more rigorous results than could be obtained in the absence of experimental parameters.

Neutron-Nucleus Interation Theory

The ultimate goal is to describe the thermal energy region nuclear interactions by fitting experimental data as just described to analytic theoretical forms derived from neutron-nucleus interaction theory. There are a limited number of nuclear interactions of interest in the thermal range, all of which may be constructed from three fundamental theoretical forms (Table 3). A modified Adler-Adler formalism is used to describe fission and capture cross sections; while coherent, incoherent, and total scattering are described by the multi-level Breit-Wigner formalism. Finally, an unnamed spin-dependent resonance formalism had to be invented to model data forms

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involving v because of the energy-dependence of v in the thermal energy range. Absorption and total cross sections and the ratios of interest may be constructed from these fundamental theoretical forms as shown in Table 4. Using the same construction logic, any theoretical form may be combined with any second theoretical form that does not involve v in two-component sums and ratios. This feature allows simultaneous multi-isotope fitting when there exist data dependent upon two isotopes such as a limited purity sample with a single contaminant (e.g., ²³⁹Pu with ²⁴⁰Pu contaminant) of data measured relative to a standard with non-trivial shape uncertainty (e.g., $\sigma_{\mathbf{f}}^{49}/\sigma_{\mathbf{f}}^{25}$).

One of the primary reasons for choosing these theoretical forms is the commonality of physical theory parameters between forms. The whole purpose of performing simultaneous fitting would be lost were this commonality absent, for there would then be no competing constraints to compromise. Indeed, in some cases it is only through these competing constraints that some parameters are even marginally determinable. Furthermore, one can obtain indirect evidence of conflicting data when parameters become unphysical or exhibit large uncertainties due to these competing constraints.

The Parameters of the Model

Now that both the theory forms have been described, a complete list of the parameters can be tabulated (see Table 5). Obviously, in any real problem, the number of parameters could be fairly lange. In general, the quality and quantity of data are inadequate to determine all of these parameters, especially when there is a high degree of correlation between some of them. Furthermore, some of the parameters are generally known with fair accuracy from prior evaluations, and expediency demands that some use be made of this a priori knowledge. In our model there are two methods available by which this information can be used to limit the region of parameterspace to be searched. The first method is the case of setting a parameter to a fixed constant. In preliminary fitting in particular, where one may be interested in examining data for systematic bias, this option is very useful. Conversely, in the final stages of fitting, one would like to determine as many parameters as possible from the data alone, but subject to restricting the range of certain of the parameters to values which are physically

plausible or which are demonstrably optimal from evidence of prior fitting. The second method allows one to do just that by treating a parameter estimate which has an associated uncertainty as a datum. Consequently, although the full dimensionality of the parameter-space is used, there are constraints which limit the freedom of parameter variation in some dimensions.

Summary of the Model

In the non-linear parameter estimation technique we used, the data are transformed via theory to remove systematic bias attributable to normalization or energy-scale errors. Weight-adjustment may be used if necessary to satisfy the common variance assumption. A collection of theoretical forms derived from neutron-nucleus interaction theory based on a common set of physical parameters has been chosen to provide competing constraints in fitting the various data forms. There is arbitrary freedom in choosing which parameters are to be varied and which are to remain fixed in the fitting algorithm. Furthermore, any subset of the variable parameters may be constrained, forcing each parameter of the subset to lie in the neighborhood of its a priori estimate.

Fitting for 240 Pu

The low-energy region in ²⁴⁰Pu is dominated by the 1 eV resonance, but to accurately model the region a bound level and the 20 eV resonance were included in the fit with all parameters fixed, the bound level as a mirror image of the 20 eV resonance. The data base used in the studies include the capture data of Weston and Todd, ⁽⁶⁾ the total data of Leonard, et. al., ⁽⁷⁾ and Block, ⁽⁸⁾ and normalization points (see Table 6) for capture, ⁽⁹⁾ scattering⁽¹⁰⁾ and fission. ⁽¹¹⁾ The total data of Leonard through the resonance were corrected for Doppler broadening, and on advice from Leonard the energy scale was allowed to adjust. The capture data of Weston and Todd show evidence of ²³⁹Pu contaminant and were fit as the sum of ²⁴⁰Pu capture and ²³⁹Pu capture with the impurity concentration of ²³⁹Pu being an adjustable parameter. Both of these data sets, along with Block's total data, were allowed to renormalize. Furthermore, the data set weights of these three data sets were internally adjustable. This was especially important for the Weston and Todd capture data, since in the absence of measurement uncertainties, the data weights were ar-

bitrarily set to correspond to a 5% data uncertainty with internal adjustment of the data weights allowed. The preliminary results for the 2200 m/s zerokelvin cross sections and the parameters of the 1 eV resonance are shown in Table 7. The cross sections generated using these parameters were Dopplerbroadened to 293.6K, weighted with a 293.6K Maxwellian spectrum to 5 kT (\sim .1275 eV) and a 1/E spectrum above 5 kT, and integrated to obtain group-averaged cross sections in the 78 thermal fine groups (10^{-5} to 3.05 eV). The resonance integral (from 0.8 to 1.3 eV) is 1.9% larger than the ENDF/B-IV value.

The ratio of this data to ENDF/B-IV data is shown in Figure 1. The large spike at 0.5 eV is probably due to an error in processing the ENDF/B-IV data. This error is not significant in reactivity calculations, because the cross section is small at this energy (Figure 2). The unusual shape at 1 eV is due to a small shift in the location of the resonance.

itting for 239Pu

processes a strong bound level just below zero neutron energy, the evidence of an even pendence for v and non-negligible Doppler-broadening effects in viewed at v0.3 eV. Furthermore, the experimental differential data sets anticipated to be the most significant do not seem to be in agreement, which leads to biased fits compromising the integrity of least-squares analysis. This apparent disagreement may be the result of several inter-related factors, such as

- Sample contamination by higher Pu isotopes, especially ²⁴⁰Pu and ²⁴¹Pu (along with ²⁴¹Am daughter)
- Misinterpretation of reported uncertainty measures
- Unaccounted for resolution effects
- Slight differences in the reported energy-scale
- Inadequacy of the theoretical model.

Care has been taken to minimize the effects of each of these by using the very general theoretical model described above (which includes a theoretical method for data adjustment).

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The alternate ²³⁹Pu nuclear data used in this study were taken from preliminary fitting results whose range did not extend to 3 eV. However, the extrapolation of the fit is acceptable for reactor calculations, for the only cross section poorly represented (radiative capture >1.5 eV) is of little consequence over the range of its extrapolation. Table 8 shows the parameters of the preliminary data analysis, while Figures 3-7 exhibit group-averaged values. The discontinuities just below 1 eV appear to be due to a processing error in the ENDF/B-IV data, but are inconsequential for the reactor calculations presented in this report.

Figures 3 and 4 show 78-group values of the ENDF/B-IV absorption and fission cross section taken from the ORNL processed library. The ratio of the new data relative to ENDF/B-IV data is shown in Figures 5 and 6 for absorption and fission, respectively. Figure 7 shows the production-to-absorption ratio (n) derived from the ENDF/B-IV data. Shown in Figure 8 is the ratio of n for the preliminary fit to n for ENDF/B-IV data. Note the increase in the vicinity of 0.3 eV and the increase above 0.8 eV. The latter increase reflects a significantly different interpretation of the 239 Pu capture cross section in the region subject to large uncertainties due to 240 Pu contamination and is not inconsistent with the measured n data on the falling side of the resonance. No attempt is made here to assign uncertainties to the alternate data, since they result from a biased fit and have been forced to produce the best estimate thermal zero-kelvin cross sections indicated in Table 8.

Two notable features of these results are the upward revision of the thermal fission cross section and the variation of v with energy in the thermal range. The change in the fission cross section is due almost entirely to recent measurements of the ²³⁹Pu half-life⁽¹²⁾ (generally used for sample assay of Pu foils) leading to an estimate of $T_{1/2} = 24134 \pm 8$ yr in contrast to the commonly used value of $T_{1/2} = 24395 \pm 10$ yr. This revision of $T_{1/2}$ corresponds to $\sim 1.1\%$ increase in the normalization of fission data where the sample assay was determined by α -counting. The variation of v with energy, fitted to recent measurements (a few meV) to the peak at 0.3 eV with recovery to the first value at higher energies. Introduction of energy variation in v

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helps to explain the differences between monoenergetic neutron n measurements and the ratio of cross sections, σ_f/σ_a .

The 2200 m/s parameters resulting from the new fit are compared with ENDF/B-IV data in Table 9. The ratio of neutrons produced per neutron absorbed (n) is a good indicator of the reactivity effect. It has increased only 0.23%.

THE SCATTERING CROSS SECTION FOR HYDROGEN BOUND IN WATER

The scattering of low-energy neutrons involves not only the nuclear properties of the scattering nucleus, but also the dynamics of the molecule. The hindered rotations, translations, and vibrations of the molecule in a bound system are important contributors to the scattering process. An analysis of the scattering cross section must include these effects.

The scattering cross section is composed of both a coherent and an incoherent component. The incoherent component of the scattering cross section describes the dynamics of a single molecule in the bound system. The coherent component of the scattering cross section describes the correlated dynamics of the system of molecules. For water, the coherent component composes approximately 2% of the total scattering.

Models which treat scattering as completely incoherent will provide a reasonable representation of the behavior of scattering in water, and permit calculational simplifications. The scattering cross section per hydrogen atom in water using the incoherent scattering approximation can be written as

$$\sigma_{s}(E \rightarrow E^{\prime}, \mu) = \frac{\sigma_{b}}{4\pi kT} \left(\frac{E^{\prime}}{E}\right)^{1/2} e^{-\beta/2} S(\alpha, \beta)$$
(1)

where

- $\sigma_s(E+E^*,\mu) =$ the differential scattering cross section (barns/ ev-steradian)
- σ_b = the bound atom scattering cross section
 k = the Boltzmann constant
 T = the temperature of the scattering system

E	=	initial energy
E*	=	final energy
μ	. =	cosine of the scattering angle
S(α,β)	=	the scattering law

In this expression α and β are the square of the momentum transfer and energy transfer in dimensionless units. They are related to the initial and final neutron energies and the systems temperature by

$$x = \frac{E + E' - 2\mu\sqrt{EE'}}{AkT}$$
(2)
$$B = \frac{E' - E}{kT}$$

where

A = the mass of the scattering atoms divided by the neutron mass.

The expression for the scattering cross section depends only on the scattering law and known numerical factors. Given a form for the scattering law, the cross sections which are needed in reactor analysis can be determined. The entire problem of evaluating thermal neutron scattering becomes a matter of evaluating the scattering law.

Many different techniques have been used to evaluate the scattering law. Each technique differs in basic data, theoretical assumptions, and numerical methodology. The differences in any of these areas can produce a different evaluation.

In this study three different evaluations of the scattering law were used. They are for convenience denoted as TISK, TISK-Koppel, and GASKET. All of the evaluations use the same basic assumption. This assumption is that the dynamics of a molecule in a bound system can be expressed in terms of a phonon spectrum. The TISK and TISK-Koppel evaluations are both new. The GASKET evaluation is the evaluation provided in the ENDF/B-IV data file.

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Since the purpose of this work was to investigate the sensitivity of integral experiments to the scattering cross section, an effort was made to eliminate the sensitivity of the scattering cross section to the details of the processing and handling routines. The evaluated scattering laws were

calculated on the same numerical grid as the present ENDF/B-IV values.

Both new evaluations were processed into a 78-group set of cross sections using the FLANGE-II⁽¹⁶⁾ computer code. Each of the three scattering laws and the phonon spectrum are described separately.

TISK Scattering Law

The scattering law in the $TISK^{(17)}$ formulation is written as

$$S(\alpha,\beta) = \frac{1}{\pi} \int_{0}^{\infty} e^{-\alpha W(t)} \cos(\beta t) dt$$
(3)

where W(t) is a width function related to the mean squared displacement of an atom from its initial position.

The width function can be expressed in terms of the fundamental parameter of a bound system, the phonon spectrum, as

$$W(t) = \int_{0}^{\infty} \rho(\beta) \left[\frac{\cosh(\beta/2) - \cos(\beta t)}{\beta \sinh(\beta/2)} \right] d\beta$$
(4)

where

$\rho(\beta)$ = the phonon spectrum.

No restriction has been placed on the form of the phonon spectrum in (4). In general, it can be any representation which describes the dynamics of the molecular system. Most functional representations require a numerical evaluation of the integral in (4).

In the TISK method, the Lindenmeier-Gibbs form of the phonon spectrum is used. This form is a series of modulated Gaussian peaks. The representation allows flexibility in modeling the peaks and valleys of the phonon

spectrum, which correspond to the hindered rotations, vibrations, and translations of the molecule, while allowing an analytic integration of (4).

The phonon spectrum in the Lindenmeier-Gibbs formulation can be written as

$$\rho(\beta) = \rho_0(\beta) + \sum_{i=1}^{N} \frac{F_i\beta \sinh(\beta/2)}{2\sqrt{\pi\delta_i}} e^{-\delta_i/4} \left[\frac{e^{-(\beta-\gamma_i)^2/4\delta_i} - (\beta+\gamma_i)^2/4\delta_i}{\gamma_i\sinh(\gamma_i/2) + \delta_i\cosh(\gamma_i/2)} \right] (5)$$

where γ_i and δ_i are parameters which describe the resonance-like peaks of the spectrum, and F_i is a weighting factor which represents the fractional contribution of a particular peak to the spectrum.

The term $\rho_0(\beta)$ accounts for the diffusive motion of the system. For a solid this form is zero. For a gas it is a delta function. For a liquid the exact form is not known, but Egelstaff and Schofield⁽¹⁸⁾ have recommended the form

$$\rho_0(\beta) = \frac{0.16}{\pi} \frac{\sinh(\beta/2)}{\beta} (\beta\sqrt{10^4 + 0.25}) K_1(\beta\sqrt{10^4 + 0.25})$$
(6)

where K_1 is a Bessel function.

Equation (4) can be integrated to give

$$W(t) = W_{0}(t) + \sum_{i=1}^{N} F_{i}[A_{i} - B_{i}e^{-\delta}i^{t^{2}}\cos(\gamma_{i}t)]$$
(7)

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where

$$A_{i} = \frac{\cosh(\gamma_{i}/2)}{\gamma_{i} \sinh(\gamma_{i}/2) + \delta_{i} \cosh(\gamma_{i}/2)}$$
$$B_{i} = \frac{e^{-\delta_{i}/4}}{\gamma_{i} \sinh(\gamma_{i}/2) + \delta_{i} \cosh(\gamma_{i}/2)}$$

 $W_0(x) = 0.08 [(x^2 + 10^4 + 0.25)^{1/2} - 100]$

This eliminates the necessity of performing two numerical integrations. The integral in (3) must still be performed numerically to determine the scattering law from the displacement function. This integral is ideally suited for evaluation using extremely fast and accurate fast-Fourier pressform techniques.⁽¹⁹⁾

These techniques were incorporated in the TISK computer code. For large values of the energy and momencum transfer an asymptotic expansion was used to evaluate the scattering law.

H₂0 Scattering Law Based on Anisotropic Molecular Vibrations

In order to provide an additional H_2O scattering kernel for sensitivity calculations, the Lindenmeier-Gabbs (L-G) formalism employed in program TISK⁽¹⁷⁾ was modified to take into account the anisotropy of the molecular vibrations. For this purpose Koppel's simplified dynamical model of H_2O vibrations⁽²⁰⁾ was adapted to the L-G formalism by assuming that each of the L-G modulated Gaussion peaks in the phonon spectrum can be associated uniquely with one of Koppel's modes (stretching, bending, hindered rotation or hindered translation). In principle the combined TISK-Koppel formalism should be a refinement of the standard TISK formalism, ⁽¹⁷⁾ which is based on the assumption of isotropic vibrations, and Koppel's original work,⁽²⁰⁾ which employed Nelkin's delta-function phonon spectrum and an axially symmetric distribution of polarization vectors.

The scattering law averaged over all orientations of the water molecule is

$$(\delta(\alpha,\beta) >> = \frac{1}{\pi} \int_{0}^{\infty} dt << \exp[-\alpha W(t)] >> \cos(\beta t)$$
(8)

where S is the scattering law for an arbitrary molecular orientation

W(t) is the corresponding width function (dependent on orientation)

and

 α and β have been defined previously

and <<Z>> = average of Z over all orientations.

Instead of working cirectly with equation (8), we adopt the method used in Reference 17 to improve the accuracy of integration at large values of t. The averaged scattering law is rewritten as

$$\langle \langle S(\alpha,\beta) \rangle = \langle \langle S(\alpha,\beta) \rangle \rangle_1 + \langle \langle S(\alpha,\beta) \rangle \rangle_2$$
(9)

where

$$<>_1 = \frac{1}{\pi} \int_0^\infty dt <<\exp[-\alpha W_{\infty}(t)]>>\cos(\beta t)$$
(10)

$$\langle \mathsf{S}(\alpha,\beta) \rangle_{2} = \frac{1}{\pi} \int_{0}^{\infty} dt \langle \exp[-\alpha \mathsf{W}(t)] - \exp[-\alpha \mathsf{W}_{\infty}(t)] \rangle \langle \mathsf{st}(\beta,t) \rangle$$
(11)

$$W_{m}(t) = asymptotic (large t) form of W(t).$$

There are now two Fourier transforms, but the one in equation (10) can be done analytically due to the simple form of $W_{\infty}(t)$. Indicating the orientation dependence of W(t) explicitly, we have

$$W(t,\phi,\theta) = W_{d}(t) + W_{c}(\phi,\theta) + W_{T}(t,\phi,\theta)$$
(12)

where $W_d(t)$ is the isotropic diffusion component, $W_c(\phi, \theta)$ is the time-independent component due to vibratory modes, and $W_T(t, \phi, \theta)$ is the time decaying component due to vibratory modes.

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Thus we have

$$W_{\infty}(t) = W_{d}(t) + W_{c}(\phi, \theta)$$
⁽¹³⁾

Suppressing the independent variables, we have

$$\langle \langle S \rangle \rangle_1 = \langle \langle \exp[-\alpha W_c] \rangle \rangle \frac{1}{\pi} \int_0^\infty dt \, \exp[-\alpha W_d] \cos(\beta t)$$
 (14)

$$<~~_{2} = \frac{1}{\pi} \int_{0}^{\infty} dt \exp[-\alpha W_{d}] \left\{ <<\exp[-\alpha (W_{c} + W_{T})] >> \right.~~$$

$$-<<\exp[-\alpha W_{c}] >> \left\} \cos(\beta t)$$

$$(15)$$

The explicit formulas for the components of W(t) are

$$W_d(t) = 2d [(t^2 + c_0^2 + 0.25)^{1/2} - c_0]$$
 (16)

where d and \boldsymbol{c}_{0} are known constants related to diffusion,

$$W_{c}(\phi,\theta) = e' + a \sin^{2}\theta \cos^{2}\phi + b \sin^{2}\theta \sin^{2}\phi + c \cos^{2}\theta$$
(17)

where θ and ϕ are suitable spherical polar coordinates

$$c = \text{ largest of quantities a', b' and c'}$$

$$b = \text{ intermediate of quantities a', b' and c'}$$

$$a = \text{ smallest of quantities a', b' and c'}$$

$$a' = 3A_sF_s$$

$$b' = A_rF_r + 3\sum_{b=1}^{2} A_bF_b$$

$$c' = 2A_rF_r$$

$$e' = \sum_{t=1}^{2} A_t F_t$$

$$W_c(\phi, \theta) + W_T(t, \phi, \theta) = e'' + \underline{a} \sin^2\theta \cos^2\phi + \underline{b} \sin^2\theta \sin^2\phi + (18)$$

$$C = \cos^2\theta$$

where

Subscripts s, b, r, t indicate stretching, bending, rotational, translational mode peaks.

 $\textbf{A}_{i}, \ \textbf{B}_{i}, \ \textbf{Y}_{i}, \ \text{and} \ \ \delta_{i} \ \text{are L-G parameters for the i-th mode peak.}$

 F_i = weight of the i-th mode peak.

It is explicitly assumed here that there are 2 low energy translational peaks, 1 medium energy rotational peak, 2 medium energy bending peaks, and 1 (consolidated) high-energy stretching peak for H_2O .

Using the explicit formulas for the width components in equations (16), (17) and (18) we can exhibit final formulas for $\langle\langle S \rangle\rangle_1$. Let

$$\langle \langle S \rangle \rangle_1 \equiv QS_d$$
 (19)

where

 $Q \equiv \langle \exp[-\alpha W_{c}] \rangle \rangle$ $S_{d} \equiv \frac{1}{\pi} \int_{0}^{\infty} dt \exp(-\alpha W_{d}) \cos(\beta t)$

The formula for S_d can be integrated analytically to give

$$S_{d} = \frac{Texp(Tc_{0})xK_{1}(x)}{\pi(T^{2} + \beta^{2})}$$
 (20)

where

$$T = 2d \alpha$$

$$x = \sqrt{(c_0^2 + 0.25)(T^2 + \beta^2)}$$

$$K_1 \text{ is a Bessel function}$$

The orientation-averaged quantity Q can be written as a double integral

$$Q = \frac{1}{4\pi} \int_{0}^{2\pi} d\phi \int_{-1}^{1} d(\cos\theta) \exp[-\alpha W_{c}(\phi,\theta)]$$

where $W_C^{}(\varphi,\theta)$ is defined in equation (17). The integral over θ can be done analytically to yield

$$Q = \frac{\exp[-\alpha(e' + c)]}{4\sqrt{\pi}} \int_{0}^{2\pi} d\phi \frac{\exp(\alpha q) \operatorname{erf} \sqrt{\alpha q}}{\sqrt{\alpha q}}$$
(21)

where

$$q \equiv c - b + (b - a)\cos^2\phi$$

The remaining integral over ϕ is done numerically by trapezoidal integration.

The integrand for $\langle \langle S \rangle \rangle_2$ in equation (15) includes Q and another orientation-averaged quantity P(t) defined by

$$P(t) \equiv \langle \exp[-\alpha(W_{c} + W_{T})] \rangle$$
(22)

Again, the integration over θ can be performed analytically to yield

$$P(t) = \frac{\exp(-\alpha[e'' + \underline{c})]}{4\sqrt{\pi}} \int_{0}^{2\pi} d\phi \frac{\exp(\alpha p) \operatorname{erf} \sqrt{\alpha p}}{\sqrt{\alpha p}}$$
(23)

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where

$$p(t) \equiv \underline{c} - \underline{b} + (\underline{b} - \underline{a})\cos^2\phi$$

The integral in equation (23) is done numerically by trapezoidal integration, and the cosine transform in equation (15) is done by a Fast Fourier Transform subroutine.

The numerical cosine transform method just described gives inaccurate results for large values of β . Thus it is necessary to supplement it with an alternative formulation. Although the saddle point method used in Reference 18

would probably be more accurate for this purpose, it was thought to be easier and quicker to formulate a generalization of the short collision time method used in program FLANGE-II. (16) The method uses the scattering law for a free gas at an effective temperature related directly to the phonon spectrum of the scattering material. The formula for a material having isotropic vibrations is

$$S_{sct}(\alpha,\beta,R) = \frac{\exp\left[-\frac{\beta}{2} - \frac{(\alpha - \beta)^2}{4\alpha R}\right]}{\sqrt{4\pi\alpha R}}, \quad \beta > 0$$
(24)

where

 $R = T_{eff}/T$

In the L-G formalism the temperature ratio is

$$R = \sum_{i} \frac{F_{i}}{2} \int_{0}^{\infty} d\beta \ \beta \operatorname{coth}(\beta/2) \rho_{i}(\beta)$$
(25)

where $\rho_i(\beta)$ are the normalized L-G peak functions.

For an anisotropic oscillator the ratio R is orientation dependent since the factor F_i is replaced by $F_i\Gamma_i(\phi,\psi,\theta)$. For the simplified Koppel dynamical model for H₂O the formulas for Γ_i for the various modes of vibration are

 $\Gamma_{\rm s} = 3 \cos^2 \theta \tag{26}$ $\Gamma_{\rm b} = 3 \cos^2 \phi$

 $\Gamma_{r} = \cos^{2}\phi + 2\cos^{2}\psi$ $\Gamma_{t} = \Gamma_{d} = 1,$

where the subscripts s, b, r, t, d indicate stretching, bending, rotational, translational, and diffusive modes, and ϕ , ψ , θ are angles relative to x, y, z axes.

Since we could not perform the orientational integrations analytically, we approximated the double integral by a weighted sum of integrand values calculated for a preselected set of directions (or points on a unit sphere).⁽²¹⁾ Actually 2 different schemes were tested and found to give equivalent results. They are the 72-point 14th-degree formula of McLaren and the 128-point 15thdegree spherical product Gauss formula (FORTRAN functions S3S14 and S3S15 of Reference 21). Thus the final formula for the averaged short collision time scattering law is

$$\langle \langle S_{sct}(\alpha,\beta) \rangle = \sum_{j} W_{j} S_{sct}(\alpha,\beta,R_{j})$$
 (27)

where j is the index of directions specified by angles θ_{i} , and ψ_{j} , and w_{i} is the corresponding weight.

Phonon Spectrum

In order to evaluate the scattering law for water in both the TISK and TISK-Koppel models, a phonon spectrum must be available. The experimental data of both Harling⁽²²⁾ and Haywood⁽²³⁾ for the phonon spectrum of hydrogen bound in water were combined. The Harling data was used for beta greater than 2.5 and the Haywood data for small beta. The experimental phonon spectrum was fitted using the nonlinear least squares techniques of the LEARN⁽²⁴⁾ computer code. Table 10 displays the values of the parameters for a 5-peak representation. An additional high-energy peak is included for the unresolved vibrational modes at a beta of 18. Figure 9 shows both the experimental and the functional evaluation of the phonon spectrum.

ENDF Scattering Law⁽²⁵⁾

The scattering law for H_20 was calculated for ENDF with the GASKET⁽²⁶⁾ computer code based on a model which retained the essential features of the Nelkin model. Between 0.04 and 0.165 eV the single delta function oscillator of the Nelkin model was replaced with a broad band of distributed modes for the hindered rotations. The data for the band of hindered rotations was taken from the work of Haywood.⁽²³⁾ Below 0.04 eV it was smoothly joined to a parabola. The original spectrum given by Haywood showed several peaks in this low-frequency range, corresponding to translational vibrations of the H_20 molecule as a whole. These modes were replaced by free translations of weight 1/18 in order to avoid numerical difficulties. The discrete internal modes of vibration of the H_20 molecule were taken from the Nelkin model with weights of 1/6 for the 0.205 eV mode and 1/3 for the 0.48 eV oscillator. The torsional band was then normalized to 4/9 in order to give the proper overall normalization.

Comparison of Scattering Models

The three different evaluations of the scattering cross section for a single hydrogen atom bound in a water molecule are displayed in Figures 10a and 10b. Both the TISK and TIKS-Koppel evaluations appear to be approximately 10% low in reproducing the cross section in the 1 to 3 eV range. At the other end of the spectrum (low energy) both the TISK and TISK-Koppel models are high in reproducing the scattering cross section. From 0.1 to 1.0 eV the three evaluations all reproduce the scattering cross section reasonably well.

Figures 11, 12, and 13 display the differential scattering cross section for fine group 173 (1.09-1.10 eV) from ENDF, TISK, and TISK-Koppel. Only the down scattering portion of the cross section is shown since the upscattering is related to the downscattering by detailed balance. The inscattering contribution is much larger in both the TISK and TISK-Koppel models to the ENDF model.

Figure 14 shows the ratio of the TISK and TISK-Koppel scattering models to the ENDF model. The differences in the structure of the differential scattering from both TISK and TISK-Koppel can be seen in the ratio graphs.

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The ratio of TISK-Koppel to TISK scattering is shown in Figure 15. The deviation from 1.0 is a representation of the anisotropy effect. The broadgroup transfer cross sections (barns/atom) for the three water kernels for the 25-group structure are displayed in Tables 11 to 23. From these tables it is apparent that the phenomenon seen in fine-group 173 does not hold for all other groups.

RESULTS

STAINLESS STEEL

Reactivity values for Benchmarks 15a and 15b (homogeneous plutonium spheres) were determined with XSDRNPM. A summary of the results and a brief description of each system are given in Table 24. Each system is reflected with water, thus a portion of the neutrons thermalized in the reflector are absorbed in the stainless steel shell. As the shell thickness is increased the fraction of neutrons absorbed in the shell is increased as shown on line 5. The k_{eff} values given in Table 24 indicate that the absorption rate in the shell is too high because k_{eff} decreases as the shell thickness increases. Assuming other parameters are calculated accurately, the stainless steel absorption rate would have to decrease 8% to obtain identical k_{eff} values.

Reactivity values for Benchmarks 42a and 42b lead to an opposite conclusion as to the stainless steel cross sections. These benchmarks are enriched UO_2 lattices using the same fuel at the same lattice pitch. One has stainless steel clad while the other has aluminum clad. The results are summarized in Table 25. The reactivity effect of changing the clad is compensated by changing the core size; and hence, the neutron leakage from the system. The k_{eff} values given in Table 25 indicate that the absorption rate in the stainless steel is too low because k_{eff} increases as aluminum is replaced by stainless steel. If other parameters are calculated accurately or have cancelling effects, the absorption rate in stainless steel would have to increase by 9% to obtain identical k_{eff} values. Since the leakage fraction is quite different for the two systems, an error in the leakage calculation would lead to an erroneous conclusion.

Based on the results for the two pairs of benchmarks, no conclusion can be drawn as to the adequacy of stainless steel cross sections. Reported crosssection uncertainties for the constituents result in an uncertainty of less than 2% for the 2200 m/s cross section of stainless steel and an uncertainty of 10% for the resonance integral of stainless steel. For the lattices, 85% of the stainless steel absorptions are in the thermal energy range while for the solutions 98% of the absorptions are in the thermal energy range. The spread in range of composition of stainless steel leads to a larger spread

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in the 2200 m/s cross section than the uncertainty due to cross-section measurements.

REACTIVITY VALUES WITH ENDF/B-IV DATA

Reactivity values for all of the homogeneous plutonium benchmarks given in Reference 1 were obtained with NITAWL and either XSDRNPM or KENO-IV using 25-group ENDF/B-IV cross sections. The results are shown in Figure 16 as a function of H/Pu ratio. Values of k_{eff} are $\sim 2\%$ high for most of the systems indicating an error(s) in the cross-section data or the theoretical methods. The uncertainties associated with the Monte Carlo results are 5 to 7 mk. As H/Pu decreases, the neutron spectrum becomes harder and non-thermal cross sections have a greater impact on reactivity. The reactivity effect of ²⁴⁰Pu becomes greater as H/Pu decreases. There is no discernible trend with H/Pu ratio or with different percentages of ²⁴⁰Pu. Thus, the results shown in Figure 16 do not suggest any particular cross section being in error. The six benchmarks listed in Table 26 were chosen to evaluate the effects of data changes.

EFFECT OF CHANGING 239Pu DATA

Shown in Figure 17 are the ratios of k_{eff} values using the preliminary ²³⁹Pu fit to k_{eff} values using ENDF/B-IV data. The new data give k_{eff} values which are 0.3 to 0.8% higher than the k_{eff} values calculated with ENDF/B-IV data, with the effect increasing as H/Pu ratio decreases. The changes in reaction rates in the vicinity of the 0.3 eV resonance are the major cause of the increase in k_{eff} . Broad group 20 is most important, followed by group 19. As H/Pu ratio decreases, the fraction of ²³⁹Pu absorptions in the 0.3 eV resonance increases. As shown in Figure 8, n has increased by 2-3% around 0.3 eV. For Benchmark 2, 30% of the absorptions occur in groups 18, 19, and 20. For Benchmark 4, 14% of the absorptions occur in groups 18, 19, and 20; hence, the reactivity effect is much less.

The increase in n above 0.5 eV (Figure 8) does not affect the reactivity of the more thermal systems (high H/Pu). For low H/Pu systems k_{eff} is increased by 0.2%.

EFFECT OF CHANGING 240 Pu DATA

Shown in Figure 18 are the ratios of k_{eff} values using the new ²⁴⁰Pu data to k_{eff} values using ENDF/B-IV data. For all systems the new data changes k_{eff} by less than 0.1%. The largest reactivity effects should be in systems with a low H/Pu ratio or systems with a high ²⁴⁰Pu content. In Benchmark 2 (low H/Pu) only 8% of the absorptions occur in the vicinity of the 1 eV ²⁴⁰Pu resonance. Thus, it would take at least a 12% increase in the resonance integral to effect a 1% decrease in k_{eff} . In Benchmark 14 (high ²⁴⁰Pu) only 10% of the absorptions occur near the ²⁴⁰Pu resonance.

EFFECT OF CHANGING THE H20 KERNEL

The reactivity effect of replacing the modified Haywood kernel (ENDF) with a TISK kernel is shown in Figure 19 as the ratio of k_{eff} values. The reactivity effect is negative for Benchmark 2 (low H/Pu) .rd Benchmark 14 (high ²⁴⁰Pu content). For the other systems the reactivity effect is positive. Shown in Figure 20 is the reactivity effect of going from the TISK kernel to the TISK-Koppel kernel. The changes are 0.2% at the most. As discussed earlier, the total cross section and the energy transfer matrix of hydrogen bound in water for the TISK kernel is quite different from the ENDF/B-IV kernel. Because of these differences one might expect to see differences in flux as a function of energy and/or space or a difference in the radial leakage. The differences between the TISK kernel and the TISK-Koppel kernel are not nearly as large.

The group fluxes for Benchmarks 2, 4, and 14 at the center of the system are shown in Tables 27, 28, and 29 respectively using the three kernels. They are normalized to the same fission source. In each case the flux at the high end of the thermal energy range is increased significantly. This is due to both the smaller total scattering cross section and less energy loss per scattering event. Increasing the flux tends to increase the radial leakage and hence, decrease k_{eff} . If the ²⁴⁰Pu concentration is very high, k_{eff} would also decrease because of the increased absorption rate. For Benchmark 4 the increased absorption in the 1 eV ²⁴⁰Pu resonance is worth -0.2% in going to the TISK kernel. For Benchmark 2 the effect is -0.4% and for Benchmark 14 it is -0.7%.

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In going to the TISK-Koppel kernel, there is a very little change in the fluxes for groups 13-17. Therefore, the reactivity effect is small.

The second area of interest is in groups 19-21 which encompass the 0.3 eV resonance of 239 Pu. If the flux increases in these groups, k_{eff} will decrease because of the lower value of n compared to the rest of the thermal energy range. In all cases the flux does increase; however, not enough to affect the reactivity significantly.

The flux in group 25 obtained with the TISK kernel is significantly lower for all three systems. The TISK kernel scatters only half as many neutrons from group 24 to group 25 as the ENDF kernel.

The last area of interest is the radial leakage. Shown in Table 30 is the difference in radial leakage from the fissile region in going to the TISK kernel expressed as percentage of total neutrons absorbed in the system and leaking from the system. For reflected systems this is the difference between leakage out and leakage into the fission region. For all systems the leakage is reduced which leads to an increase in reactivity. Benchmark 14 has much less leakage than the other systems; hence, the change in leakage is worth less in terms of reactivity.

Although small, all systems exhibit a reduction in the fast-energy neutron leakage. This is due to a change in the spatial fission rate, most of which is in the bottom 6 groups. The TISK kernel has led to a flux distribution which is reduced at the edge of the fissile region.

The leakage in group 13, the top of the thermal calculation, increases appreciably for the unreflected systems. This could be due to the increase in flux as shown in Tables 27-29. However, the flux is also increased in groups 14-17 with no increase in leakage. In group 18 neutron leakage is decreased significantly yet the flux is increased 5-7%. In groups 21-23 (0.225 to 0.030 eV) the neutron leakage is decreased significantly for Benchmarks 4 and 7 but not for the other systems.

In going from the TISK kernel to the TISK-Koppel kernel there is very little change in leakage. The reactivity worth is less than 0.1%.

For the kernels used in this study, two parameters were sensitive to the type of kernel. Absorption in the 240 Pu resonance was increased and leakage from the system was decreased in the going to the TISK kernel. For the benchmarks considered in this study the effects were of the same order of magnitude. The leakage effect ranged from +0.1 to +0.7% in reactivity. The 240 Pu absorption effect ranged from -0.2 to -1.0% in reactivity. For other systems one or the other may dominate.
CONCLUSIONS AND RECOMMENDATIONS

Neutronics analyses of critical systems were performed to identify where certain cross sections may be deficient. The integral reactivity parameter, k_{eff} , was used to make judgements about the cross sections. The cross sections of interest are stainless steel, ²³⁹Pu thermal, ²⁴⁰Pu resonance (1 eV), and scattering of hydrogen bound in water.

A limited number of experiments were available to evaluate stainlesssteel data. The calculation of these experiments led to conflicting conclusions concerning biases. Other uncertainties or biases in the experiments and/or calculations were concluded to be large enough to preclude the determination of biases in the cross-section data. For the systems used in this study, uncertainties in k_{eff} due to uncertainties in the elemental cross sections are small compared to the other calculational biases and uncertainties. Although this study cannot demonstrate a need to improve the cross-section data for the elements of stainless steel, it would be desirable to design and perform benchmark experiments more appropriate for the evaluation of stainless-steel cross-section data.

Results of a preliminary fit of ²³⁹Pu data were used to calculate plutonium benchmarks. Calculated values of k_{eff} for several homogeneous plutonium benchmarks were compared with values obtained with ENDF/B-IV data. The new data resulted in k_{eff} values which ranged from 0.3 to 0.8% higher than the values calculated with ENDF/B-IV data. The primary cause of the increase is due to reactions in the 0.3 eV resonance. The production-toabsorption ratio, $n = v\sigma_f/\sigma_a$, is higher for the new data. Uncertainties in 2200 m/s ENDF/B-IV data lead to small uncertainties in k_{eff} . No uncertainties have been generated for the new cross-section data. However, the ²³⁹Pu data is known least accurately in the vicinity of the 0.3 eV resonance. Consequently, a good measurement of the data between 0.0 and 0.5 eV should be performed.

A least squares fit of ²⁴⁰Pu data from 0 to 3 eV was performed to obtain a best estimate of the cross section. The new fit resulted in a resonance integral which is i.9% larger than ENDF/B-IV data. This small change nad a negligible effect on k_{eff} (≤ 0.1 %) for the plutonium systems considered in

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this study. Since the cross-section uncertainty is $\sim 2\%$, there is not a need to improve the accuracy of the data. Uncertainties (or errors) in the theoretical methods used to calculate ²⁴⁰Pu reaction rates are much larger than uncertainties due to the cross-section data.

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Two kernels for hydrogen bound in water were generated. Reactivity calculations for several plutonium benchmarks using these two kernels were compared to calculations using the ENDF kernel (modified Haywood). The first kernel was generated with TISK assuming isotropic scattering. Three major differences between the ENDF and TISK kernels are apparent. First, the scattering from TISK is more peaked, thus the spectrum is harder. Hence, the flux in the vicinity of 1 eV was increased by ~10%. A second difference between the TISK and ENDF kernels is the low total scattering cross section generated by TISK between 1 and 3 eV. The third difference between the kernels is the higher total scattering cross section generated by TISK below 0.0253 eV. The increased cross section at low energies has a positive effect on keff because it decreases neutron leakage from the systems. The increased absorption rate in 240 Pu is worth -0.2 to -0.7% in reactivity for the plutonium benchmarks considered. The reduced neutron leakage is worth +0.1 to +0.6% in reactivity for the plutonium benchmarks considered. The magnitudes of these effects suggest that the model for neutron thermalization could be causing a significant error in the calculated reactivity of plutonium systems. The TISK kernel generated for this study needs to be refined because of the total cross section mismatch between it and the ENDF kernel. The results obtained in this study indicate that kernel effects can have a significant impact on calculated reactivity values for plutonium systems. Thus, a thorough evaluation of neutron scattering in water is recommended.

A second kernel (TISK-Koppel) was generated with TISK by modifying the code to include anisotropic scattering. It is substantially different from the kernel generated assuming isotropic scattering. However, reactivity results obtained using the TISK-Koppel kernel were essentially the same as those using the TISK kernel. The reactivity changes are of the order of 0.1%. However, for geometrically more complex systems, anisotropic scattering could be very important. Further, comparisons should be performed for systems of fuel rods in water to determine if the anisotropic effect is significant.

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TABLE 1. 25 Broad-Group Structure

	Energy Ran		
Gp. No.	Upper	Lower	<u> </u>
1	2.0 +7*	3.0 +6	1.89712
2	3.0 +6	1.4 +6	0.76214
3	1.4 +6	9.0 +5	0.44183
4	9.0 +5	4.0 +5	0.81093
5	4.0 +5	1.0 +5	1.38629
6	1.0 +5	1.7 +4	1.77196
7	1.7 +4	3.0 +3	1.73460
8	3.0 +3	5.5 +2	1.69645
9	5.5 +2	1.0 +2	1.70475
10	1.0 +2	30	1.20397
11	30	10	1.09861
12	10	3.05	1.18744
13	3.05	1.77	0.54417
14	1.77	1.30	0.30861
15	1.30	1.13	0.14015
16	1.13	1.00	0.12222
17	1.00	0.80	0.22314
18	0.80	0.40	0.69315
19	0.40	0.325	0.20764
20	0.325	0.225	0.36772
21	0.225	0.100	0.81093
22	0.100	0.050	0.69315
23	0.050	0.030	0.51082
24	0.030	0.010	1.09862
25	0.010	15	6.90775

*Read as 2.0 x 10^7

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TABLE 2. Homogeneous Plutonium Benchmarks

No.	H/Pu Atom Ratio	% ²⁴⁰ Pu	Pu Density, g/cm ³	Geometry
1	3695	0	0.007	Infinite
2*	125	5	0.172	Sphere
3*	980	1	0.026	Sphere
4*	758	5	0.034	Sphere
5	15	2	1.12	Parallelepiped
6	0	5	15.6	Sphere
7*	422	5	0.058	Slab
8	910	14	0.028	Cylinder
9	50	18	0.37	Parallelepiped
10	210	8	0.116	Cylinder
11	0	18	5.8	Parallelepiped
12	5	11	2.3	Parallelepiped
13	0	20	15.7	Sphere
14*	623	43	0.041	Cylinder
15a*	1067	5	0.024	Sphere
156	1031	5	0.025	Sphere

TABLE 3. Fundamental Theoretical Forms

Modified Adler-Adler Formalism

$$\sigma_{\mathbf{x}}(\mathbf{E})\sqrt{\mathbf{E}} = \frac{\pi\hbar^2}{2M_n} \begin{bmatrix} NR & \frac{g_{\mathbf{r}}\Gamma_{\mathbf{n}\mathbf{r}}^{\circ}\Gamma_{\mathbf{x}\mathbf{r}} + A_{\mathbf{x}\mathbf{r}}(\mathbf{E}-\mathbf{E}_{\mathbf{r}})}{(\mathbf{E}-\mathbf{E}_{\mathbf{r}})^2 + (\Gamma_{\mathbf{r}}(\mathbf{E})/2)^2} + \sum_{b=1}^{NB} B_{\mathbf{x}b}\mathbf{E}^{b-1} \end{bmatrix}$$

$$\mathbf{x} = \gamma, \mathbf{f}$$

Multi-Level Breit-Wigner Formalism

$$\sigma_{coh}(E)/4\pi = [g_{+}b_{+}(E) + g_{-}b_{-}(E)]^{2} + [g_{+}d_{+}(E) + g_{-}d_{-}(E)]^{2}$$

$$\sigma_{inc}(E)/4\pi = g_{+}g_{-}[(b_{+}(E) - b_{-}(E))^{2} + (d_{+}(E) - d_{-}(E))^{2}]$$

$$\sigma_{s}(E)/4\pi = g_{+}^{2}[b_{+}^{2}(E) + d_{+}^{2}(E)] + g_{-}[b_{-}^{2}(E) + d_{-}^{2}(E)]$$

$$b_{\pm}(E) = R + \frac{\hbar}{\sqrt{8M_{n}}} \sum_{\substack{r=\pm}}^{\Sigma} \frac{\Gamma_{nr}^{\circ}(E-E_{r})}{(E-E_{r})^{2} + (\Gamma_{r}(E)/2)^{2}}$$

$$d_{\pm}(E) = \frac{\hbar}{\sqrt{32M_{n}}} \sum_{\substack{r=\pm}}^{\Sigma} \frac{\Gamma_{nr}^{\circ}\Gamma_{r}}{(E-E_{r})^{2} + (\Gamma_{r}(E)/2)^{2}}$$

Spin-Dependent Resonance Formalism

$$v(E)\sigma_{f}(E)\sqrt{E} = v_{+}\sigma_{f}^{+}(E)\sqrt{E} + v_{-}\sigma_{f}^{-}(E)\sqrt{E} + v_{b}\sigma_{f}^{b}(E)\sqrt{E}$$

$$\sigma_{f}^{\pm}(E)\sqrt{E} = \frac{\pi\hbar^{2}}{2M_{n}} \sum_{\substack{r=\pm}}^{\Sigma} \frac{g_{r}\Gamma_{nr}^{\circ}\Gamma_{fr} + A_{fr}(E-E_{r})}{(E-E_{r})^{2} + (\Gamma_{r}(E)/2)^{2}}$$

$$\sigma_{f}^{b}(E)\sqrt{E} = \frac{\pi\hbar^{2}}{2M_{n}} \sum_{\substack{b=1\\b=1}}^{NB} B_{fb}E^{b-1}$$

$$v_{b} = \lambda v_{+} + (1-\lambda)v_{-}$$

NOTE: For all forms $\Gamma_r(E) = \Gamma_{fr} + \Gamma_{\gamma r} + \Gamma_{nr}^{\circ} \sqrt{E}$

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TABLE 4. Combinations of Fundamental Theoretical Forms

Absorption

$$\sigma_{a}(E)\sqrt{E} = \sigma_{f}(E)\sqrt{E} + \sigma_{v}(E)\sqrt{E}$$

Total

$$\sigma_{+}(E)\sqrt{E} = \sigma_{a}(E)\sqrt{E} + \sigma_{c}(E)\sqrt{E}$$

Alpha

$$\alpha(E) = \sigma_{e}(E) \sqrt{E} / \sigma_{f}(E) \sqrt{E}$$

Eta

 $\eta(E) = (v(E)\sigma_f(E)\sqrt{E})/\sigma_a(E)\sqrt{E}$

Nu

$$v(E) = (v(E)\sigma_{f}(E)\sqrt{E})/\sigma_{f}(E)\sqrt{E}$$

Sums*

$$S(E) = \lambda \sigma_v^{Z}(E) + (1-\lambda) \sigma_v^{Z}(E)$$

(possibly with \sqrt{E} multiplier)

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Ratios*

$$R(E) = \sigma_x^{Z}(E)/\sigma_x^{Z}(E)$$
 (possibly with \sqrt{E} cancelling)

*Sums and ratios may be formed with any theory form x for isotope z and any theory form x' for isotope z', except n and v.

TABLE 5. The Parameters of the Model

	Resonance Parameters	Non-Resonance Parameters		
Er	Resonance Energy (eV)	B _{f1} , B [*] _{f2} , B [*] _{f3}	Coefficients of back-	
r°nr	Reduced Neutron width $(eV^{1/2})$	$B_{\gamma 1}^{}, B_{\gamma 2}^{*}, B_{\gamma 3}^{*}$	and fission and capture	
^r fr	Fission width (eV)	R	Potential scattering radius $(b^{1/2})$	
ryr	Capture width (eV)	ν ₊ , ν ₋ , ν _b	Neutrons per fission in	
Afr	Fission asymmetry coefficient ($eV^{1/2}$)		and non-resonance fission respectively	
Ayr	Capture asymmetry coefficient ($eV^{1/2}$)			

Theory Parameters for Each Isotone

Input constant - statistical weight factor) (gr

Experimental Parameters

N _s *	Normalization factor for ath data set
α _s *, β _s *	Energy-scale adjustment parameters for sth data set
	$E = E_m (\alpha_s + \beta_s \sqrt{E_m})$
λs*	Compostition parameter for sth data set, if applicat

Compostition parameter for sth data set, if applicable

* Indicates that parameter does not have to be present

TABLE 6. Absolute Data for 240Pu Used for Normalization

Cross Section	Datum	Fitted Value
σ _γ (.0253)	289.5 ± 1.4b	289.41 ± 1.63b
σ _s (.08)	$1.54 \pm .05b$	1.537 ± .059b
of PEAK	33 ± 3b	33.00 ± 3.55b

TABLE 7. Preliminary Results of ²⁴⁰Pu Data Analysis

2200	m/s	Cross	Sections	1 eV	Re	sonance Parameters
σt°	=	291.3	± 1.64b	Eo	=	1.0594 ± .008 eV
σγ°	=	289.4	± 1.63b	۲'n°	=	2.451 \pm .0026 meV/eV $^{1/2}$
σs°	=	1.813	± .060b	Γ _γ	=	29.72 ± .41 meV
				Гf	=	5.76 ± .60 µeV

1/V Capture Background at Thermal is 10.4 \pm 2.1b Fitted $^{239}\text{Pu}\,\sigma_{_{\rm Y}}$ impurity in Weston and Todd data (.82 \pm .09%)

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Parameter	Bound Level	Visible Level
E _o (eV)	071876	.29687
$r_n^o(\mu eV/\sqrt{eV})$	48.963	149.46
$\Gamma_{\gamma}(meV)$	38.892	39.508
$\Gamma_{f}(meV)$	405.75	59.990
$A_{f}(\mu eV/\sqrt{eV})$	2.2702	5.8061

TABLE 8. Resonance Parameters from the Preliminary Fit of ²³⁹Pu Data

TABLE 9. 2200 m/s Parameters for ²³⁹Pu

Parameter	ENDF/B-IV	Preliminary New Data
σt	1019.9	1027.1
σc	270.2	271.5
σf	741.7	748.5
νt	2.8733	2.8766
α	0.3643	0.3627
η	2.1061	2.1109

TABLE 10. Parameters for the Six Peaks of the Phonon Spectrum

Peak	Υ _i	δ _i	Fi
1	0.1647	0.1941	0.0279
2	0.8794	0.2216	0.0105
3	2.1629	0.6402	0.3401
4	2.6258	0,1814	0.1905
5	7.9479	0.2597	0.1099
6	17.4520	0.6903	0.3206

TABLE 11. Comparison of H₂O Kernels for Broad Group 13

FINAL GP. NO.	ENDF	TISK	TISK-Koppel
13	5.750	5.420	5.559
14	4.098	3.656	3.791
15	1.485	1.253	1.337
16	1.133	0.934	1.000
17	1.739	1.412	1.516
18	3.464	2.860	2.823
19	0.645	0.546	0.487
20	0.852	0.725	0.621
21	1.039	0.861	0.705
22	0.387	0.289	0.232
23	0.145	0.093	0.075
24	0.117	0.070	0.057
25	0.035	0.018	0.015
TOTAL	20.889	18.139	18.216

TABLE 12. Comparison of H₂O Kernels for Broad Group 14

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FINAL GP. NO.	ENDF	TISK	TISK-Koppel
13	0.007	0.006	0.006
14	4.195	4.353	4.506
15	2.313	2.201	2.123
16	1.695	1.591	1.571
17	2.625	2.400	2.476
18	5.294	4.591	4.875
19	0.982	0.817	0.925
20	1.287	1.058	1.196
21	1.492	1.211	1.351
22	0.487	0.393	0.442
23	0.154	0.124	0.142
24	0.110	0.091	0.106
25	0.030	0.024	0.028
TOTAL	20.670	18.860	19.748

FINAL GP. NO.	ENDF	TISK	TISK-Koppel
14	0.052	0.047	0.050
15	2.837	3.161	3.462
16	2.437	2.313	2.240
17	3.254	3.119	2.825
18	6.549	5.987	6.196
19	1.230	1.081	1.082
20	1.615	1.396	1.490
21	1.875	1.595	1.786
22	0.612	0.514	0.591
23	0.0193	0.162	0.190
24	0.0138	0.119	0.143
25	0.037	0.031	0.037
TOTAL	20.828	19.525	20.093

TABLE 13. Comparison of H20 Kernels for Broad Group 15

TABLE 14. Comparison of H₂O Kernels for Broad Group 16

FINAL GP. NO.	ENDF	TISK	TISK-Koppel
15	0.123	0.106	0.118
16	2.873	3.156	3.480
17	4.208	4.002	3.833
18	7.342	6.881	6.908
19	1.403	1.267	1.255
20	1.845	1.646	1.597
21	2.148	1.877	1.937
22	0.701	0.606	0.679
23	0.221	0.191	0.221
24	0.157	0.140	0.165
25	0.042	0.036	0.043
TOTAL	21.063	19.910	20.236

FINAL GP. NO	ENDF	TISK	TISK-Koboel
15	0.081	0.070	0.078
- 17	4.354	4.586	5.002
18	9.124	8.704	9.268
19	1.647	1.525	1.659
20	2.190	1.995	2.072
21	2.553	2.313	2.265
22	0.834	0.748	0.747
23	0.261	0.235	0.244
24	0.185	0.172	0.184
25	Ú.049	0.044	0.049
TOTAL	21.278 -	20.392	20.567

TABLE 15.

Comparison of H₂O Kernels for Broad Group 17

TABLE 16. Comparison of H₂O Kernels for Broad Group 18

FINAL GP. NO.	ENDF	TISK	TISK-Koppel
17	0.028	0.026	0.027
18	9.613	9.754	10.250
19	2.942	2.807	2.680
20	3.641	3.472	3.216
21	4,105	3.905	3.674
22	1.304	1.233	1.233
23	0:402	0.382	0,403
24	0.279	0.276	0.302
25	0.073	0.070	0.080
TOTAL	22.387	21.925	21.865

TABLE 17.	Comparison or	f H_20 Kernels for	Broad Group 19
FINAL GP. NO.	ENDF	TISK	TISK-Koppel
18	0.437	0.383	0.416
19	6.913	7.425	8.285
20	6.748	6.392	6.447
21	7.046	6.736	6.009
22	2.174	2.080	1.787
23	0.649	0.619	0.542
24	0.435	0.432	0.390
25	0.110	0.107	0.100
TOTAL	24.511	24.174	23.976

TABLE 18. Comparison of H₂O Kernels for Broad Group 20

FINAL GP. NO.	ENDF	TISK	TISK-Koppel
18	0.019	0.017	0.016
19	0.457	0.401	0.441
20	10.238	10.830	11.962
21	10.503	9.952	9.542
22	3.179	3.004	2.660
23	0.976	0.922	0.823
24	0.656	0.643	0.581
25	0.165	0.157	0.144
TOTAL	26.192	25.927	26.168

TABLE 19.	Comparison of	f H ₂ O Kernels for	Broad Group 21
FINAL GP. NO.	ENDF	TISK	TISK-Koppel
19	0.007	0.006	0.006
20	0.453	0.402	0.424
21	18.808	19.967	21.375
22	7.599	6.751	6.546
23	2.092	2.042	1.841
24	1.345	1.318	1.204
25	0.324	0.292	0.273
TOTAL	30.629	30.778	31.669

TABLE 20. Comparison of H_2O Kernels for Broad Group 22

FINAL GP. NO.	ENDF	TISK	TISK-Koppel
20	0.015	0.013	0.012
21	2.673	2.250	2.239
22	25.086	28.560	29.852
23	6.938	5.187	5.307
24	2.669	2.496	2.365
25	0.631	0.650	0.606
TOTAL	38.013	39.156	40.381

TABLE 21.	Comparison o	f H ₂ 0 Kernels for	Broad Group 23
FINAL GP. NO.	ENDF	TISK	TISK-Koppel
21	0.909	0.873	0.787
22	8.657	6.424	6.573
23	26.898	34.864	35.621
24	9.063	6.127	6.250
25	0.723	0.637	0.626
TOTAL	46.257	48.930	49.862

TABLE 22. Comparison of H₂O Kernels for Broad Group 24

FINAL GP. NO.	ENDF	TISK	TISK-Koppel
21	0.554	0.509	0.463
22	3.183	2.847	2.698
23	8.625	5.667	5.781
24	40.852	53.238	53.744
25	5.746	2.141	2.155
TOTAL	58.963	64.405	64.845

TABLE 23. Comparison of H₂O Kernels for Broad Group 25

FINAL GP. NO.	ENDF	TISK	TISK-Koppel
21	0.557	0.467	0.437
22	3.197	3.215	2.993
23	2.931	2.543	2.499
24	24.332	9.322	9.383
25	48.074	97.537	97.922
TOTAL	79.095	113.087	113.238

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TABLE 24. Evaluation of Stainless Steel Using Homogeneous Plutonium Benchmarks

Parameter	15a	15b
SS Thickness, cm	0.122	0.325
Pu Density, g/cm ³	0.0244	0.0252
H/Pu Atom Ratio	1067	1031
k _∞	1.4895	1.4995
SS Absorptions	0.0225	0.0466
k _{eff}	1.0207	1.0187

TABLE 25. Evaluation of Stainless Steel Using Enriched UO2 Lattice Benchmarks

Parameter	42a	42b
Clad Material	SS	Al
k∞	1.1777	1.2941
Clad Absorptions	0.0733	0.0047
^k eff	0.9973	0.9917
Critical Number of Rods	1766	950
Leakage Fraction	0.153	0.234

Benchmark No.	H/Pu	% ²⁴⁰ Pu	Pu Density, g/cm ³	Geometry	Radius or Thickness, cm
2	125	4.5	0.172	Sphere	19.32
3	980	0.5	0.026	Sphere*	17.78
4	758	4.5	0.034	Sphere	19.32
7	422	4.6	0.058	Slab	16.91
14	623	42.9	0.041	Cylinder*	30.51
15a	1067	4.5	0.024	Sphere*	19.32

TABLE 26. Description of Benchmarks Used to Evaluate Data Changes

*Reflected with H_20 ; other systems are unreflected.

TABLE 27. Group Fluxes for Benchmark 2 Using Various Water Kernels

Gp. No.	ENDF	TISK	% Difference	TISK-Koppel	% Difference
13	22.033	25.982	+17.9	26.098	+0.4
14	12.587	14.620	+16.2	14.232	-2.7
15	5.514	6.228	+13.0	6.149	-1.3
16	2.543	2.732	+ 7.4	2.736	+0.1
17	7.943	8.597	+ 8.2	8.731	+1.6
18	24.788	26.114	+ 5.4	27.128	+3.9
19	4.315	4.431	+ 2.7	4.599	+3.8
20	4.836	4.881	+ 0.9	4.951	+1.4
21	18.277	18.468	+ 1.0	18,448	-0.1
22	19.254	19.079	- 0.9	18,689	-2.0
23	10.853	10.498	- 3.3	10.236	-2.5
24	8.816	8.549	- 3.0	8.309	-2.8
25	1.729	1.511	-12.6	1.467	-2.9

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-	-	-	-
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1 M	DL	E .	60.

Group Fluxes for Benchmark 4 Using Various Water Kernels

Gp. No.	ENDF	TISK	% Difference	TISK-Koppel	% Difference
13	21.248	25.213	+18.7	25.318	+0.4
14	12.312	14.370	+16.7	13.955	-2.9
15	5.625	6.398	+13.7	6.310	-1.4
16	4.260	4.718	+10.8	4.722	+0.1
17	8.941	9.812	+ 9.7	9.949	+1.4
18	29.527	31.561	+ 6.9	32.957	+4.4
19	8.126	8.563	+ 5.4	9.136	+6.7
20	14.023	14.540	+ 3.7	15.343	+5.5
21	70.820	71.568	+ 1.1	72.615	+1.5
22	130.978	131.998	+ 0.8	130.319	-1.3
23	94.240	94.358	+ 0.1	92.963	-1.5
24	91.974	93.851	+ 2.0	92.280	-1.7
25	20.558	19.717	- 4.1	19.354	-1.9

TABLE 29. Group Fluxes for Benchmark 14 Using Various Water Kernels

Gp. No.	ENDF	TISK	% Difference	TISK-Koppel	% Difference
13	21.199	25.147	+18.6	25.291	+0.6
14	12.278	14.305	+16.5	13.917	-2.7
15	5.196	5.859	+12.8	5.791	-1.2
16	1.664	1.765	+ 6.1	1.770	+0.3
17	7.303	7.880	+ 7.9	8.024	+1.8
18	26.722	28.209	+ 5.6	29.552	+4.8
19	7.831	8.171	+ 4.3	8.770	+7.3
20	14.445	14.840	+ 2.7	15.810	+6.5
21	74.823	74.467	- 0.5	75.917	+1.9
22	142.78	141.80	- 0.7	140.61	-0.8
23	103.61	102.32	- 1.2	101.26	-1.0
24	101.61	102.33	+ 0.7	101.08	-1.2
25	22.756	21.563	- 5.2	21.261	-1.4

Gp. No.	N	No Reflector			Reflected		
	2	4	7	3	14	15a	
1	+.02	+.02	+.01	+.03	+.02	+.02	
2	+.02	+.03	+.02	+.04	+.03	+.04	
3	+.01	+.01	+.01	+.02	+.01	+.02	
4	+.01	+.01	+.01	+.02	+.01	+.02	
5	+.01	+.01	+.01	+.02	+.01	+.02	
6	0	+.01	0	+.01	+.01	+.01	
7	0	0	0	0	0	0	
8	0	0	0	0	0	0	
9	0	0	0	0	0	0	
10	0	0	0	0	0	0	
11	0	0	0	0	0	0	
12	0	0	0	0	0	0	
13	04	05	05	02	0	02	
14	0	01	0	+.02	+.01	+.02	
15	+.01	0	+.01	+.01	+.01	+.01	
16	+.01	0	+.01	+.02	+.01	+.02	
17	+.01	+.01	+.02	+.03	+.01	+.03	
18	+.07	+.06	+.10	+.12	+.03	+.11	
19	+.01	+.02	+.03	+.03	+.01	+.03	
20	+.01	+.03	+.04	+.04	+.01	+.04	
21	+.03	+.12	+.10	+.02	02	+.02	
22	+.03	+.16	+.11	02	04	01	
23	+.01	+.10	+.06	01	02	0	
24	+.01	+.07	+.04	+.02	0	+.02	
25	0	+.03	+.01	0	0	0	
Total	+.23	+.63	+.54	+.40	+.10	+.40	

TABLE 30. Reactivity Effect of Water Kernel on Leakage

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Energy, eV



52

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996 151







Energy, eV

FIGURE 4. ENDF/B-IV Fission Cross Section for 239Pu

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Energy, eV















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Energy, eV



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996 157



Energy Transfer (Beta)





Energy, eV



996. 158











FIGURE 11. Transfer Cross Section from Group 173 for ENDF Hydrogen Bound in Water



Energy, eV

FIGURE 12. Transfer Cross Section from Group 173 for TISK Hydrogen Bound in Water 996 161

63

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FIGURE 13. Transfer Cross Section from Group 173 for TISK-Koppel Hydrogen Bound in Water

162

096



FIGURE 14. Ratio of Transfer Cross Sections from Group 173 for Hydrogen Bound in Water 996 163

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Cross-Section Ratio

66

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Parts.





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17. KEY WORDS AND	DOCUMENT ANALYSIS	17a. DESCRI	PTORS		
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