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Author(s):	Kiedrowski, Brian C.
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IMPORTANCE OF SCATTERING DISTRIBUTIONS ON CRITICALITY

Brian C. Kiedrowski
Los Alamos National Laboratory
P.O. Box 1663 MS A143, Los Alamos, NM 87545
bckiedro@lanl.gov

ABSTRACT

MCNP6 has the capability to compute sensitivity coefficients for k from scattering distributions as a function of scattering cosine. A new capability has been prototyped, and will hopefully available in a future release, that takes those results and converts them into sensitivities for Legendre scattering moments, which is discussed. Results are shown for a variety of criticality benchmarks for elastic scattering, and it appears that the P_1 elastic scattering Legendre moment (i.e., average scattering cosine $\bar{\mu}$) may indeed have a significant effect in fast, bare and reflected systems with significant leakage. The results also show that higher elastic moments and all inelastic moments are typically not important to criticality.

Key Words: MCNP, sensitivity, uncertainty, Legendre moments

1. INTRODUCTION

MCNP6.1 [1], the first production version of MCNP6, has a new capability to compute sensitivity coefficients for the effective multiplication k from continuous-energy nuclear data [2]. The code can generate sensitivity coefficients to cross sections, fission ν and χ, as well as scattering distributions. The scattering distributions have typically not been a major focus until recently when Aliberti and McKnight [3] showed that the average scattering cosine $\bar{\mu}$ can have a significant impact in bare spherical systems. They were also able to take these sensitivities and convolve them with Evaluated Nuclear Data File (ENDF) covariance data, which is represented as covariances for Legendre moments ($\bar{\mu}$ is the P_1 Legendre moment) as a function of incident energy.

The capability in MCNP6.1, however, cannot estimate the sensitivity to $\bar{\mu}$ directly, but rather does so as a function of scattering cosine μ. To facilitate comparisons to published results as well as uncertainty propagation, a new capability to take the sensitivities as a function of scattering cosine into sensitivities to Legendre scattering moments has been developed and is planned to be released in the next version of MCNP6.

This paper discusses the new method, and applies it to 22 criticality benchmarks from the International Criticality Safety Benchmark Experiment Project (ICSBEP) Handbook [4]. The results show that the P_1 elastic scattering distribution has a significant effect on criticality for fast bare and reflected systems where leakage is significant. The continuous-energy Monte Carlo results shown are in general agreement with those from Aliberti and McKnight, which are from multigroup deterministic calculations. The results also show that the higher elastic Legendre moments and inelastic distributions do not have a significant effect on criticality, implying that having only $\bar{\mu}$ covariances (which is all that is currently available for some isotopes in ENDF/B-VII.1) is sufficient for uncertainty quantification for most criticality applications.

2. METHOD

The sensitivity coefficient of k with respect to parameter x is defined as

$$S_{k,x} = \frac{x}{k}\frac{dk}{dx}. \tag{1}$$

Here the parameter x is taken to be some nuclear data, e.g., cross section, prompt fission spectra, etc. This can be found from perturbation theory as a ratio of adjoint-weighted integrals:

$$S_{k,x} = -\frac{\left\langle \psi^{\dagger}, (\Sigma_x - \mathcal{S}_x - \lambda\mathcal{F}_x)\psi \right\rangle}{\langle \psi^{\dagger}, \lambda\mathcal{F}\psi \rangle}. \tag{2}$$

Here ψ is the angular (forward) flux and $\psi^{\dagger}$ is its adjoint function. Σ_x is the cross section corresponding to x if x is a cross section, and zero otherwise (e.g., fission χ). $\mathcal{S}_x$ is the integral scattering operator for x if x is a scattering cross section or law [includes elastic, inelastic, (n,2n), etc.], and zero otherwise. $\mathcal{F}_x$ is the integral fission operator for x if x is a fission cross section, fission ν, or fission χ and zero otherwise. The quantity $\lambda = 1/k$ and the brackets denote integration over all phase space.

The adjoint-weighted integrals are computed by special tallies within MCNP using the iterated fission probability method [5].

For scattering distributions, the Σ_x and $\mathcal{F}_x$ in Eq. (2) terms are always zero. Furthermore, the scattering law is integrated over some cosine bin, where i represents the index for left edge of the bin and $i + 1/2$ represents the bin center. The simplified version for Eq. (2) is therefore

$$S_{k,f,i+1/2} = \frac{\left\langle \psi^{\dagger}, \mathcal{S}_{x,i}\psi \right\rangle}{\langle \psi^{\dagger}, \lambda\mathcal{F}\psi \rangle}, \tag{3}$$

where the i subscript on $\mathcal{S}_x$ represents that the integration of the forward scattering source is only over cosine bin i.

The sensitivities computed by Eq. (3) are not entirely correct because they do not account for the fact that they need to be renormalized such that the integral of the probability function is preserved. In other words, the sensitivity represents some small increase of the data in some energy range, which needs to be offset by decreases elsewhere. There are many possible methods for doing this; MCNP uses a classic approach where the entire distribution is renormalized by a constant factor after the hypothetical increase. This renormalization can be taken into account by

$$\hat{S}_{k,f,i+1/2} = S_{k,f,i+1/2} - F_{i+1/2}S_{k,f} \tag{4}$$

Here $S_{k,f,i+1/2}$ represents the sensitivity coefficient for f if the distribution were left unnormalized, $F_{i+1/2}$ represents the bin-integrated cumulative density function (CDF) obtained from

$$F_{i+1/2} = \int_{\mu_i}^{\mu_{i+1}} d\mu\, f(\mu), \tag{5}$$

and $S_{k,f}$ is given by

$$S_{k,f} = \sum_{i=0}^{N-1} S_{k,f,i+1/2}, \tag{6}$$

where there are $N-1$ cosine bins and N bin edges.

The ENDF covariance data for scattering distributions, however, is represented as uncertainties and correlations of Legendre scattering moments. It is therefore beneficial to convert the sensitivities into that format as well. Let $f(\mu)$ be the probability density function (PDF) of a neutron scattering with cosine μ (the incident and outgoing energy dependence are not included for notational brevity). The scattering PDF may be reconstructed by its Legendre moments through

$$f(\mu) = \sum_{\ell=0}^{\infty} \frac{2\ell+1}{2} P_\ell(\mu) f_\ell, \tag{7}$$

where the ℓth Legendre moment is found by

$$f_\ell = \int_{-1}^{1} d\mu \; P_\ell(\mu) f(\mu). \tag{8}$$

Using the definition of the sensitivity coefficient in Eq. (1), the relative change in k from a relative change in f may be found by

$$\frac{\Delta k}{k} = \int_{-1}^{1} d\mu \; \frac{\Delta f(\mu)}{f(\mu)} \hat{s}_{k,f}(\mu). \tag{9}$$

Here $\hat{s}_{k,f}(\mu)$ is the sensitivity density, which is the bin-integrated sensitivity from Eq. (4) per unit cosine. The sensitivity density and the bin-integrated sensitivities are related by

$$\hat{S}_{k,f,i+1/2} = \int_{\mu_i}^{\mu_{i+1}} d\mu \; \hat{s}_{k,f}(\mu). \tag{10}$$

The integer values of i represent bin edges and the bin-integrated sensitivities are taken at bin centers or $i+1/2$. If the binning is fine enough, the central difference may be used to adequately approximate the relationship between the two:

$$\hat{s}_{k,f,i+1/2} = \frac{\hat{S}_{k,f,i+1/2}}{\mu_{i+1}-\mu_i}. \tag{11}$$

Likewise, MCNP may estimate the scattering CDF $F_{i+1/2}$ where Eq. (9) requires the PDF. Again, for a fine enough binning, central differencing may be used as well:

$$f_{i+1/2} = \frac{F_{i+1/2}}{\mu_{i+1}-\mu_i}. \tag{12}$$

Going back to Eq. (9), suppose the ℓth Legendre moment is perturbed by a multiplicative factor of $1+p$ where p is small. The change in the scattering distribution Δf is then

$$\Delta f(\mu) = \frac{2\ell+1}{2} P_\ell(\mu) f_\ell p. \tag{13}$$

Assuming that the binning is fine enough that midpoint integration is valid, Eq. (9) may be written in a discrete form:

$$\frac{1}{p}\frac{\Delta k}{k} = \frac{2\ell+1}{2} f_\ell \sum_{i=0}^{N-1} \left(\mu_{i+1}-\mu_i\right) \frac{P_\ell(\mu_{i+1/2})}{f_{i+1/2}} \hat{s}_{k,f,i+1/2}. \tag{14}$$

The left-hand side is the relative change in k divided by the relative change in the Legendre moment f_ℓ, so that is the sensitivity coefficient for the ℓth Legendre moment by the definition of the sensitivity coefficient.

Substituting the CDFs in place of the PDFs using the central differencing approximation, the final result for the Legendre moment is obtained:

$$\hat{S}_{k,f,\ell} = \frac{2\ell+1}{2} f_\ell \sum_{i=0}^{N-1} \left(\mu_{i+1} - \mu_i\right) \frac{P_\ell(\mu_{i+1/2})}{F_{i+1/2}} \hat{S}_{k,f,i+1/2}. \tag{15}$$

There still remains the task of computing the Legendre moment f_ℓ, which is done by midpoint integration:

$$f_\ell = \sum_{i'=0}^{N-1} F_{i'+1/2} P_\ell(\mu_{i'+1/2}). \tag{16}$$

Here the dummy index i' is used to delineate between the index i.

The implementation of solving for $\hat{S}_{k,f,\ell}$ is as follows: First, a cosine grid is created at problem setup. The user may provide one, and if not, a default of 200 equally spaced cosine intervals of width 0.01 is used. Note that in MCNP6, these scattering cosines and all calculations are in the reference frame of the table, which is usually the center-of-mass frame. MCNP obtains random samples of the renormalized sensitivities and the scattering CDFs on the cosine grid every block of cycles or iterations in the eigenvalue calculation, and applies Eq. (15) to estimate the random samples of the Legendre scattering moment sensitivities. This process is repeated again and again and the random samples are averaged to provide the final estimate of the Legendre scattering moment sensitivities.

The estimate of the Legendre moment sensitivity should be accurate if the cosine grid is a fine enough representation (the default has empirically been found to be good enough) and there are no negative scattering probabilities, which MCNP does not treat. Sometimes with Legendre expansion representations in ENDF, small amounts of unphysical negative scattering occurs. When the data is processed by NJOY, these negative regions are zeroed out or ignored. Should the data have significant amounts of negative scattering, estimates obtained by MCNP for the Legendre moment sensitivities will not be accurate. Then again, negative scattering is unphysical anyway, and the data representation should have used more Legendre moments for a more accurate representation of the scattering distribution.

To verify this method, fictitious multigroup cross sections were created, and a perturbed cross section library was created by directly changing either the P_1 or P_2 scattering moment. For each case, two calculations were run, one with the reference data, and the other with the perturbed data, and the difference in k was used to estimate the Legendre sensitivities. These results were compared to the Legendre scattering moment sensitivities obtained from perturbation theory. The results show agreement and are published elsewhere [6].

3. RESULTS

To show the impact of scattering distributions, 22 benchmarks were selected from the ICSBEP Handbook to cover a variety of fissile isotopes, geometries, and neutron spectra. ENDF/B-VII.1 nuclear data [7] was used for all calculations. The default of 200 equally-spaced cosine bins was used.

Tables I and II show P_1 through P_5 elastic scattering Legendre moments sensitivities to k for selected isotopes from each of the 22 benchmarks summed over incident energies from 0 to 10 MeV. An incident energy grid with 0.1 MeV intervals was used for each.

Table I. Legendre elastic scattering moment sensitivities to k for fast/intermediate benchmarks

Benchmark	Isotope	P_1	P_2	P_3	P_4	P_5
hmf-001	^{235}U	-0.10396	0.00401	0.00004	-0.00019	0.00050
hmf-004	^{1}H	0.00013	0.00000	0.00000	0.00000	0.00000
	^{16}O	-0.01021	0.00384	-0.00032	0.00005	0.00000
	^{235}U	-0.05046	0.00112	-0.00042	-0.00044	0.00152
hmf-028	^{235}U	-0.03883	0.00119	-0.00103	0.00049	0.00025
	^{238}U	-0.11071	0.01589	-0.00467	0.00139	0.00151
hmf-072	^{56}Fe	-0.01716	0.00101	0.00036	0.00016	0.00014
	^{235}U	-0.00845	0.00054	-0.00029	0.00083	-0.00009
hmi-006	C	-0.01259	0.00183	-0.00006	0.00001	0.00002
	^{235}U	-0.00312	0.00111	-0.00064	0.00014	0.00012
hci-003	^{1}H	0.00028	0.00000	0.00000	0.00000	0.00000
	^{235}U	-0.02399	0.00065	-0.00076	0.00043	0.00035
	^{238}U	-0.04202	0.00474	-0.00301	0.00209	0.00018
imf-003	^{235}U	-0.04066	0.00056	-0.00084	0.00057	0.00032
	^{238}U	-0.07188	0.00147	-0.00145	0.00091	0.00111
mmf-008	^{235}U	0.00082	0.00007	0.00007	-0.00040	-0.00003
	^{238}U	0.00985	0.00040	-0.00397	0.00241	-0.00031
pmf-001	^{239}Pu	-0.08958	0.00551	-0.00379	0.00224	0.00134
pmf-002	^{239}Pu	-0.07224	0.00394	-0.00309	0.00221	0.00089
	^{240}Pu	-0.01516	0.00045	-0.00172	0.00147	0.00011
pmf-006	^{238}U	-0.13136	0.02764	-0.00909	0.00271	0.00106
	^{239}Pu	-0.03421	0.00086	-0.00195	0.00210	0.00018
pmf-018	^{9}Be	-0.04174	0.01282	-0.00138	0.00006	0.00000
	^{239}Pu	-0.05124	0.00178	-0.00256	0.00171	0.00087
smf-008	^{235}U	-0.08178	0.00205	-0.00106	-0.00001	0.00075
	^{237}Np	-0.00312	-0.00005	-0.00035	0.00033	0.00001
umf-001	^{233}U	-0.09876	0.00648	-0.00112	-0.00008	0.00133
umf-004	^{182}W	-0.01423	0.00153	0.00030	0.00019	-0.00032
	^{183}W	-0.00679	0.00033	0.00046	-0.00008	-0.00010
	^{184}W	-0.01664	0.00168	0.00039	0.00035	-0.00042
	^{186}W	-0.01768	0.00222	0.00032	0.00046	-0.00051
	^{233}U	-0.06769	0.00299	-0.00098	0.00073	0.00100

Table II. Legendre elastic scattering moment sensitivities to k for thermal benchmarks

Benchmark	Isotope	P_1	P_2	P_3	P_4	P_5
hst-013	^{1}H	0.00040	0.00000	0.00000	0.00000	0.00000
	^{16}O	-0.00599	0.00117	0.00005	0.00000	-0.00001
	^{235}U	0.00000	0.00000	0.00000	0.00000	0.00000
ict-002	^{1}H	0.00025	0.00000	0.00000	0.00000	0.00000
	^{16}O	-0.00520	0.00046	-0.00008	0.00004	-0.00001
	^{235}U	-0.00005	-0.00001	-0.00004	0.00001	-0.00002
	^{238}U	-0.00062	-0.00015	-0.00008	0.00011	0.00000
lct-008	^{1}H	0.00002	0.00000	0.00000	0.00000	0.00000
	^{16}O	-0.00139	-0.00008	-0.00010	0.00000	0.00000
	^{235}U	-0.00004	-0.00010	-0.00002	-0.00000	0.00001
	^{238}U	-0.00233	0.00020	-0.00088	0.00016	0.00014
lst-002	^{1}H	0.00024	0.00000	0.00000	0.00000	0.00000
	^{16}O	-0.00528	0.00045	-0.00001	-0.00001	0.00000
	^{235}U	-0.00001	0.00000	0.00000	0.00000	0.00000
	^{238}U	-0.00043	-0.00027	0.00005	0.00006	0.00005
mct-001	^{1}H	0.00033	-0.00001	0.00000	0.00000	0.00000
	^{16}O	-0.00960	0.00174	0.00000	-0.00004	0.00000
	^{238}U	-0.00267	-0.00027	-0.00006	0.00052	0.00008
	^{239}Pu	-0.00043	0.00002	-0.00022	0.00013	-0.00002
pst-009	^{1}H	0.00014	0.00000	0.00000	0.00000	0.00000
	^{16}O	-0.00263	0.00011	0.00011	-0.00003	0.00001
	^{239}Pu	-0.00001	0.00000	0.00000	0.00000	0.00000
uct-002	^{1}H	0.00041	0.00000	0.00000	0.00000	0.00000
	^{16}O	-0.01171	0.00149	-0.00004	-0.00002	0.00000
	^{232}Th	-0.01315	0.00139	-0.00141	0.00110	-0.00014
	^{235}U	-0.00044	-0.00010	0.00006	0.00001	-0.00002

The results show that fast criticals are far more sensitive than the thermal ones to the angular distributions of elastic scattering. This is expected because scattering becomes more isotropic at lower incident neutron energies.

The amount of leakage and the proximity of materials to the system boundary in the fast criticals also plays a significant role as well. For example, hmf-028 and pmf-006, the Flattop experiment with the highly-enriched uranium (HEU) and plutonium cores respectively and a natural uranium reflector, have the highest sensitivities to the ^{238}U P_1 elastic moment. The sign of these is negative because increasing P_1 increases leakage and leads to a corresponding decrease in k.

On the other extreme is mmf-008, the Zebra-8 experiment, which is modeled as an infinitely reflected fast unit with a square 37.5 w/o enriched uranium metal plate and natural uranium reflector plates. The ^{238}U has a lower sensitivity to P_1 than the others, but has a positive sign, unlike all the other major P_1 moment sensitivities reported because the effect of backscattering neutrons into the HEU plate and not having any leakage to prevent.

For the thermal systems, the P_1 elastic moment sensitivities are typically an order of magnitude lower than in the fast ones. The ^{16}O is the significant contributor in the water moderated systems, which these all are. In some cases, the actinides of ^{238}U or ^{232}Th provide significant neutron reflection, and those tend to be more significant in those particular cases.

For this wide selection of benchmarks, rarely does any moment above P_1 have a significant effect. The reasons for this are two-fold. First, the neutrons in a typical fast assembly are 1-2 MeV or lower and in that regime, much of the anisotropy can be described through only the first Legendre moment. In other words, the number of neutrons where a high-order Legendre polynomial is necessary are small and therefore do not contribute much to the overall multiplication of the system. Second, increasing a higher moment tends to both increase forward scattering and backscattering simultaneously, leading to competing effects on the multiplication.

Figures 1 and 2 give the P_1 through P_5 moments for pmf-001 (Jezebel) and hmf-028 (Flattop with the HEU core) as a function of incident neutron energy. In both cases, the P_1 is clearly dominant, and peaks at about 500 keV and then decreases as higher Legendre moments are needed to treat scattering. The higher moments peak at higher energies, but are much less in magnitude for the reasons just discussed.

The results from Aliberti and McKnight have their Jezebel P_1 sensitivity peaking at a few MeV as opposed to 500 keV. This makes sense as their deterministic code can only handle P_1 scattering, so all the anisotropy has to be described with only the first Legendre moment. The sum over incident energies shows agreement, however. Their result is approximately -0.10, whereas this result is -0.09, which is good agreement considering the different methods and cross section treatments.

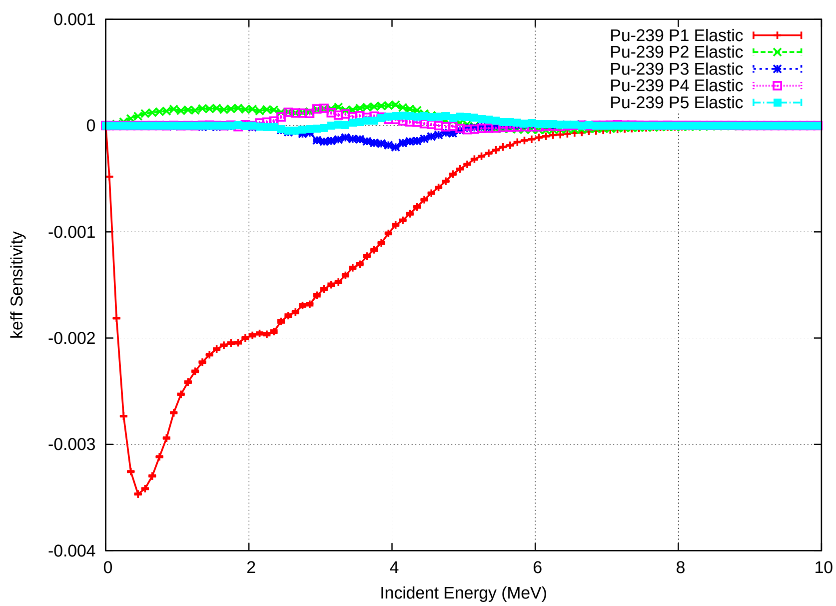

Figure 1. Elastic Legendre moment sensitivities of ^{239}Pu in Jezebel.

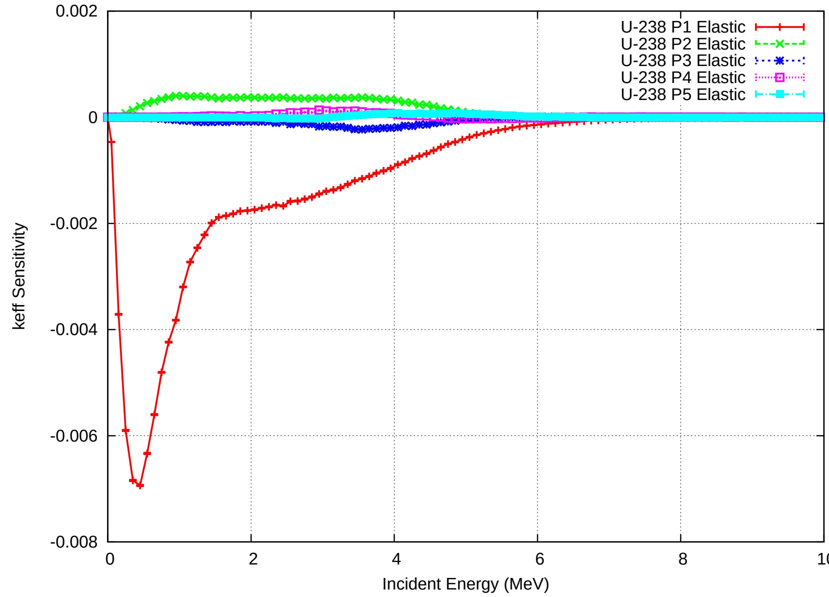

Figure 2. Elastic Legendre moment sensitivities of ^{238}U in Flattop with the HEU core.

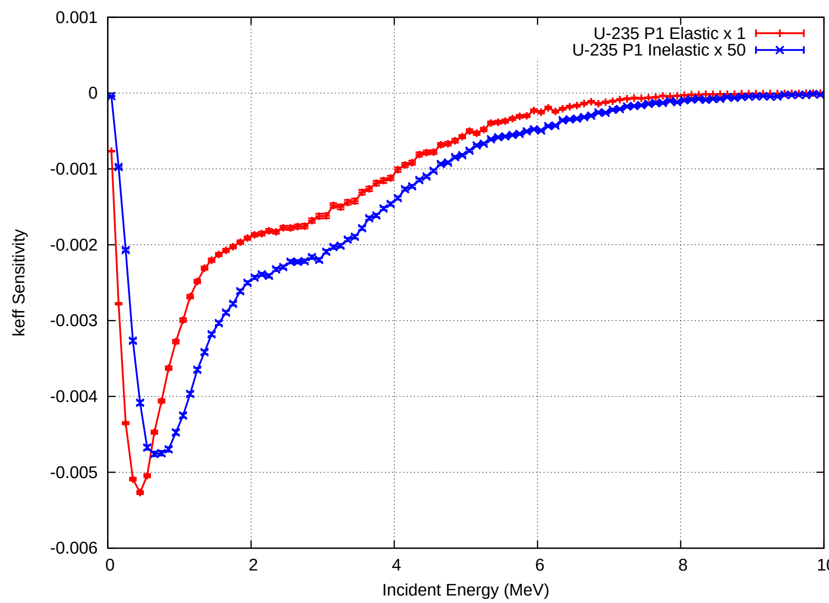

Figure 3. Elastic and Inelastic P_1 Legendre moment sensitivities in Lady Godiva.

Figure 3 shows the elastic and inelastic P_1 moments for ^{235}U in hmf-001 (Lady Godiva). Note that he inelastic moment in is multiplied by 50 to make the curves appear on the same scale. The P_1 inelastic moment has a similar shape to the elastic, but peaks at higher energies and is (unscaled) much smaller in magnitude. Never in any of the cases run does the P_1 inelastic case compare significantly with the elastic one. For criticality, therefore, it is probably safe to neglect Legendre moments of inelastic scattering when doing sensitivity/uncertainty analysis.

4. CONCLUSIONS

A new method was implemented in MCNP6 to calculate k sensitivities to Legendre scattering moments, and is planned to be released in the future. This method was applied to 22 benchmark experiments from the ICSBEP Handbook; the benchmarks cover a variety of isotopes, geometries, and neutron spectra. The results are quite consistent showing that most of the sensitivity to k comes from the elastic P_1 moment with the highest effects being those where leakage has a significant impact on criticality. Inelastic scattering moments typically have a negligible effect on criticality.

In the future, the plan is to take these sensitivities and convolve them with ENDF covariance data to provide estimates on the uncertainties. It is expected based on the magnitudes of both that the P_1 elastic scattering moment is a significant source of uncertainty and needs to be considered in data adjustment exercises.

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REFERENCES

[1] MCNP6 Development Team: J.T. Goorley, M.R James, T.E. Booth, F.B. Brown, J.S. Bull, L.J. Cox, J.W. Durkee, J.S. Elson, M.L. Fensin, R.A. Forster, J.S. Hendricks, H.G. Hughes, R.D. Johns, B.C. Kiedrowski, R.L. Martz, S.G. Mashnik, G.W. McKinney, D.B. Pelowitz, R.E. Prael, J.E. Sweezy, L.S. Waters, T. Wilcox, T.J. Zukaitis, "Initial MCNP6 Release Overview", *Nucl. Technol.*, **180**, pp. 298-315 (2012).

[2] B.C. Kiedrowski, F.B. Brown, "Adjoint-Based k-Eigenvalue Sensitivity Coefficients to Nuclear Data Using Continuous-Energy Monte Carlo," *Nucl. Sci. Eng.*, **174**, in publication (2013).

[3] G. Aliberti, R. D. McKnight, "Mu-Bar Sensitivities," *Trans. Am. Nucl. Soc.*, **107**, pp. 1093-1096 (2012).

[4] J.B. Briggs (Ed.), "International Handbook of Evaluated Criticality Safety Benchmark Experiments", Nuclear Energy Agency, NEA/NSC/DOC(95)03/I, Paris, France (2012).

[5] B.C. Kiedrowski, F.B. Brown, P.P.H. Wilson, "Adjoint-Weighted Tallies for k-Eigenvalue Calculations with Continuous-Energy Monte Carlo," *Nucl. Sci. Eng.*, **168**, pp. 226-241 (2011).

[6] B.C. Kiedrowski, "K-Eigenvalue Sensitivity Coefficients to Legendre Scattering Moments," *Trans. Am. Nucl. Soc.*, **109** (2013).

[7] M.B. Chadwick, et. al., "ENDF/B-VII.1 Nuclear Data for Science and Technology," *Nucl. Data Sheets*, **112** (12), 2887-2996 (2011).