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Author(s): Kiedrowski, Brian C.
Brown, Forrest B.

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K-EIGENVALUE SENSITIVITIES OF SECONDARY DISTRIBUTIONS OF CONTINUOUS-ENERGY DATA

Brian C. Kiedrowski and Forrest B. Brown

Los Alamos National Laboratory
P.O. Box 1663 MS A143, Los Alamos, NM 87545
bckiedro@lanl.gov; fbrown@lanl.gov

ABSTRACT

MCNP6 has the capability to produce energy-resolved sensitivity profiles for secondary distributions (fission χ and scattering laws). Computing both unconstrained and constrained profiles are possible. Verification is performed with analytic test problems and a comparison to TSUNAMI-3D, and the comparisons show MCNP6 calculates correct or consistent results. Continuous-energy calculations are performed for three fast critical experiments: Jezebel, Flattop, and copper-reflected Zeus. The sensitivities to the secondary distributions (integrated over chosen energy ranges) are of similar magnitude to those of many of the cross sections, demonstrating the possibility that integral experiments are useful for assessing the fidelity of these data as well.

Key Words: MCNP, nuclear data, benchmark

1. INTRODUCTION

The U.S. DOE/NNSA Nuclear Criticality Safety Program sponsors efforts to do critical (integral) experiments to provide measurements for code and nuclear data validation. Multigroup Monte Carlo methods (such as those found in TSUNAMI-3D [1]) have been able to compute sensitivity coefficients for several years [2], and MCNP6 [3] has a new continuous-energy capability for this purpose as well [4,5]. Recently, at Los Alamos National Laboratory (LANL), the “Chi-Nu Experiments” at the LANSCE particle accelerator have been initiated to focus on performing high-fidelity differential measurements of fission emission distributions (fission χ) [6]. Also at LANL, covariance data libraries to fission χ of the major actinides [7] have been released in ENDF/B-VII.1 [8], offering the possibility of uncertainty quantification. Finally, operations at the National Critical Experiments Research Center (NCERC) in Nevada have begun, and new integral experiments are being performed [9]. This convergence of experimental, codes, and data efforts offers opportunities to address the need for assessing the impact of secondary distributions such as fission χ on nuclear criticality.

This paper specifically focuses on MCNP6 capabilities for generating sensitivity coefficients to secondary distributions. While some details of the method are given herein, readers are encouraged to see a companion paper [10], which goes much more in depth, and focuses on verification and code performance. This paper specifically focuses on computing sensitivity coefficients arising from the normalization requirements of secondary distributions (i.e., unconstrained versus constrained sensitivities). Two multigroup, infinite-medium test problems are defined, analytic solutions for unconstrained and constrained fission- χ and scattering law sensitivities are obtained, and results are compared with MCNP6. A comparison is also made of an energy-resolved constrained fission- χ sensitivity obtained by TSUNAMI-3D for a published benchmark exercise [11]. The results of both agree within a few percent or better.

Continuous-energy secondary distribution sensitivities are then obtained for three fast critical assemblies in the International Handbook of Criticality Safety Benchmark Experiments (ICSBEP) [12]: Jezebel, Flattop, and copper-reflected Zeus. Comparisons are made with cross-section sensitivities, and, when integrated over energy ranges of interest, the magnitudes of the secondary distribution are comparable. This indicates that measurements of integral experiments may be useful for helping determine the fidelity of these data, much the same as is done today for cross sections or fission ν .

2. BACKGROUND

The sensitivity coefficient of k to nuclear data x of isotope j is

$$S_{k,x}^j = \frac{x^j}{k} \frac{dk}{dx^j} = - \frac{\langle \psi^\dagger, (\Sigma_x^j - \mathcal{S}_x - \lambda \mathcal{F}_x) \psi \rangle}{\langle \psi^\dagger, \lambda F \psi \rangle}. \quad (1)$$

Here ψ is the angular (forward) flux and ψ^\dagger is its adjoint function. Σ_x^j is the cross section corresponding to x^j if x is a cross section, and zero otherwise (e.g., fission χ). \mathcal{S}_x is the integral scattering operator for x^j if x^j 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^j if x^j 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.

This is a ratio of two adjoint-weighted integrals. The tallies needed to estimate these integrals are given in the companion paper [10]. The adjoint weighting is done with the Iterated Fission Probability method [13].

For this paper, the sensitivities of interest are for the secondary distributions, so Σ_x^j is zero, leaving either the scattering or fission term. The secondary distribution is $f(E' \rightarrow E, \mu)$ where E' is the incident energy, E is the exiting energy, and $\mu = \hat{\Omega}' \cdot \hat{\Omega}$ and is the cosine of the scattering angle; $\hat{\Omega}'$ and $\hat{\Omega}$ are entering and exiting directions respectively. In MCNP6, the exiting energies and scattering cosines used are those that are in the processed data files. The convention used is that all scattering laws except the correlated energy-angle scatter law (ENDF law 67) have E and μ specified in the center-of-mass frame.

The secondary distribution is normalized such that

$$\int_0^\infty dE \int_{-1}^1 d\mu f(E' \rightarrow E, \mu) = 1, \quad (2)$$

which provides a constraint upon the sensitivity coefficient. An increase in some energy or cosine range must be offset by decreases elsewhere to preserve the normalization. Correspondingly, the sensitivity coefficient integrated over all E and μ must be zero.

There are infinitely many ways one could enforce the normalization. A standard approach (also used in TSUNAMI-3D) involves two steps. First, the distribution is increased in some energy range g spanning E_{g-1} to E_g and some angle range n spanning μ_{n-1} to μ_n by some small multiplicative factor c . Second, the distribution is renormalized everywhere by decreasing the amount of emission by a uniform multiplicative factor of c times the probability of emission in the energy-angle range. The sensitivity coefficient is where the multiplicative factor c approaches zero in the limit.

The standard approach leads to a constrained sensitivity coefficient denoted by $\hat{S}_{k,x}^j$. This can be found from knowing the unconstrained sensitivity coefficient from Eq. (1) and the value of the secondary

distribution f by

$$\hat{S}_{k,f}^j(\mu, E, E') = S_{k,f}^j(\mu, E, E') - f(E' \rightarrow E, \mu) \int_0^\infty dE \int_{-1}^1 d\mu S_{k,f}^j(\mu, E, E'). \quad (3)$$

Note that this constrained sensitivity is the result that MCNP6 normally reports, and is also now the default in the newer versions of TSUNAMI-3D. In reality, MCNP6 must integrate this over a bin for tallying. The bin-integrated value reported by MCNP6 is defined by

$$\hat{S}_{k,f,g,g',n}^j = S_{k,f,g,g',n}^j - f_{g,g',n}^j S_{k,f,g'}^j. \quad (4)$$

The bin-integrated unconstrained sensitivity is

$$S_{k,f,g,g',n}^j = \int_{E_{g'-1}}^{E_g} dE' \int_{E_{g-1}}^{E_g} dE \int_{\mu_{n-1}}^{\mu_n} d\mu S_{k,f}^j(\mu, E, E'). \quad (5)$$

The term on the right is integrated over all outgoing energies and angles of direction change μ , but is only integrated over a specific incident energy bin.

The term $f_{g,g',n}^j$ is the bin averaged transfer distribution. An important point is that this one number may fail to capture needed detail if the incident energy grid is too coarse. In the limit where the incident energy grid is infinitely fine, the sum of $\hat{S}_{k,x}^j$ (calculated in each incident energy range) over all incident energies approaches a steady value. Conversely, different estimates of $\hat{S}_{k,x}^j$ on varying incident energy grids that are too coarse do not sum to the same value. This is in contrast to either the unconstrained sensitivity coefficients or the constrained ones in the exiting energy or cosine dimensions; these are always additive regardless of the energy or cosine grid selected.

The necessary spacing of the incident energy grid depends on the amount variation of the secondary distribution with incident energy. For fission χ , the dependence upon incident energy is relatively weak for neutron energies typical in fast critical assemblies, and therefore this is a minor consideration. This difference does, however, become quite evident for scattering laws, which have outgoing energy and angular dependence that tend to be strong functions of incident energy, and care must be taken to choose an appropriate incident energy grid. For now, this is left up to the user, but future research will be done to automate this.

MCNP6 computes a secondary-production weighted averaged distribution for the transfer function f in Eq. (4). This is done by

$$f_{g,g',n}^j = \frac{\int_{\mu_{n-1}}^{\mu_n} d\mu \int_{E_{g-1}}^{E_g} dE \int_{E_{g'-1}}^{E_g'} dE' f(E' \rightarrow E, \mu) m(E') N^j \sigma_x^j(E')}{\int_{-1}^1 d\mu \int_0^\infty dE \int_{E_{g'-1}}^{E_g'} dE' f(E' \rightarrow E, \mu) m(E') N^j \sigma_x^j(E')}, \quad (6)$$

where N^j is the atomic density of isotope j , and m is the multiplicity of the reaction [e.g., (n,2n) has $m = 2$, fission has $m = \nu(E')$, etc.], and σ_x is the corresponding reaction cross section.

3. VERIFICATION

Demonstrating that MCNP6 is calculating these sensitivities correctly is done in three different ways: comparisons to (1) analytic solutions, (2) direct perturbations, and (3) results from other software.

Table I. Nuclear Data for the First Analytic Problem

g	σ_t	σ_c	σ_f	ν	χ	σ_{sg1}	σ_{sg2}	σ_{sg3}
1	2	1/2	0	–	5/8	1	1/2	0
2	4	1	0	–	1/4	0	1	2
3	4	1/2	3/2	8/3	1/8	0	0	2

Table II. Fission- χ Sensitivity Results for the First Analytic Problem

x	$S_{k,x}$			$\hat{S}_{k,x}$		
	Exact	MCNP6 Adjoint	C/E	Exact	MCNP6 Adjoint	C/E
χ_1	+5/12	+0.4169 ± 0.09%	1.001	–5/24	–0.2080 ± 0.12%	0.999
χ_2	+1/3	+0.3334 ± 0.07%	1.000	–5/24	–0.2080 ± 0.12%	0.999
χ_3	+1/4	+0.2497 ± 0.06%	0.999	+1/8	+0.1246 ± 0.17%	0.997

The first analytic test problem is an infinite medium case with three energy groups. The features of the problem physics are as follows: fission may only occur in group 3 (the lowest energy group), fission neutrons may appear, however, in all energy groups, downscattering is restricted to subsequent groups (e.g., groups 1 to 2), and there is no upscattering. This is the same problem given in the companion paper, except that now sensitivities to fission χ (both constrained and unconstrained) are estimated. The data is also identical (see Table I), and is chosen to give $k = 1$.

The analytic solution for k is

$$k = \frac{\nu_3 \sigma_f \sigma_{s23}}{\sigma_{R2} \sigma_{R3}} \left[\frac{\sigma_{s12}}{\sigma_{R1}} \chi_1 + \chi_2 + \frac{\sigma_{R2}}{\sigma_{s23}} \chi_3 \right]. \quad (7)$$

Differentiating this equation with respect to χ_1 , χ_2 , and χ_3 give the unconstrained sensitivity coefficients. The constrained sensitivity coefficients are found by applying Eq. (4).

MCNP6 is also used to obtain estimates of these. The calculated (labeled ‘‘MCNP6 Adjoint’’) and analytic reference values are given in Table II. Also given is the C/E , which is the ratio of the MCNP6 calculated value with respect to the ‘‘expected’’ or reference value. The results show that MCNP6 can accurately calculate these quantities to within a few tenths of a percent.

A second analytic problem is done that looks at sensitivities to scattering laws. The problem is also an infinite medium, but contains four groups and the data are given in Table III (which again are chosen to make $k = 1$). This problem is somewhat unphysical in that neutrons in group 1 can downscatter into any of the three other groups, but downscattering in groups 2 and 3 can only occur into the subsequent group. There is no upscattering, fission neutrons are only produced in group 1, and fission can only occur in group 4.

The analytic solution for k is

$$k = \left(\frac{\nu_4 \sigma_f \sigma_{s1}}{\sigma_{R1} \sigma_{R2} \sigma_{R3} \sigma_{R4}} \right) [f_{14} \sigma_{R2} \sigma_{R3} + f_{34} \sigma_{s3} (f_{13} \sigma_{R2} + f_{12} f_{23} \sigma_{s2})]. \quad (8)$$

Table III. Nuclear Data for the Second Analytic Problem

<i>g</i>	σ_t	σ_c	σ_f	ν	χ	σ_{sg1}	σ_{sg2}	σ_{sg3}	σ_{sg4}
1	3	1	0	–	1	1	1/2	1/4	1/4
2	4	1	0	–	0	0	2	1	0
3	4	2	0	–	0	0	0	1	1
4	6	3	2	12	0	0	0	0	1

Table IV. Group-1 Scattering Law Sensitivity Results for the Second Analytic Problem

<i>x</i>	$S_{k,x}$			$\hat{S}_{k,x}$			
	Exact	MCNP6 Adjoint	<i>C/E</i>	Exact	MCNP6 Direct	MCNP6 Adjoint	<i>C/E</i>
f_{11}	+1/2	+0.504 ± 1.5%	0.995	–1/4	–0.257	–0.250 ± 0.1%	1.001
f_{12}	+1/5	+0.199 ± 1.1%	1.015	–7/40	–0.180	–0.175 ± 0.1%	0.999
f_{13}	+1/5	+0.203 ± 1.1%	1.015	+1/80	+0.013	+0.012 ± 1.4%	0.994
f_{14}	+3/5	+0.598 ± 0.4%	0.997	+33/80	+0.405	+0.413 ± 0.1%	1.000

Here f_{ij} is the probability of scattering from group *i* to *j*, and $\sigma_{sij} = f_{ij}\sigma_{si}$.

Sensitivity results (constrained and unconstrained) are specifically obtained for scattering with incident neutrons in group 1. Direct perturbation results are obtained by increasing the group-to-group scattering cross section by some small amount (in this case 1%), calculating a new *k* to find a Δk , and then approximating the (constrained) sensitivity from the definition. MCNP6 results are also given, along with *C/E* values. These are shown in Table IV, where the sensitivity coefficients computed by the adjoint methods are labeled “Adjoint” and those computed directly are labeled “Direct” and the *C/E* values are Adjoint to Exact. The MCNP6 Adjoint calculations agree to within a few percent of the Direct results (uncertainties of about 5%) confirming the consistency between the calculations. The adjoint-based sensitivity coefficients agree with the analytic solutions within the 2- σ statistical uncertainties, which are all under 2%.

Of course, these calculations are multigroup, and MCNP6 is capable of computing sensitivity coefficients with continuous energy. A comparison can be made with TSUNAMI-3D. While the TSUNAMI-3D method is multigroup, there is special handling to correct for the self-shielding induced by the group collapse, so the results should match.

Figure 1 gives constrained fission- χ sensitivities for an established benchmark, which is a mixed-oxide lattice of fuel pins with specifications found in Ref. [11], from MCNP6 and TSUNAMI-3D. As seen from the curves, the two curves agree well with differences usually being on the order of a few percent – where the sensitivity is near zero, the agreement is still good, even though, strictly speaking, the percent difference is high. This demonstrates that MCNP6 is computing constrained fission- χ sensitivities consistently with TSUNAMI-3D.

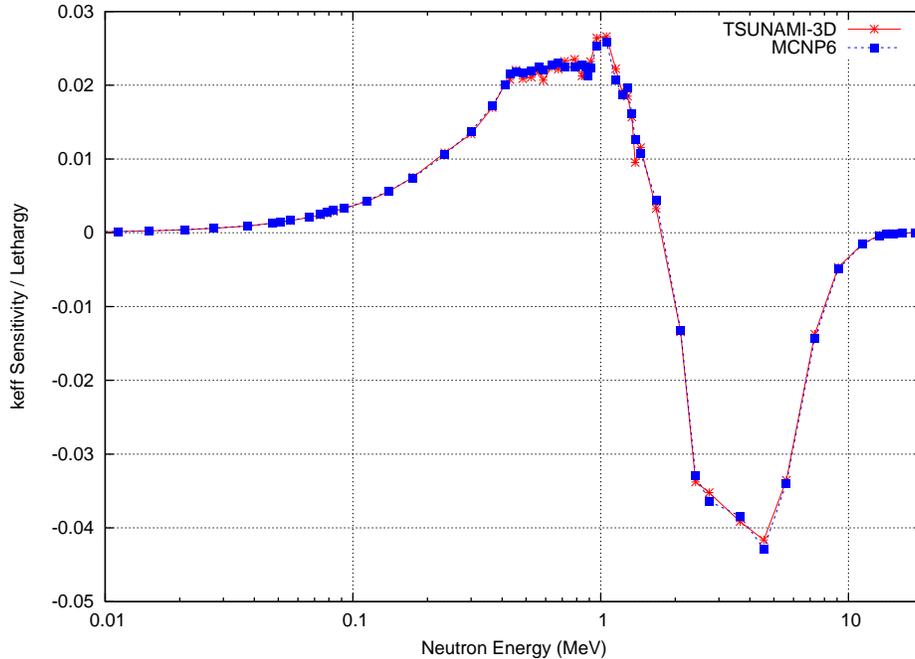


Figure 1. Comparison of constrained ^{239}Pu fission- χ sensitivities for a MOX lattice benchmark.

4. FAST BENCHMARK RESULTS

Fission- χ and scattering distribution sensitivities are computed for three fast critical assembly benchmarks, which may all be found in the ICSBEP. The incident energy grid used contains 100 keV intervals from 0 to 20 MeV. The results are then summed over all incident energy grids to obtain the final result. A parametric study of the grid resolution shows consistency of results when the incident energy grid is refined, indicating that it is sufficiently fine. The results for fission- χ sensitivities are presented with 100 uniform lethargy bins each decade from 0.1 keV to 10 MeV, with 100 keV bins from 10 to 20 MeV. The scattering distributions are given with respect to outgoing direction cosines in 1 degree intervals.

4.1. Jezebel

Jezebel was a nearly-spherical mass of plutonium. The experiments were performed at Los Alamos Scientific Laboratory in the 1950s. The benchmark evaluation in the ICSBEP is PU-MET-FAST-001, and approximates the experiment with a bare sphere. A revision is underway to provide a more detailed specification. For these calculations, the revised, detailed model was used [14], and preliminary results show only small deviation in sensitivities from the simplified sphere model.

The constrained fission- χ sensitivity of ^{239}Pu is displayed in Fig. 2. Notice that the sensitivity profile is negative below the mean emission energy and positive above. This indicates that faster neutrons are more effective at driving a chain reaction relative to slower ones. This result is a consequence of ν increasing for faster neutron energies. There is also a sudden peak starting at about 6 MeV. This corresponds to where the fission cross section increases because of second-chance fission.

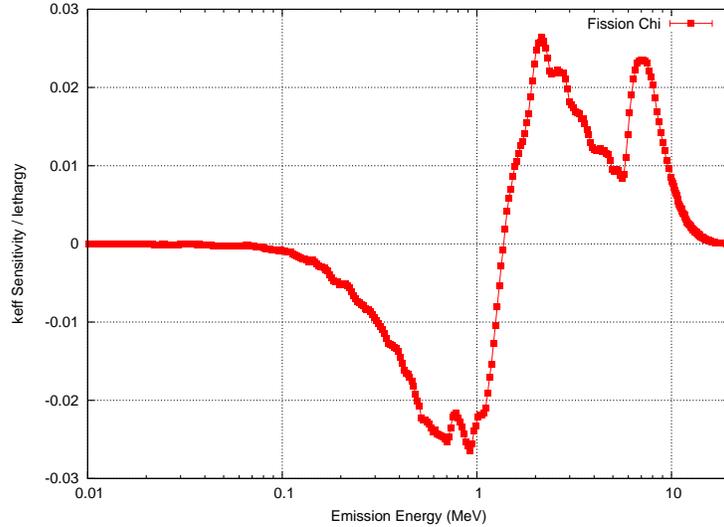


Figure 2. Constrained fission- χ sensitivity profile for ^{239}Pu in Jezebel.

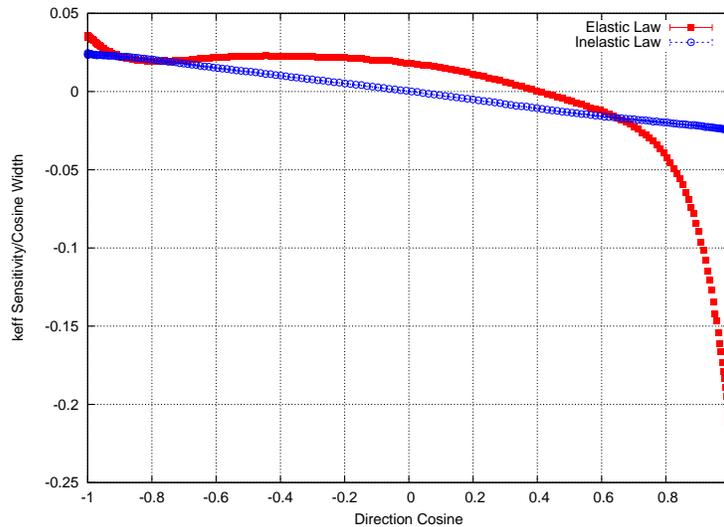


Figure 3. Constrained scattering law sensitivity profiles for ^{239}Pu in Jezebel.

The elastic and inelastic scattering distribution (constrained) sensitivities for ^{239}Pu are given in Fig. 3. Forward-peaked elastic scattering has a relatively strong negative effect on the reactivity of the system, whereas neutrons exiting collisions not going as forward tend to have less of a positive effect. This is expected as this system is fast and the main loss mechanism is through leakage. Increasing the amount of elastic scattering going forward relative to those going backward would increase loss through leakage, therefore decreasing k . Inelastic scattering shows a much smaller, linear variation with outgoing direction.

As for significance, the integral of the above 6 MeV fission- χ sensitivity peak and the elastic scattering from 0-30 degrees have about the same magnitude of 0.02, which is a similar effect of ^{240}Pu fission or ^{239}Pu inelastic scattering. While this is not a dominant effect, it cannot be neglected either.

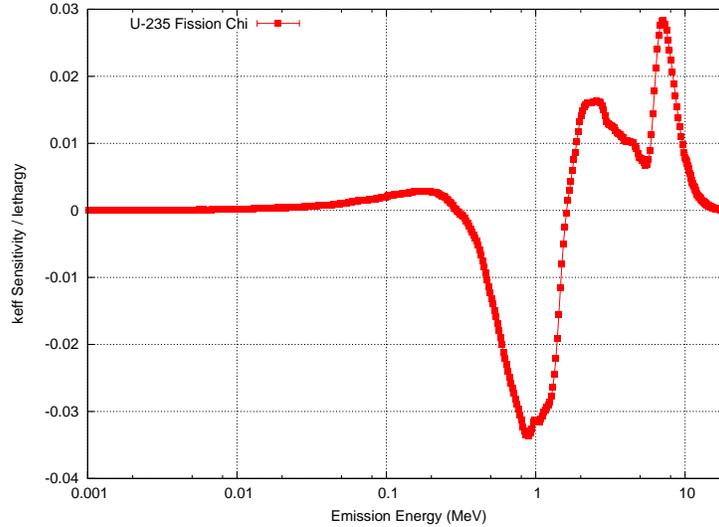


Figure 4. Constrained fission- χ sensitivity profile for ^{235}U in Flattop.

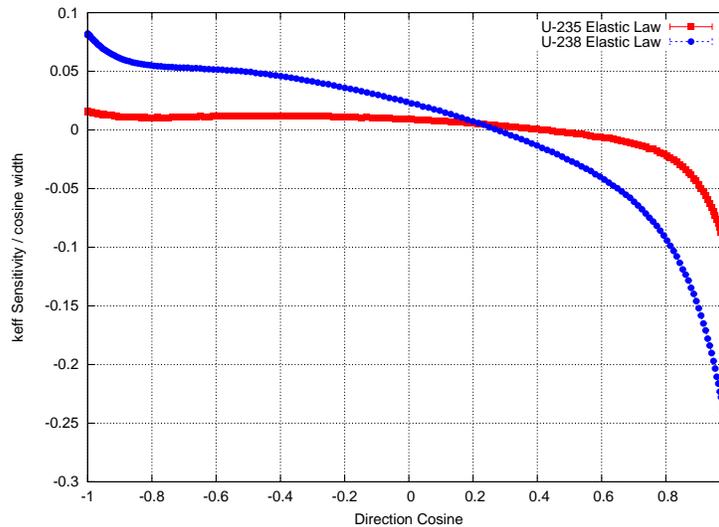


Figure 5. Constrained elastic scattering law sensitivity profiles for $^{235/238}\text{U}$ in Flattop.

4.2. Flattop

Flattop is a subcritical sphere of highly-enriched uranium (HEU) brought to criticality by a natural uranium spherical reflector shell. The ICSBEP evaluation for this is HEU-MET-FAST-028, and the benchmark model contained therein is used for the calculations.

The ^{235}U fission- χ sensitivity is given in Fig. 4. It is similar in shape to that seen for ^{239}Pu in Jezebel, except that the above 6 MeV peak is relatively higher than the peak from about 1.5-6 MeV. The reason for this is because of fission in the ^{238}U reflector, which produces neutrons that would have leaked from a bare configuration. This suggests that reflected fast critical assemblies may be more sensitive to high-energy

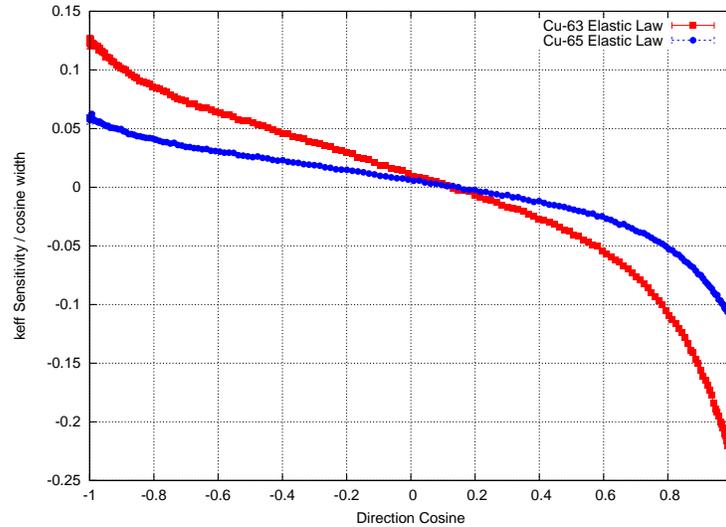


Figure 6. Constrained elastic scattering law sensitivity profiles for $^{63/65}\text{Cu}$ in Copper-Reflected Zeus.

fission emission.

The elastic scattering distribution sensitivities for ^{235}U and ^{238}U are given in Fig. 5. As expected, forward scattering in both produce a negative effect on k , with ^{238}U being more important as a consequence of having a large amount of it near the edge of the assembly where it would control leakage. These have similar magnitudes to those seen for Jezebel.

4.3. Copper-Reflected Zeus

The previous two benchmarks are quite simple geometrically, or can at least be approximated by simple sphere models. A more complicated experiment is Zeus, which has 3-D detail. The Zeus experiments use thin plates of HEU, and are done bare and with reflectors in various configurations to achieve criticality. Recently, the copper-reflected Zeus experiment was redone at NCERC [15] (a previous run of the experiment was done about a decade earlier at Los Alamos), and this motivates the choice of using it as a test problem. Note that the model used was from the ICSBEP (identifier HEU-MET-FAST-072), which is the Los Alamos experiment, and is slightly different than the NCERC experiment because of differences between the two facilities.

The purpose of this experiment is to look at the fast copper cross sections, which are suspected to be the cause of poor predictions in k [16]. Elastic scattering in copper is a dominant component of the k , having an energy-integrated sensitivity of just under 0.3 (both isotopes). The sensitivities of elastic scattering distributions of both isotopes of copper are given in Fig. 6. Again, similar behavior to what is seen for the uranium isotopes in Flattop is seen, and their relative magnitudes appear to be mostly driven by their natural abundance, suggesting the two isotopes have similar fast neutron scattering properties. Note that scattering in ^{235}U is not significant, so it is not presented here.

5. CONCLUSIONS

The ability to compute sensitivity coefficients to secondary distributions using both multigroup and continuous-energy data has been implemented into MCNP6. Verification has been performed using multigroup calculations in MCNP6, and comparing answers to analytic solutions yields favorable results. Comparison of continuous-energy results to those from multigroup TSUNAMI-3D also show favorable agreement. Calculations of sensitivity coefficients of secondary distributions are performed on three fast critical assemblies, and all show similar trends.

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