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Title: A Comparison of MCNP5 Perturbation Estimates of k_eff Sensitivities with TSUNAMI-3D Results for a Homogeneous Thermal Sphere (U)

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SUBJECT: A Comparison of MCNP5 Perturbation Estimates of k_{eff} Sensitivities with TSUNAMI-3D Results for a Homogeneous Thermal Sphere (U)

Abstract

The MCNP5 perturbation capability was tested for energy-integrated k_{eff} sensitivities in a continuous-energy homogeneous spherical $U(2)F_4$/paraffin test problem. Perturbation estimates were compared with direct central-difference estimates for the sensitivities to the total isotopic cross sections. Results suggested that the perturbation capability would be accurate for ^{235}U and ^{238}U but not accurate for C and ^{19}F; results for ^{1}H were ambiguous. Sensitivities to individual reactions were compared with TSUNAMI-3D results. Sensitivities to reactions in hydrogen agreed well, as did sensitivities to fission and the important capture reactions in all isotopes, but sensitivities to elastic and total scattering in isotopes other than ^{1}H disagreed by no less than 15%. This difference in sensitivities to scattering deserves more study. A comparison of TSUNAMI-3D results with the direct MCNP5 results suggested that the MCNP5 perturbation estimates should match the TSUNAMI-3D results. An important conclusion of this paper is a table showing the MCNP5 PERT card RXN numbers that correspond with TSUNAMI-3D reactions.

I. Introduction

The MCNP5 perturbation capability[1] was recently tested for the analysis of k_{eff} sensitivities to cross-section data in multigroup problems for which the exact sensitivities could be calculated or estimated by directly manipulating the cross sections.[2] Such problems are physically realistic and interesting, and much insight was gained.

In this paper, the perturbation capability is used to compute k_{eff} sensitivities in a continuous-energy problem. Continuous-energy problems present difficulties because there is no direct method of obtaining the exact sensitivities, except for energy-integrated sensitivities to total cross sections. Thus, in this paper a comparison is made with results from the TSUNAMI-3D sequence[3,4] of the SCALE code.[5] The test problem is a homogeneous sphere of UF_4 (enriched to 2%) and paraffin.[6]

In order to compare results, the reaction numbers on the MCNP5 perturbation cards must correspond to TSUNAMI-3D reactions, which are given by reaction name rather than MT number. The correspondence turned out to be surprisingly difficult to obtain. This paper discusses the conclusions that were reached, but only five isotopes have been tested so far.

The next section of this paper is a brief review of sensitivity concepts. Section III describes the test problem. Section IV identifies the appropriate MT numbers to use in MCNP5 to correspond to TSUNAMI-3D reactions. Section V discusses the applicability of the differential operator method of MCNP5 to the test problem by using direct total cross section perturbations. In Sec. VI the MCNP5 and TSUNAMI-3D sensitivities are compared.

II. Review of Sensitivity Principles

The *sensitivity* of a response k to cross section σ_x is defined as

$$S_{k,\sigma_x} \equiv \frac{\sigma_{x,0}}{k_0}\frac{dk}{d\sigma_x}, \tag{1}$$

where $k_0 = k(\sigma_{x,0})$ is the reference value of the response. Letting the cross section vary with a parameter p_x as

$$\sigma_x = \sigma_{x,0}(1+p_x) \tag{2}$$

and using this in Eq. (1) yields

$$S_{k,\sigma_x} = \frac{\sigma_{x,0}}{k_0}\frac{dk}{dp_x}\frac{dp_x}{d\sigma_x} = \frac{1}{k_0}\frac{dk}{dp_x}. \tag{3}$$

As explained in Ref. 2, the sensitivity is obtained from the first-order Taylor term of the MCNP5 perturbation capability, Δk_1, using

$$S_{k,\sigma_x} = \frac{\Delta k_1}{k_0\, p_x}. \tag{4}$$

Thus, the user must post-process MCNP5 perturbation output to obtain sensitivities. The sensitivities are independent of the perturbation parameter p_x. The statistical relative uncertainty in the sensitivity is given by the usual propagation of errors formula to be

$$\frac{s_S}{S} = \sqrt{\left(\frac{s_{\Delta k_1}}{\Delta k_1}\right)^2 + \left(\frac{s_{k_0}}{k_0}\right)^2} \tag{5}$$

(where s_x^2 is the variance of quantity x), assuming that Δk_1 and k_0 are uncorrelated, which is not true if they are computed using the same set of histories but which is nevertheless a common approximation.

When the cross section can be directly perturbed, the derivative in Eq. (3) is estimated using a central difference:

$$S_{k,\sigma_x} \approx \frac{1}{k_0}\frac{k(p_{x+}) - k(p_{x-})}{p_{x+} - p_{x-}} = \frac{k(p_{x+}) - k(p_{x-})}{2k_0 p_{x+}}, \tag{6}$$

where $p_{x-} = -p_{x+}$ for a central difference. When $k(p_{x+})$, $k(p_{x-})$, and k_0 are all estimated using uncorrelated Monte Carlo calculations, the relative statistical uncertainty in S_{k,σ_x} is

$$\frac{s_S}{S} = \sqrt{\frac{s_{k_+}^2 + s_{k_-}^2}{(k_+ - k_-)^2} + \frac{s_{k_0}^2}{k_0^2}}, \tag{7}$$

where $k_\pm \equiv k(p_{x\pm})$.

III. Problem Description

The test problem has been used before for TSUNAMI-3D tests[6]; it "is based on an unreflected rectangular parallelepiped consisting of a homogeneous mixture [of] UF_4 and paraffin with an enrichment of 2% in ^{235}U. The H/^{235}U atomic ratio is 293.9:1." The material composition is given in Table I. As in Ref. 6, the experiment was modeled as a homogeneous sphere with a radius of 38.50 cm. The calculations used ENDF-VI cross sections (".60c") and the lwtr.60t $S(\alpha,\beta)$ table for consistency with recent TSUNAMI-3D results. The reference (track-length) value of k_{eff} was 1.00149 ± 0.000254755, obtained using 60,000 neutrons per cycle, 20 settle cycles, and 340 active cycles. The KENO-V.a value of k_{eff} was 1.00782 ± 0.00099 (more details on this calculation will be given in Sec. VI).

Table I. $U(2)F_4$ Material.

Isotope	Atom density (at/bn·cm)
^{235}U	0.00013303
^{238}U	0.006437
^{1}H	0.039097
C	0.018797
^{19}F	0.02628
Total	0.09074403

IV. Appropriate RXN Identifiers

In the TSUNAMI-3D output, reactions are identified with words rather than specific MT numbers. The conversion is given in Table II. However, MT numbers in SCALE do not correspond directly with MT numbers in MCNP5. To compare MCNP5 results with TSUNAMI-3D results, it is necessary to identify the appropriate MT or FM numbers to use on the RXN keywords of the PERT cards.

Table II. Reaction Sensitivity Types Computed by TSUNAMI-3D. Table Adapted from Ref. 7.

MT	Reaction	SCALE identifier
0[a]	Sum of scattering[a]	scatter
1	Total	total
2	Elastic scattering	elastic
4	Inelastic scattering	n,n'
16	n,2n	n,2n
18	Fission	fission
101	Neutron disappearance	capture
102	n,γ	n,gamma
103	n,p	n,p
104	n,d	n,d
105	n,t	n,t
106	n,^{3}He	n,he-3
107	n,α	n,alpha
452[b]	$\overline{\nu}$	nubar[b]
1018[b]	χ	Chi[b]

[a] MT = 0 is the sum of MT = 2, 4, and 16.
[b] Nubar and chi can not be perturbed in MCNP5.

The subsections that follow identify the MT or FM numbers to use in MCNP5 so that results for specific reactions correspond with TSUNAMI-3D results. The TSUNAMI-3D results are referenced in this section but are not discussed in detail until Sec. VI.

IV.A. Total

Using “RXN = 1” and “RXN = –1” gave identical sensitivities for each isotope in this problem. “RXN = 1” is recommended. (In track-length tallies without perturbations, reaction 1 on an FM card gave the same result as reaction –1 for each isotope except ^{1}H. This difference seems inconsistent with the PERT results.)

IV.B. Elastic

Using “RXN = 2” and “RXN = –3” gave identical results for each isotope except ^{1}H. (In track-length tallies without perturbations, reaction 2 on an FM card gave the same result as reaction –3 for each isotope except ^{1}H.) “RXN = 2” is recommended for all isotopes except those associated with an $S(\alpha,\beta)$ table.

At this point only ^{1}H has been tested with an $S(\alpha,\beta)$ table. For ^{1}H, the TSUNAMI-3D elastic and scatter results are identical and no n,n′ result is given. However, in MCNP5 the result of “RXN = 2 4” closely matched the TSUNAMI-3D result for elastic scattering in hydrogen, even though MT = 4 is supposed to indicate inelastic scattering (according to Appendix B of the ENDF manual[8]). The reason seems to be that the $S(\alpha,\beta)$ table also uses MT = 4 for incoherent thermal neutron scattering. (However, in a track-length tally without perturbations, reaction 4 on an FM card with only ^{1}H gave zero.) “RXN = 2 4” appears to be correct for elastic scattering in ^{1}H and probably for other materials using $S(\alpha,\beta)$ tables.

IV.C. n,n′

According to Appendix B of the ENDF manual,[8] MT = 4 is supposed to be the sum of MT = 51 to 91. However, because of a historic quirk in the format of the neutron data tables, in no case was the result of “RXN = 4” and “RXN = 51 i39 91” the same. The result of “RXN = 4” was 0 for ^{19}F, C, and ^{238}U but nonzero for ^{1}H and ^{235}U. The n,n′ reaction should be represented by “RXN = 51 39i 91”.

IV.D. n,2n

There appears to be no other option for the n,2n reaction but "RXN = 16".

IV.E. Scatter

In MCNP5, the total scattering must *not* be requested using "RXN = 2 4 16". Generally, total scattering is given by "RXN = 2 16 51 39i 91". For ^{1}H in this problem, total scattering actually is given by "RXN = 2 4 16" (or by "RXN = 2 4" since there is no n,2n). For higher-*Z* elements such as zirconium for which $S(\alpha,\beta)$ tables exist, there may be inelastic scattering. Thus, for isotopes associated with $S(\alpha,\beta)$ tables, total scattering should be given by "RXN = 2 4 16 51 39i 91".

IV.F. Fission

For ^{235}U, the result of "RXN = –6" matched that of "RXN = 18" but not that of "RXN = 19 20 21 38" (from Appendix G of the MCNP5 manual[1]). For ^{238}U, the situation was reversed. For the non-matching RXN numbers, the k_{eff} sensitivities were non-zero, even though the reaction numbers actually do not exist in those cases. This is a probable bug in the code. "RXN = –6" is recommended for fission.

IV.G. Capture (Neutron Disappearance)

According to Appendix G of the MCNP5 manual,[1] MT =2 is supposed to mean the same thing as FM = 101. However, the result of "RXN = 101" was zero for all isotopes. (In track-length tallies without perturbations, reaction 101 on an FM card gave zero for all isotopes in this problem.) "RXN = –2" is recommended for total capture.

IV.H. Other reactions

The (n,gamma), (n,p), (n,d), (n,t), (n,he-3), and (n,alpha) reactions are specified with the MT numbers shown on Table II. Nubar and chi can not be perturbed in MCNP5.

IV.I. Summary

Table III summarizes the conclusions of this section. Note that only the five isotopes in the UF_4/paraffin test problem (Table I) have been tested in this way so far. There may be surprises when other isotopes are used, especially with $S(\alpha,\beta)$ tables.

Table III. Reaction Sensitivity Types for Comparing TSUNAMI-3D and MCNP5 Results.

Reaction	SCALE identifier	MCNP5 PERT RXN
Sum of scattering	scatter	2 16 51 39i 91 [add 4 for $S(\alpha,\beta)$[a]]
Total	total	1
Elastic scattering	elastic	2 [add 4 for $S(\alpha,\beta)$[a]]
Inelastic scattering	n,n'	51 39i 91
n,2n	n,2n	16
Fission	fission	–6
Neutron disappearance	capture	–2
n,γ	n,gamma	102
n,p	n,p	103
n,d	n,d	104
n,t	n,t	105
n,^{3}He	n,he-3	106
n,α	n,alpha	107

[a] Only ^{1}H has been tested.

Since sensitivities add linearly,[2] the total (sum of) scattering can be obtained (for isotopes other than hydrogen) without a PERT card by summing the elastic, inelastic (n,n′), and n,2n results. However, doing it this way and using the standard propagation of errors formula for the standard deviations leads to slightly different uncertainty estimates than using a PERT card for the sum because the sensitivities are correlated. The maximum difference was for ^{235}U, for which the standard deviation of the sum was almost 2% smaller than the standard deviation from the single PERT card.

Interestingly, although RXN = 2 and RXN = 4 are not needed separately for ^{1}H, treating them separately led to a difference of 580% in the standard deviation than when they were treated as a sum on a single PERT card (the standard deviation of the external sum was a factor of 6.8 larger), suggesting a very large correlation term. Caution should always be used when combining correlated Monte Carlo results.

V. Testing the Applicability of the Differential Operator Method

There is one direct sensitivity calculation that users can do to test the applicability of the differential operator method used in the MCNP5 perturbation capability. Since an isotopic total cross section perturbation is the same as an isotopic density perturbation, the k_{eff} sensitivity to a total isotopic cross section can be computed directly using Eq. (6). The perturbation parameter p must be small enough that the three points ($-p$, k_-), (0, k_0), and ($+p$, k_+) are in a line, but large enough that the numerator of Eq. (6) is statistically significant. The result can be compared with the result of Eq. (4), which uses the MCNP5 perturbation capability, but which is independent of the size of p.

Direct calculations were done with p = 5% and a different random number seed for each run. For ^{1}H, ^{235}U, and ^{238}U, the calculations used 120,000 neutrons per cycle, 20 settle cycles, and 680 active cycles; for C and ^{19}F, the calculations used 240,000 neutrons per cycle, 20 settle cycles, and 1360 active cycles. The perturbation calculations were done in a single run with 60,000 neutrons per cycle, 20 settle cycles, and 340 active cycles.

Results are shown in Table IV. The difference is the average,

$$\text{Difference} = \frac{S_1 - S_2}{\frac{1}{2}(S_1 + S_2)}, \tag{8}$$

with S_1 as the perturbation estimate and S_2 as the direct calculation. In addition, Ns is the difference represented as the number of standard deviations apart the results are, calculated by equating

$$S_1 \pm N s_1 = S_2 \mp N s_2 \tag{9}$$

and solving for N to find

$$N = \frac{|S_1 - S_2|}{s_1 + s_2}. \tag{10}$$

In the direct calculations, the least-squares best-fit lines through the three points had correlation coefficients greater than 0.9996 (in magnitude) except for ^{19}F, which was 0.9987.

Table IV. Energy-Integrated Total Sensitivities from MCNP5.

Isotope	Direct	PERT	Difference	*Ns*
^{1}H	2.310E-01 ± 0.771%	2.215E-01 ± 0.811%	–4.210%	2.662
C	2.506E-02 ± 3.487%	1.981E-02 ± 2.644%	–23.401%	3.757
^{19}F	3.937E-02 ± 2.198%	3.432E-02 ± 1.931%	–13.716%	3.307
^{235}U	2.536E-01 ± 0.724%	2.559E-01 ± 0.074%	0.922%	1.159
^{238}U	–2.110E-01 ± 0.846%	–2.130E-01 ± 0.245%	0.933%	0.857

The results of Table IV suggest that the MCNP5 perturbation method should be accurate, in this test problem, for the uranium isotopes. The accuracy will probably not be high for C or ^{19}F. Results for ^{1}H are more ambiguous. The relative difference is only ~ 4%, but it is outside two standard deviations.

Note that the MCNP5 output was modified to print more digits for both the perturbation result and its standard deviation (from FORTRAN `0pf17.5,f12.5` to `1pe17.5,e12.5`) and the track-length k_{eff} and its standard deviation (from `f12.5,f16.5` to `1p2e14.5`). These modifications are not available in any public version of MCNP5 but they should be added.

VI. Sensitivities and Comparison with TSUNAMI-3D Results

TSUNAMI-3D results for this problem were provided by B. T. Rearden (Oak Ridge National Laboratory). It is the same problem whose results appear in Table IV in Ref. 6. Dr. Rearden provided new results using 238 energy groups, ENDF-VI cross sections, and a light water scattering kernel; thus, there are differences from Ref. 6, which used 44 energy groups, ENDF-V cross sections, and a polyethylene scattering kernel. These changes resulted in a change in k_{eff} from 1.00416 ± 0.00037 (Ref. 6) to 1.00782 ± 0.00099.

MCNP5 perturbation estimates of the energy-integrated k_{eff} sensitivities are compared with TSUNAMI-3D results in Table V. Differences were computed using Eq. (8) with S_1 as the MCNP5 result and S_2 as the TSUNAMI-3D result. The number of standard deviations separating the results, *Ns*, was computed using Eq. (10). Rows with differences greater (in magnitude) than 10% but less than 20% are blue. Rows with differences greater than 20% are red.

Table V. Energy-Integrated Sensitivities.

Isotope	Reaction	MCNP5	TSUNAMI-3D	Difference	*Ns*
^{1}H	Total	2.215E-01 ± 0.811%	2.203E-01 ± 0.091%	0.527%	0.583
	Scatter	3.223E-01 ± 0.559%	3.220E-01 ± 0.061%	0.073%	0.117
	Elastic	3.223E-01 ± 0.559%	3.220E-01 ± 0.061%	0.073%	0.117
	Capture	–1.008E-01 ± 0.055%	–1.017E-01 ± 0.012%	–0.918%	13.589
	n,γ	–1.008E-01 ± 0.055%	–1.017E-01 ± 0.012%	–0.918%	13.589
C	Total	1.981E-02 ± 2.644%	2.416E-02 ± 0.059%	–19.760%	8.072
	Scatter	2.048E-02 ± 2.558%	2.484E-02 ± 0.058%	–19.248%	8.106
	Elastic	2.028E-02 ± 2.585%	2.462E-02 ± 0.058%	–19.301%	8.043
	n,n′	1.963E-04 ± 6.872%	2.250E-04 ± 0.069%	–13.618%	2.102
	n,2n	–5.743E-10 ± 68.561%	N/A[a] ± N/A[a]	200%	1.459
	Capture	–6.681E-04 ± 0.125%	–6.855E-04 ± 0.012%	–2.570%	18.972
	n,γ	–4.943E-04 ± 0.055%	–4.996E-04 ± 0.012%	–1.053%	15.630
	n,p	–5.963E-08 ± 9.406%	–2.975E-08 ± 0.827%	66.877%	5.104
	n,d	–1.595E-07 ± 11.192%	–5.932E-08 ± 1.169%	91.542%	5.401
	n,α	–1.735E-04 ± 0.447%	–1.858E-04 ± 0.031%	–6.843%	14.752
^{19}F	Total	3.432E-02 ± 1.931%	4.139E-02 ± 0.048%	–18.680%	10.356
	Scatter	3.983E-02 ± 1.667%	4.698E-02 ± 0.043%	–16.472%	10.454
	Elastic	2.564E-02 ± 2.431%	2.980E-02 ± 0.058%	–15.002%	6.493
	n,n′	1.419E-02 ± 1.351%	1.612E-02 ± 0.034%	–12.699%	9.757
	n,2n	0.000E+00 ± 0.000%	2.779E-06 ± 0.130%	–200%	771.951
	Capture	–5.609E-03 ± 0.081%	–5.592E-03 ± 0.014%	0.298%	3.126
	n,γ	–2.361E-03 ± 0.054%	–2.391E-03 ± 0.011%	–1.274%	19.648
	n,p	–2.332E-04 ± 0.215%	–2.380E-04 ± 0.026%	–2.018%	8.412
	n,d	–1.114E-05 ± 0.581%	–1.256E-05 ± 0.035%	–12.056%	20.667
	n,t	–2.052E-06 ± 1.269%	–2.625E-06 ± 0.058%	–24.514%	20.796
	n,α	–3.002E-03 ± 0.125%	–2.948E-03 ± 0.024%	1.804%	12.058
^{235}U	Total	2.559E-01 ± 0.074%	2.504E-01 ± 0.017%	2.165%	23.429
	Scatter	5.524E-04 ± 10.911%	4.421E-04 ± 0.028%	22.188%	1.827
	Elastic	3.255E-04 ± 17.420%	2.052E-04 ± 0.053%	45.351%	2.118
	n,n′	2.118E-04 ± 7.960%	2.196E-04 ± 0.021%	–3.607%	0.460
	n,2n	1.506E-05 ± 11.372%	1.727E-05 ± 0.026%	–13.664%	1.286
	Fission	3.657E-01 ± 0.046%	3.629E-01 ± 0.015%	0.777%	12.824
	Capture	–1.103E-01 ± 0.054%	–1.129E-01 ± 0.011%	–2.274%	35.215
	n,γ	–1.103E-01 ± 0.054%	–1.129E-01 ± 0.011%	–2.274%	35.215
^{238}U	Total	–2.130E-01 ± 0.245%	–2.049E-01 ± 0.012%	3.859%	14.752
	Scatter	3.522E-02 ± 1.392%	4.885E-02 ± 0.012%	–32.422%	27.465
	Elastic	2.315E-02 ± 2.005%	3.488E-02 ± 0.014%	–40.424%	25.018
	n,n′	1.109E-02 ± 1.251%	1.293E-02 ± 0.023%	–15.318%	12.982
	n,2n	9.833E-04 ± 1.483%	1.032E-03 ± 0.029%	–4.806%	3.253
	Fission	3.441E-02 ± 0.050%	3.350E-02 ± 0.016%	2.685%	40.440
	Capture	–2.826E-01 ± 0.050%	–2.873E-01 ± 0.008%	–1.625%	28.505
	n,γ	–2.826E-01 ± 0.050%	–2.873E-01 ± 0.008%	–1.625%	28.505

[a] Not reported in TSUNAMI-3D output file.

For hydrogen, the MCNP5 and TSUNAMI-3D results agree to within 1%, but the sensitivities to capture are far outside one standard deviation of each other. For the other isotopes, the sensitivities to capture and fission are within 2.7%, but in terms of standard deviations the differences are huge. This reflects the fact that the results are well converged but the calculations are fundamentally different (multigroup vs. continuous-energy, etc.).

For all isotopes except hydrogen, the differences in the sensitivities to total scattering and elastic scattering are very large, none smaller than 15%. These differences are responsible for almost all of the differences in the sensitivities to the total reaction cross sections. Thus, there seems to be a difference in the way MCNP5 and TSUNAMI-3D treat scattering in isotopes other than hydrogen. There is not an obvious bias. The MCNP5 estimated sensitivity to scattering in ^{235}U is larger than the TSUNAMI-3D value, but the other MCNP5 values are smaller then the corresponding TSUNAMI-3D values. Why are the scattering results so different? This is an issue that needs more study.

These code to code comparisons are fraught with ambiguity. It would be wrong to declare a priori that the TSUNAMI-3D sensitivities are correct. They may be so for the group structure, cross-section data, and other parameters used in the KENO calculation, but the MCNP5 calculation uses different data and methods and there is no completely fair way to compare.

However, it has already been shown (Table IV of Sec. V) that the differential operator method is expected to have some trouble with the carbon and fluorine in this problem. The comparison with TSUNAMI-3D (Table V) suggests that the trouble is in the scattering reactions.

Another fruitful way to analyze the results is to compare the total sensitivities computed directly with MCNP5 (shown in Table IV) with the TSUNAMI-3D results for the total cross section (shown in Table V). This is done in Table VI. The direct MCNP5 results and the TSUNAMI-3D results are all within 5% of each other. Table VI shows that if the MCNP5 perturbation sensitivities to the total cross sections were accurate, they would be within a few percent of the TSUNAMI-3D sensitivities. This does not prove that the TSUNAMI-3D results are correct for all reactions in all isotopes, but it does suggest as much for the major reactions.

Table VI. Energy-Integrated Total Sensitivities.

Isotope	Direct MCNP5	TSUNAMI-3D	Difference	*Ns*
^{1}H	2.310E-01 ± 0.771%	2.203E–01 ± 0.091%	–4.736%	5.394
C	2.506E-02 ± 3.487%	2.416E–02 ± 0.059%	–3.684%	1.021
^{19}F	3.937E-02 ± 2.198%	4.139E–02 ± 0.048%	4.996%	2.278
^{235}U	2.536E-01 ± 0.724%	2.504E–01 ± 0.017%	–1.243%	1.666
^{238}U	–2.110E-01 ± 0.846%	–2.049E–01 ± 0.012%	–2.927%	3.366

In summary, MCNP5 and TSUNAMI-3D estimated k_{eff} sensitivities to scattering do not agree except for ^{1}H. The direct evidence is that the MCNP5 perturbation sensitivities should match the TSUNAMI-3D sensitivities for the total reactions in Table V. The circumstantial evidence is that the sensitivities should match for the other reactions as well. Differences are likely due to the effect of spatial and spectral fission source shifts induced by the perturbation, which are neglected by the differential operator method but accounted for (to first order) by the use of the adjoint flux in TSUNAMI-3D.

Hydrogen is a special case. The MCNP5 and TSUNAMI-3D results for the total cross section agree to within ~ ½% on Table V, but Table IV shows that the MCNP5 perturbation result for the total cross section is actually in error by ~ 4%. Thus the MCNP5 and TSUNAMI-3D agreement for ^{1}H on Table V should not be construed to suggest that the MCNP5 perturbation results are more correct for ^{1}H than for the other isotopes. Such are the difficulties of code-to-code comparisons.

VII. Summary and Conclusions

A homogeneous spherical test problem was run for k_{eff} sensitivities to isotopic reaction cross sections. First, the problem was used to identify the correct MT or FM numbers to use on the MCNP5 PERT card RXN keyword so that MCNP5 results could be compared with TSUNAMI-3D results. It is important to *not* use the MT numbers from the TSUNAMI-3D documentation (i.e., Table II). The correct numbers are given in Table III. It would be possible to add reaction 0 to indicate total scattering on the PERT card RXN keyword.

Next, the k_{eff} sensitivities to the total isotopic cross sections were estimated directly using perturbed materials in MCNP5 calculations and a central-difference approximation for the derivatives. These direct results were compared with MCNP5 energy-integrated PERT results. It was clear that k_{eff} sensitivities to carbon and fluorine cross sections would be troublesome but that sensitivities to uranium cross sections would be well estimated with the perturbation capability.

Finally, MCNP5 perturbation estimates of the sensitivities were compared with TSUNAMI-3D results provided by B. T. Rearden. Sensitivities to reactions in hydrogen agreed well. Sensitivities to fission and the important capture reactions agreed well. Sensitivities to scattering reactions in isotopes other than hydrogen did not agree.

Comparing the direct MCNP5 results with the TSUNAMI-3D results led to the conclusion that the MCNP5 perturbation sensitivities should match the TSUNAMI-3D sensitivities for isotopes other than ^{1}H. Differences may be due to the effect of spatial and spectral fission source shifts induced by the perturbation, which are neglected by the differential operator method but accounted for (to first order) by the use of the adjoint flux in TSUNAMI-3D. However, if this were the case, then it is unclear why MCNP5 and TSUNAMI-3D results actually do agree for scattering in hydrogen, which should have a bigger spectral effect than scattering in carbon or fluorine.

In a 30-group fast reflected problem, the k_{eff} sensitivities to scattering cross sections were also poorly estimated using the MCNP5 perturbation capability, but in that problem the estimates for hydrogen were worse than for other scattering isotopes.[2]

Thus, the k_{eff} sensitivity to scattering in MCNP5 is an issue that needs to be addressed.

An issue needing immediate attention is that the MCNP5 perturbation capability gives nonzero Δk_{eff} results for fission reactions that do not exist, such as MT = 18 in ^{238}U. Another question is why the PERT results for ^{1}H using “RXN = 1” and “RXN = –1” were identical even though tallies using FM cards with reactions 1 and –1 were not identical (in an unperturbed problem). This behavior might or might not indicate a bug, but it is suspicious.

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