LA-UR-11-06503

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Title:	Temperature Effects of Resonance Scattering for Epithermal Neutrons in MCNP
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Intended for:	PHYSOR-2012 ANS Reactor Physics Topical Meeting Knoxville, TN, 15-20 April 2012

Form 836 (7/06)

PHYSOR 2012 – Advances in Reactor Physics – Linking Research, Industry, and Education
Knoxville, Tennessee, USA, April 15-20, 2012, on CD-ROM, American Nuclear Society, LaGrange Park, IL (2012)

TEMPERATURE EFFECTS OF RESONANCE SCATTERING FOR EPITHERMAL NEUTRONS IN MCNP

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ABSTRACT

Epithermal neutron elastic scattering can be significantly affected by the thermal motion of target nuclides. Since the 1950s continuous-energy Monte Carlo codes have generally accounted for the target motion using a free gas scattering model, with the assumption that the scattering cross-section is constant in energy. Recent work has shown the importance of resonance scattering, and several methods for an improved free-gas treatment have been developed. We have implemented a rejection-based sampling scheme in the MCNP free-gas treatment to account for cross-section variation. The modified MCNP code was used to investigate a number of practical concerns: results for an LWR Doppler defect benchmark; computational costs; and energy limits for the free-gas treatment. Additionally, the impact on a suite of ICSBEP criticality benchmark problems (at room temperature) was determined to be negligible, an important result since such problems are used extensively in testing and evaluating revisions to ENDF/B-VII nuclear data.

Key Words: free gas, elastic scatter, Monte Carlo

1. INTRODUCTION

Continuous-energy Monte Carlo codes have traditionally used 3 different models for simulating elastic collisions between a neutron and a target nuclide: At high neutron energies, target thermal motion is neglected, and a target-at-rest elastic scattering model is used. At epithermal neutron energies (a few eV to 10s or 100s of eV), a free gas elastic scattering model is used to account for thermal motion of the target nuclides. At thermal neutron energies (up to a few eV), an $S(\alpha,\beta)$ thermal scattering treatment is used to account for thermal motion and chemical binding effects (if data are available); otherwise a free gas model is used. Many minor variations on these models have been used in Monte Carlo codes for specific applications.

Free gas scattering models for epithermal neutrons were first developed in the 1950s for continuous-energy Monte Carlo codes [1]. Several assumptions were made:

- Target nuclides are unbound and distributed energy-wise according to a Maxwell-Boltzmann distribution.
- The microscopic elastic scattering cross-section is constant.

With these assumptions, the Doppler broadened scattering cross-section

$$\sigma_{eff,s}(v) = \int_{4\pi}\int_{0}^{\infty} \frac{|\mathbf{v}-\mathbf{V}|}{v}\sigma_s(|\mathbf{v}-\mathbf{V}|)P(\mathbf{V})\,d\mathbf{V}\,d\Omega \quad , \tag{1}$$

where $P(\mathbf{V}) = \left(\frac{M}{2\pi kT}\right)^{3/2} e^{-\left(M/2kT\right)\mathbf{V}^2}$, $\mathbf{v}$ is neutron velocity, and $\mathbf{V}$ is target nuclide velocity (both in laboratory system), becomes

$$\sigma_{eff,s}(v) = \sigma_s\left[\frac{e^{-\alpha v^2}}{v\sqrt{\pi\alpha}} + \left(1+\frac{1}{2\alpha v^2}\right)erf\left(v\sqrt{\alpha}\right)\right], \qquad \text{where } \alpha = \frac{M}{2kT}, \tag{2}$$

and the bivariate PDF for selecting the target nuclide speed and cosine of the angle between the incoming neutron and target nuclide direction becomes

$$P(V,\mu\,|\,v)\,dV\,d\mu = \frac{\left(\frac{\alpha}{\pi}\right)^{3/2}\sigma_s\,|\mathbf{v}-\mathbf{V}|\,V^2 e^{-\alpha V^2}\,2\pi\,dV\,d\mu}{\sigma_{eff,s}(v)} \quad . \tag{3}$$

After some manipulation, Eq. (3) can be written as

$$P(V,\mu\,|\,v)\,dV\,d\mu = C\cdot\left(P_1\cdot f_1(V)dV \;+\; P_2\cdot f_2(V)dV\right)\cdot\frac{d\mu}{2}\cdot\frac{|\mathbf{v}-\mathbf{V}|}{v+V} \quad , \tag{4}$$

where $P_1 = \dfrac{v}{v+2/\sqrt{\pi\alpha}}$, $\qquad f_1(V) = 4\sqrt{\frac{\alpha^3}{\pi}}V^2 e^{-\alpha V^2}$

$P_2 = 1-P_1$, $\qquad f_2(V) = 2\alpha^2 V^3 e^{-\alpha V^2}$

and $C = \sigma_s / \sigma_{eff,s}(v)$.

The Monte Carlo rejection scheme for sampling the free gas kernel is then:

- With probability P_1 sample V from $f_1(V)$, otherwise sample V from $f_2(V)$.
- Sample μ uniformly on [-1,1].
- With probability $|\mathbf{v}\text{-}\mathbf{V}|/(v+V)$, accept V and μ, and compute the exit neutron energy and scattering angle; otherwise reject V and μ, and resample.

In MCNP [2], the free gas model is used when neutron energy is greater than the limit of S(α,β) data (or above 0 eV if there S(α,β) data is not available). For hydrogen scattering, the free gas model is used at all higher energies; for other target nuclides, free gas scattering is used for neutron energies up to 400 *kT*, with target-at-rest kinematics at higher energies.

As noted in several recent studies [3-5], using Eq. (4) in sampling the free gas collision can lead to significant inaccuracies when the basic assumption of a constant elastic scattering cross-section is not valid. Figure 1 compares the elastic scattering cross-sections for ^{1}H and ^{238}U over the range 1 eV to 200 eV.

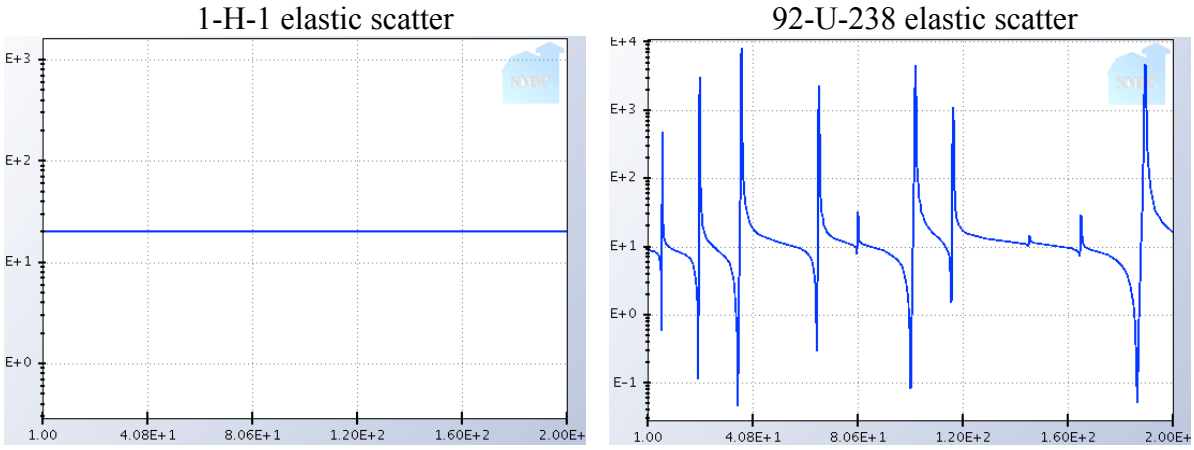

Figure 1. Elastic scattering cross-sections for ^{1}H and ^{238}U over the range 1 eV to 200 eV.

Several researchers [3-7] have shown that neglect of the significant scattering resonances in ^{238}U results in underestimating upscattering and resonance absorption, leading to a temperature-dependent bias in k_{eff}. At room temperature, neglect of the ^{238}U resonance scattering results in underestimating k_{eff} by ~100 pcm or less (1 pcm=.00001 Δk) for typical LWR problems. For hot conditions, the bias is ~200 pcm. This temperature-dependent bias can result in underestimating Doppler defect reactivity by about 10%. Further, for high temperature advanced reactors, the effects can be much larger.

When free gas scattering models were first introduced into continuous-energy Monte Carlo in the 1950s, approximations in physics modeling were considered acceptable if the impact on k_{eff} was less than ~100 pcm; due to computer limitations, statistical uncertainties were of that size or larger. With today's more powerful computers, it is common to achieve statistical uncertainties in the 10 pcm range or even lower. Hence there is a need to remove the problematic assumption in the free gas scattering model. In the following sections, we describe the improved free gas scattering tested in MCNP, results for an LWR Doppler defect benchmark, computational costs, and energy limits for the free-gas treatment. Additionally, the impact on a suite of ICSBEP [8,9] criticality benchmark problems (at room temperature) was investigated, an important consideration since such problems are used extensively in testing and evaluating revisions to ENDF/B-VII nuclear data [10].

2. IMPROVED FREE GAS MODEL

Becker [11] developed a revised rejection method for dealing with scattering cross-section variations in the free gas model. His scheme was called the Doppler Broadening Rejection Correction (DBRC). Mori [5] and Lee [4] developed schemes using a weight correction factor. We chose to largely follow Becker's DBRC scheme, independently implementing an additional rejection based on the variation in scattering cross-section. (It should be noted that independent

validation of Becker's scheme is desirable, due to the complexity of modifying the MCNP collision physics routines.)

If Eq. (1) is used directly for the Doppler broadened scattering cross-section; Eq. (2) is not used; and σ_s in Eq. (3) is replaced by $\sigma_s(|\boldsymbol{v}-\boldsymbol{V}|)$, then Eq. (4) may be written as:

$$P(V,\mu \mid v)dV\,d\mu = C' \cdot \left(P_1 \cdot f_1(V)dV \;+\; P_2 \cdot f_2(V)dV\right) \cdot \frac{d\mu}{2} \cdot \frac{|\,\mathbf{v}-\mathbf{V}\,|}{v+V} \cdot \frac{\sigma(|\,\mathbf{v}-\mathbf{V}\,|)}{\sigma_{\max}(v)}, \qquad (5)$$

where $P_1 = \dfrac{v}{v + 2/\sqrt{\pi\alpha}}$, $\qquad f_1(V) = 4\sqrt{\frac{\alpha^3}{\pi}}V^2 e^{-\alpha V^2}$

$P_2 = 1 - P_1$, $\qquad f_2(V) = 2\alpha^2 V^3 e^{-\alpha V^2}$

and $\quad C' = \sigma_{\max}(v) / \sigma_{eff,s}(v).$

The parameter $\sigma_{max}(v)$ is the largest scattering cross-section within $\pm 4/\alpha^{1/2}$ of the relative speed $|\boldsymbol{v}-\boldsymbol{V}|$. This range for the cross-section is chosen to be consistent with the NJOY Doppler broadening, in that the tail of the Maxwellian distribution of target speeds is negligible outside this range.

A separate module was created to contain all the calculations that are required to make the scattering decision regarding target atom speed and cosine of the angle between the neutron and target directions. This module contains a function that determines the decision of the second rejection test and a subroutine that reads in all the zero Kelvin scattering cross section values for ^{238}U. It also contains subroutines to determine the corresponding maximum cross section value and the scattering cross section for the relative neutron speed, and to implement the second rejection test. For most of the testing discussed below, the upper energy limit for use of the free gas scattering kernel is set to 210 eV as recommended in [3].

2.1. Comparison of Double-Differential Scattering Kernels

The double-differential scattering kernel produced by the original free gas scattering kernel in MCNP does take into account neutron up-scattering. However, it does not produce the true double-differential scattering kernel because of the simplifying assumption of using constant scattering cross sections in epithermal region. When resonance scattering is taken into account by using cross sections dependent on relative neutron speed in the free gas scattering kernel, the true double-differential scattering kernel can be found to represent correct neutron scattering behavior. Fig. 2 shows the difference in up-scattering effects in the original free gas scattering kernel in MCNP and the modified free gas scattering kernel. The scattering kernel is a function of temperature and up-scattering percentages increase as the temperature of the target material increases. Fig. 3 shows how the double-differential scattering kernel changes as a function of temperature. The scattering kernel functions were obtained using an MCNP current (F1) tally with fine energy binning. The tally was modified by a special treatment (FT card) to account for only once-collided neutrons. A monoenergetic source of neutrons was placed in a small target of ^{238}U and, and the current of once-collided neutrons was tallied and normalized. The results agree with those found in other publications.

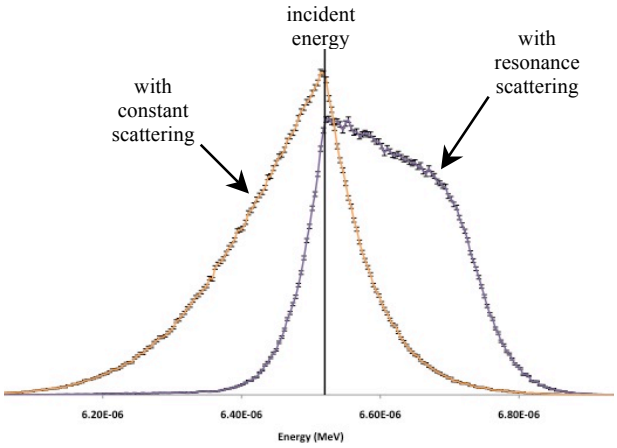

Figure 2. Comparison of Double-Differential Scattering Kernels for U-238 at 1200 K for Incident Neutron Energy of 6.52 eV

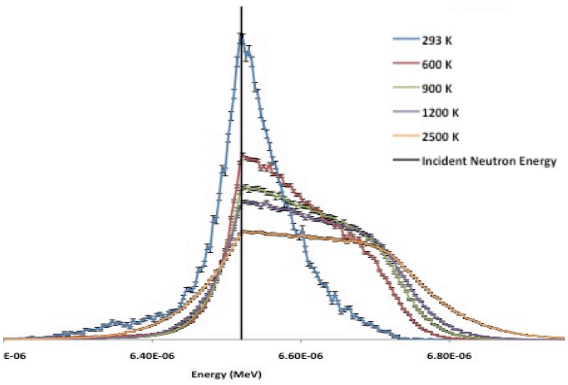

Figure 3. Scattering Kernel for U-238 at Varying Temperatures for Incident Neutron Energy of 6.52 eV

3. NUMERICAL RESULTS AND TESTING

3.1. Mosteller Benchmark Problem

The Mosteller benchmark problem [12] for LWR pin cell with UO_2 fuel is chosen to benchmark MCNP5 results with resonance scattering to the results published in [4,5,13]. ENDF/B-VII.0 cross sections are used for these calculations. In order to calculate the Fuel Temperature Coefficient (FTC), two sets of calculations are done in MCNP5. The first is at Hot Zero Power (HZP) conditions where the fuel, cladding and moderator are at a temperature of 600K. The second set of calculations is done under Hot Full Power (HFP) conditions where the fuel temperature is 900K and the cladding and moderator temperatures are 600K. The FTC is calculated using

$$FTC = \left(\frac{1}{k_{HZP}} - \frac{1}{k_{HFP}} \right) \times \frac{10^5}{\Delta T}, \qquad (6)$$

where ΔT is 300K.

The results obtained from this benchmark exercise are comparable to those presented in [4,5]. The FTC decreases when resonance scattering is taken into account. MCNP5 results with constant free gas scattering and with resonance free gas scattering are presented in Table I, and differences in k_{eff} in Table II. The differences in k_{eff} increase with fuel temperature due to resonance scattering. The difference is on the order of several hundred pcm for LWR pin cell calculations at full power. This clearly shows that resonance scattering cannot be ignored in full power reactor calculations for LWRs and VHTRs. The FTCs decrease as expected when resonance free gas scattering is taken into account. Fig. 4 illustrates the difference in Doppler coefficients computed in MCNP5 with constant and resonance free gas scattering models. The figure depicts the negative shift in FTC due to resonance scattering due to the greater likelihood of losing a neutron as they gain energy and fall into an absorption resonance in the epithermal range.

Table I. MCNP5 Results for Doppler Benchmark

	Free gas, constant σ_s			Free gas, varying σ_s		
wt%	**k_{eff} for HZP**	**k_{eff} for HFP**	**FTC (pcm/K)**	**k_{eff} for HZP**	**k_{eff} for HFP**	**FTC (pcm/K)**
0.711	0.66569 (19)	0.65987 (20)	-4.42 ± 0.21	0.66541 (22)	0.65909 (20)	-4.80 ± 0.23
1.6	0.96124 (26)	0.95295 (25)	-3.02 ± 0.13	0.96044 (26)	0.95142 (22)	-3.29 ± 0.12
2.4	1.09913 (26)	1.08986 (29)	-2.58 ± 0.11	1.09889 (27)	1.08877 (29)	-2.82 ± 0.11
3.1	1.17657 (30)	1.16777 (27)	-2.13 ± 0.10	1.17613 (26)	1.16563 (28)	-2.55 ± 0.09
3.9	1.23944 (28)	1.23009 (27)	-2.04 ± 0.09	1.23924 (29)	1.22866 (30)	-2.32 ± 0.09
4.5	1.27495 (32)	1.26542 (27)	-1.97 ± 0.09	1.27460 (25)	1.26271 (31)	-2.46 ± 0.08
5.0	1.29920 (34)	1.28911 (29)	-2.01 ± 0.09	1.29860 (29)	1.28748 (30)	-2.22 ± 0.08

Table II. K_{eff} differences: k_{eff}(FG,varying) - k_{eff}(FG,constant)

wt%	HZP (pcm)	HFP (pcm)
0.711	-28 ± 29	-78 ± 28
1.6	-80 ± 37	-153 ± 33
2.4	-24 ± 37	-109 ± 41
3.1	-44 ± 40	-214 ± 39
3.9	-20 ± 40	-143 ± 40
4.5	-35 ± 41	-271 ± 41
5.0	-60 ± 45	-163 ± 42

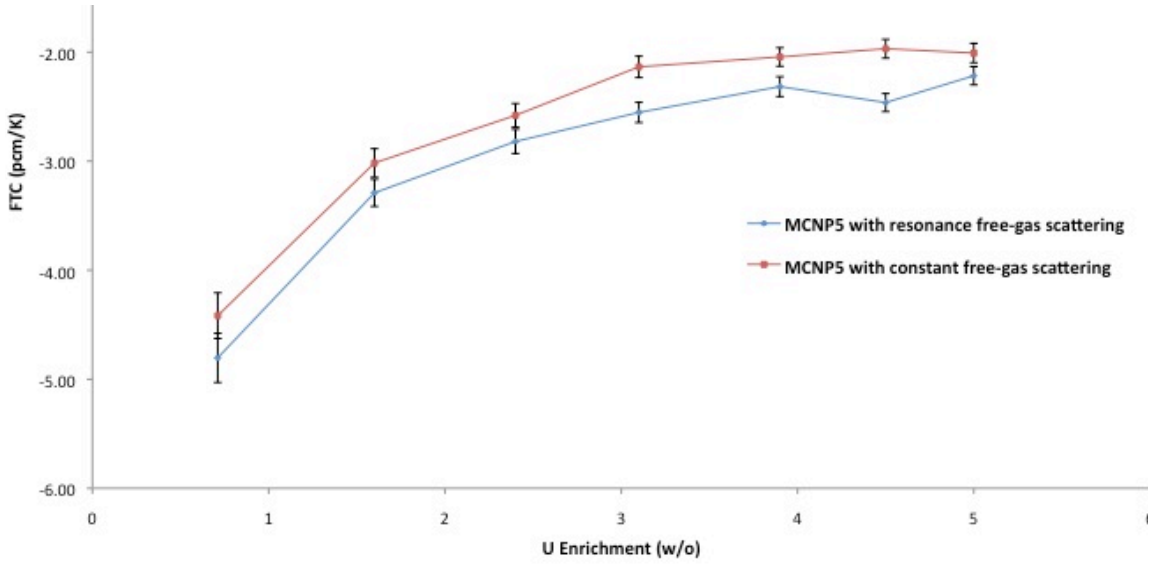

Figure 4. FTCs for UO_2 Pin Cell (LWR) Benchmark

3.2. Computational Time Study

A study on computational time was conducted for criticality calculations with resonance scattering in free gas for energies below 210 eV. The time it takes to run these criticality problems increased as temperature of the fuel increased. Table III shows that there is over a 10% increase in computational time for HFP cases and about 6 – 9 % increase in computational time for HZP cases.

Table III. Time difference (%) between Standard and Modified MCNP5

	TIME DIFFERENCE (%)	
wt%	**HZP**	**HFP**
0.711	6.45	10.47
3.1	9.17	13.13
5.0	6.09	11.56

3.3. Energy Limits for Resonance Free Gas Scattering

A study was conducted on FTC behavior when the upper energy limit at which resonance free gas scattering invoked is changed. The results from this parametric study on varying energy limits for free gas scattering is presented in Table IV.

The results show that FTCs oscillate around similar values after the upper energy limit was set above 50 eV. However, for 500 eV, FTC for 0.711 wt% U is slightly lower than other cases, however, the value is reasonable since it is within two standard deviations of the corresponding results above 50 eV upper limit. This suggests that there is no need to invoke the modified free gas scattering kernel for the entire epithermal region in U-238. However, these upper limits will be different for other nuclides since the energies at which their resonance lie are different and neutron up-scattering percentages will vary accordingly.

Table IV. k_{eff} due to varying energy limits for resonance free gas scattering

Energy Limit (eV)	**50**	**90**	**150**	**210**	**250**	**500**	**1000**
wt%	**FTC (pcm/K)**	**FTC (pcm/K)**	**FTC (pcm/K)**	**FTC (pcm/K)**	**FTC (pcm/K)**	**FTC (pcm/K)**	**FTC (pcm/K)**
0.711	-5.11 ± 0.22	-4.88 ± 0.20	-4.90 ± 0.20	-4.80 ± 0.23	-4.91 ± 0.21	-4.66 ± 0.21	-4.90 ± 0.20
3.1	-2.60 ± 0.10	-2.60 ± 0.09	-2.72 ± 0.09	-2.55 ± 0.09	-2.67 ± 0.10	-2.62 ± 0.11	-2.57 ± 0.10
5.0	-2.20 ± 0.08	-2.34 ± 0.08	-2.28 ± 0.08	-2.22 ± 0.08	-2.26 ± 0.09	-2.23 ± 0.08	-2.29 ± 0.08

3.4. MCNP Extended Criticality Validation Suite

The MCNP Extended Criticality Validation Suite [9] was run with constant free gas scattering in MCNP5 and with resonance free gas scattering below 210 eV in modified MCNP5. The Extended Criticality Validation Suite contains 119 problems from ICSBEP Handbook out of which only less than ten problems contain low-enriched uranium. The differences in criticality results were insignificant within statistics because of the nature of problems in the benchmark suite and the temperatures for the benchmark problems, which are at 300K. Resonance free gas scattering is not expected to affect criticality calculations significantly at this temperature and the benchmark calculations validated the expectations.

4. CONCLUSIONS AND FUTURE WORK

Resonance scattering is expected to affect criticality and safety studies for only very specific problems, namely those that involve high-temperature calculations. Criticality calculations vary on the order of only 10 pcm for reactor calculations at room temperature, and this suggests that resonance scattering does not make a considerable difference to criticality calculations at room temperature.

However, HFP and HZP temperature conditions in a VHTR are much higher than those for LWRs, and the up-scattering percentages for neutrons scattering off ^{238}U are higher. Studies by Lee *et. al.* [4] show k_{eff} reduction on the order of 400 pcm in VHTRs, which is significant. As a result, criticality and safety studies using resonance scattering in the free gas scattering kernel is expected to affect VHTR criticality analysis more so than LWR criticality and safety studies. This suggests that criticality and safety studies involving VHTRs should use this modified free gas scattering model that includes resonance scattering in ^{238}U.

The DBRC method developed by Becker *et. al.* [11] was correctly implemented in a test version of MCNP5. Only high-temperature applications are affected by this modification, and models at room temperature are not expected to change. For VHTR and LWR criticality calculations, this modification can change k_{eff} on the order of several hundred pcm. However, there is no need to invoke the modified free gas scattering kernel for the entire epithermal region.

It should be noted that the work described herein on modification and testing of the MCNP free gas treatment was performed with MCNP5. Because no further releases of MCNP5 are planned, the modifications to the free gas treatment will actually appear in the upcoming release of MCNP6 (currently scheduled for mid-2012).

Future work should focus on determining nuclides for which the modified free gas scattering kernel needs to be implemented and the upper energy limits at which it is invoked for these nuclides. An investigation into significance of up-scattering percentages for low-lying resonances in various nuclides needs to be conducted so that the modified free gas scattering kernel can be applied to broader applications. Additionally, the effects of the modified free gas treatment on quantities other than keff, such as local powers and depletion of specific isotopes, should be investigated.

ACKNOWLEDGMENTS

This work was supported by the US DOE/NNSA Nuclear Criticality Safety Program.

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