Corrected User Guidance to Perform Three-Dimensional Criticality Accident Alarm System Modeling with SCALE

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INTRODUCTION

SCALE includes a three-dimensional criticality safety calculation sequence, CSAS6, which is based on the KENO-VI Monte Carlo code, as well as a three-dimensional shielding sequence, MAVRIC, which is based on the Monaco Monte Carlo code [1,2,3]. Guidance is provided with SCALE to use the two sequences together for the analysis of criticality accident alarm systems (CAAS). Through a two-step process, a spatially varying fission source is generated with CSAS6 using a mesh tally, and then detector responses are calculated with MAVRIC based on the mesh source provided [4,5].

As discussed in reference 4, having Monaco add fission photons to the neutron mesh source created by KENO can accelerate the shielding portion of the CAAS analysis. The shielding portion of the CAAS analysis is accelerated because the sampling of source fission photons is biased, consistent with the input weight windows, to optimize the convergence of the photon tallies. The addition of the fission photons to the neutron mesh source results in accurately modeling the neutron and photon fission source at each initial source location in the Monaco simulation. To avoid producing too many fission neutrons and photons, subsequent fission events must be treated as absorption producing no fission neutrons or photons because all fission events are accounted for in the KENO-generated mesh source.

No method was available to avoid producing too many fission photons in SCALE 6.0. This method was implemented in SCALE 6.1 [5] and is based on an assumption that fission photon production can be entirely separated from the production of other photons generated by nonfission neutron interactions. In theory this is a reasonable assumption, but it is only possible if the photon production data are available in an amenable format. In practical application, most evaluated cross-section data, including ENDF/B-VII.1 [6] and all previous releases, are not available in a format where it is possible to entirely separate fission photon production from the production of all other photons. Therefore, the user guidance provided to account for fission photons during CAAS analysis in all previous SCALE manuals, publications, and training courses can lead to incorrect results for fast systems where the majority of fissions occur above the energies in Table I. This paper reviews the representation of fission photons in ENDF data, reviews the SCALE CAAS analysis guidance previously provided, provides the correct SCALE CAAS analysis guidance, and discusses some computational results that illustrate the difference and the types of problems impacted.

DESCRIPTION OF THE ACTUAL WORK

Fission Photons in Nuclear Data

In ENDF, photon production specifically associated with fission (MT 18) has an upper neutron energy cutoff that is below the maximum energy of the nuclear data set for nearly all the fissionable isotopes. When neutrons above these cutoff energies induce fission, no photons are produced via the MT 18 fission reaction since the fission photon yield above these neutron energies is zero. Table I lists the upper energy cutoff for a few of the major fissionable isotopes. The only isotope in Table I that has fission photon production data associated with MT 18 up to the maximum energy of the nuclear data set is ^{238}U.

Table I. Upper Neutron Energy Cutoffs for Fission Photon Production for Some of the Fissionable Isotopes in ENDF/B-VII.1

Isotope	Upper Neutron Energy Cutoff (MeV)
^{233}U	1.09
^{235}U	1.09
^{238}U	30
^{237}Np	0.54923
^{239}Pu	1.09
^{241}Pu	0.1

These missing fission photons are accounted for in ENDF and are not completely ignored, but they are not associated with MT 18. The missing fission photons are included in the photon production due to nonelastic neutron interactions (MT 3). Since the fission photon production data missing from MT 18 are included in MT 3, no data are missing, and ENDF provides all the needed data. However, dividing fission photon production data into two parts and including them in two different reaction types can lead to confusion. References 7 and 8 explain why this division of the fission photon production data for ^{235}U, ^{239}Pu, and ^{240}Pu is necessary. The references explain that, above the cutoff energies in Table I, the photon production measurements did not distinguish between neutron interaction types as was done below the cutoff energies. Therefore, photons produced by neutrons above the cutoff energies are not associated with the specific neutron interaction that produced the photon.

Rather, they are associated with the nebulous nonelastic interaction type. When a neutron with energy above the Table I cutoffs induces fission, the MT 3 multiplicity and energy distribution is used to determine the number and energy of photons produced. The MT 3 production data are due to any type of neutron interaction type, such as capture, inelastic scattering, or fission. Therefore, the MT 3 photon production multiplicity and energy distribution is an average of all interactions that produce photons. The use of MT 3 photon production data results in photon production that is uncorrelated to neutron interaction type. For example, a fission event induced by a neutron above the Table I cutoffs can produce photons that are associated with an inelastic scattering event.

This structure in the measured photon production data and subsequent evaluated data causes Monte Carlo codes to not be able to conserve energy on an event-by-event basis. It also leads to the inability of cross-section processing codes to remove just the fission photons from the (n,γ) transfer matrix because the photons produced by neutrons with energy above the Table I cutoffs are uncorrelated to the neutron interaction type that produces them. Even though reference 8 states that the upper cutoff energy to distinguish photon production for ^{238}U is 1.09 MeV, the ENDF evaluation has been updated to separate fission photon production data up to 30 MeV. In fact, this change is present as far back as ENDF/B-VI.8. Furthermore, JENDL-4.0 has separated fission photon production for all fissionable isotopes [9]. These new evaluations show that the data can be separated, but separating them requires either a new measurement of the fission photon production data or a theoretical estimate of the fission photon production data above the Table I cutoff energies.

Previous SCALE CAAS Analysis Guidance, Accounting for Fission Photons

The methodology provided with SCALE 6.1 that is recommended to perform CAAS analysis relied on the fission photons from other nonelatic photons being separable in the nuclear data, a feature that is not available in ENDF data. The previous procedure is outlined below.

1. Calculate the spatial and energy dependent fission neutron distribution using KENO-VI
   a. Set KENO parameter `cds=yes`
   b. Add grid geometry to KENO input
2. Convert the KENO neutron mesh tally to a Monaco mesh source using the MAVRIC utility MT2MSM.
3. Calculate the CAAS detector response using Monaco
   a. Input the directory paths to the neutron mesh source and `kenoNuBar.txt` files, and set the number of fissions
   b. Use the `noFissions` parameter
   c. If no photon CAAS detector response is needed use the `noSecondaries` parameter
   d. If a photon CAAS detector response is needed
      i. In the `celldata` block set the `moredata` parameter `nFisFot` equal to 1 to remove photon yields from the fission cross sections used by the MAVRIC sequence
      ii. Set the source keyword `fissPhotonZAID` to the primary fission isotope ZAID to add fission photon data to the neutron source

The brevity of this outline is intended for users familiar with the SCALE CAAS analysis capability. A more detailed explanation of each step is available in Appendix C of reference 10.

Revised CAAS Analysis Guidance, Accounting for Fission Photons

The problem with the guidance listed above occurs with step 3.d, which is removing fission photons from the (n,γ) transfer matrix (step 3.d.i) and adding fission photons to the Monaco source (step 3.d.ii). *In order to correctly account for fission photons in CAAS analysis, step 3.d should be ignored entirely.* In other words, if a photon CAAS detector response is needed, then the parameters `noSecondaries`, `nFisFot`, and `fissPhotonZAID` should **NOT** be used. This is because the data that need to be removed from the (n,γ) transfer matrix cannot be entirely removed when using cross sections based on ENDF/B-VII.1, any previously released version of ENDF, or nearly all other evaluated nuclear data files. If new evaluations separating fission photon production from all energies are included in ENDF, or if a cross-section library based on JENDL-4.0 is used, the previous CAAS user guidance, including step 3.d, is the correct procedure to perform CAAS analysis. Otherwise, step 3.d should be ignored.

Comparison of Methods

Based on the cutoff energies shown in Table I, it is apparent that issues will arise with the previous CAAS user guidance for fast systems. For thermal- and intermediate-energy systems, where the vast majority of fissions occur below this cutoff energy, the impact is minimal. In the previous CAAS guidance, the user attempts to remove all fission photons from the (n,γ) transfer matrix and includes all fission photons in the Monaco fixed source. However, only the fission photons specifically associated with MT 18 can be removed. This means that the fission photons associated with MT 3, which are due to neutrons above the cutoff energies in Table I, are included in the transport simulation twice, once in the source and again in any subsequent (n,γ) interactions. The fission photons produced by neutrons below the Table I cutoff energies are not included in the problem twice because they can successfully be removed from the (n,γ) transfer matrix. The revised CAAS user guidance avoids this issue by not removing the fission photons from the (n,γ) transfer matrix and by not adding fission photons to the Monaco fixed source.

In order to illustrate the difference between these two methodologies, the results are presented from a simple model that exacerbates the issue. The model consists of a critical sphere of metal ^{239}Pu (radius = 4.946 cm, density = 19.82 g/cm^3). The quantities that are compared are the neutron and photon kerma in air 2 meters from the surface of the critical sphere. The neutron and photon air kerma factors are those published by the ICRP and readily available in SCALE as flux-to-dose conversion factors. The comparison is made using cross-section data based on ENDF/B-VII.0 with MAVRIC/Monaco using the previous and revised CAAS user guidance. Additionally, the MAVRIC results are compared with results from XSDRNPM [11] and MCNP5 [12]. It should be pointed out that XSDRNPM is the computational tool that was used to develop the Nuclear Criticality Slide Rule [13]. The MCNP calculations used continuous-energy cross sections, while the XSDRNPM and MAVRIC calculations used multigroup cross sections. The results of these calculations are presented in Table II.

Table II. Calculated Dose Rates for a Critical ^{239}Pu Sphere[a]

Dose Rates (Air Kerma – Gy/hr/fiss/sec)	XSDRN	MCNP5	MAVRIC CAAS	
			Previous Guidance	Revised Guidance
Neutron	6.00e-14	5.99e-14	5.99e-14	5.99e-14
Photon	2.23e-14	2.23e-14	3.31e-14	2.23e-14

[a] All Monte Carlo results have a relative uncertainty of less than 0.3%.

The neutron kerma results in Table II all agree very well, as was expected. The photon kerma results produced by XSDRNPM, MCNP5, and MAVRIC using the revised CAAS guidance also agree very well. Note in the MCNP5 calculation the thick-target bremsstrahlung model was turned off, as was Doppler energy broadening for photons, and the photon cutoff energy was set of 10 keV to match the SCALE cross-section library. The largest difference in Table II is between the MAVRIC with previous guidance photon kerma and all the other photon kermas. As explained earlier, the previous guidance produces too many fission photons induced by fast neutrons. In this example, the additional fission photons with the previous guidance overestimated the photon kerma by nearly 50%.

In order to illustrate that there is minimal difference between these two methodologies for thermal-energy systems, where the vast majority of fissions occur below the Table I cutoff energies, the results are presented from another simple model. The thermal model consists of a homogenous mixture of ^{239}Pu and water in a critical spherical geometry (radius = 29.06 cm, ^{239}Pu density = 0.01324 g/cm^3, water density = 0.9982 g/cm^3). Otherwise, this model is identical to the previous metal sphere of ^{239}Pu. Therefore, the same cross-section libraries are used, with the same computational tools, and the same responses are calculated. The dose rate results calculated for the thermal model are presented in Table III.

Table III. Calculated Dose Rates for a Critical Sphere of ^{239}Pu and Water[a]

Dose Rates (Air Kerma – Gy/hr/fiss/sec)	XSDRN	MCNP5	MAVRIC CAAS	
			Previous Guidance	Revised Guidance
Neutron	1.21e-14	1.21e-14	1.22e-14	1.21e-14
Photon	1.18e-13	1.18e-13	1.18e-13	1.18e-13

[a] All Monte Carlo results have a relative uncertainty of less than 0.4%.

Like the results for the metal sphere in Table II, the neutron kerma results for the thermal model shown in Table III all agree as expected. The difference between the results in Tables II and III is that all the photon kerma results in Table III agree. Including the photon kerma results calculated with the previous and revised CAAS guidance. The results in Table III illustrate that the revised CAAS user guidance has minimal impact on thermal- and intermediate-energy systems.

RESULTS AND CONCLUSIONS

The guidance on how to use the SCALE CAAS analysis option has been revised. This revision was necessary not because of any error in the SCALE coding, but because ENDF includes fission photon production as part of two different reaction types, MT 18 and MT 3. The MT 3 reaction includes photon production due to more than one reaction type, which makes it impossible to remove just the portion due to fission. When following the revised guidance, users do not remove the fission photons from the (n,γ) transfer matrix or include fission photons in the fixed source of the Monaco calculation. With the revised guidance, fission photons are not included in the source, but are created by subsequent neutron interactions even if the neutron interactions are not fission events. Therefore, these two inconsistencies compensate for each other when calculating integral quantities. If new fission photon production data are ever measured or estimated theoretically, and if the ENDF data are reevaluated to correlate fission photon production for all incident neutron energies, SCALE will still be able to correctly perform CAAS analysis by following the previous CAAS guidance. The revised CAAS guidance that will be documented in the SCALE user manuals beginning with SCALE 6.2 can be applied to all calculations including SCALE 6.1 and 6.0 to produce correct results with all the ENDF evaluations currently available. The error is independent of the SCALE coding and is a result of the nuclear data being interpreted and applied incorrectly in the previous CAAS guidance.

Any errors using the previous CAAS guidance will only manifest themselves with fast systems. The high energy of the cutoff where the fission photons are transitioned from MT 18 to MT 3 leads to minimal differences for thermal systems whether applying the previous or revised guidance. In an example calculation, the photon kerma was overestimated by nearly 50% when the previous CAAS guidance was used to model a fast system. That translates into a 13% underestimation of the minimum accident of concern based on ANSI/ANS-8.3-1997 [14]. Underestimating the minimum accident of concern could result in the unnecessary installation of additional CAAS detectors, resulting in additional conservatism in design.

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