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A comparison of Monte Carlo fission models for safeguards neutron coincidence counters

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ABSTRACT

Monte Carlo simulation is a powerful tool used to model neutron coincidence detectors for international safeguards. The simulation has typically sampled properties such as the fission neutron multiplicity, energy, and direction, from independent probability density functions. However, multiplicity counters detect event-based neutron correlations and thus more accurate fission event modeling is needed. To respond to this need, the Fission Reaction Event Yield Algorithm (FREYA) and the Cascading Gamma-ray Multiplicity with Fission (CGMF) models were added in the newest version of MCNP, MCNP6.2. The models simulate individual fission events conserving momentum, energy, and angular momentum such that correlated particles are emitted.

The effects of the new models on simulations of safeguards neutron coincidence counters were studied and compared to standard MCNP simulations. The MCNPX-PoliMi model was also included in the comparison. The properties of fission neutrons from safeguards relevant isotopes were compared to literature references. Then a hypothetical simplified detector was modeled to isolate the effects of specific differences between models. Experimental measurements from previous work were modeled and agreements were compared. Finally, the probabilities of correlated events occurring in the experimental measurements were calculated with the different models. For example, the probability was calculated of detecting neutrons from both induced fission in uranium and spontaneous fission of Cf-252 in the same fission chain.

1. Introduction

Neutron coincidence and multiplicity detectors are widely used for the safeguards verification of nuclear material. These detectors are modeled in Monte Carlo simulations for design optimization and characterization. The standard simulations sample properties such as the number of fission neutrons and their energy and directions from independent probability density functions. However, these neutron counters detect event-based neutron correlations and so more accurate modeling is needed. In response to this need, the Fission Reaction Event Yield Algorithm (FREYA) and the Cascading Gamma-Ray Multiplicity with Fission (CGMF) models were added in version 6.2 of MCNP[1] [1,2]. The models include analog fission physics with neutron–neutron, neutron–gamma, gamma–gamma, and multiplicity correlations conserving momentum, energy, and angular momentum from individual fission events [3,4]. These models were compared with the options commonly used for safeguards simulations which is referred to as the standard model in this work, and with MCNPX-PoliMi [5].

The purpose of this work is to guide users in choosing a model. The models have different neutron multiplicity distributions, angular correlations, and energy distributions. In some cases one model is clearly more accurate than another, and in other cases experimental data is lacking and the models are simply different. Some differences have large effects and others are negligible, and the sensitivity depends on the detector. Even when a model most accurately matches a measurement it could be coincidental. Multiple incorrect effects could be balancing out and the same model could be least accurate across other measurement configurations.

The choice of model is increasingly important as Cf-252 replaces AmLi as an interrogation source. The use of Cf-252 as an interrogation source has already been studied for the Active Well Coincidence Counter (AWCC) and the Uranium Neutron Coincidence Collar (UNCL) [6,7].

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Detectors such as the Advanced Experimental Fuel Counter (AEFC) also incorporate Cf-252 [8]. AmLi sources were used because a single random (alpha,n) reaction emits a single neutron. Overlap between neutron emissions is accidental and is easily accounted for. The neutrons are produced in separate reactions and are independent with respect to multiplicity (always 1), energy, and direction. However, Cf-252 spontaneous fission emits multiple neutrons in the same event which can induce fissions that are time correlated to the other neutrons from the Cf-252 fission. Accurate modeling of correlations between these spontaneous fission neutrons is required to accurately model the system's coincidence or doubles count rate. Modeling the angular correlation is one such example. If two spontaneous fission neutrons are more likely to go in the same direction, it is more likely that two fissions will be induced at the same time. If they are more likely to go in opposite directions, one is more likely to induce fission and the other will move away from the interrogation sample.

CGMF [9] and FREYA [10] model the underlying fission event including scission and fission fragments. The emission of radioactive signatures from fission are produced by this modeling. However, when their data or models are lacking the produced signatures can have incorrect properties. The properties of interest in safeguards are the fission neutron multiplicities, neutron energies, and angles between neutrons. The multiplicities are known most accurately, followed by energies, and differences between the models were shown in this work to have the least effect. The angular correlation was not previously produced by the standard model (which used an isotropic distribution) and differences in angular correlation between models were shown to have the greatest effect. Because CGMF and FREYA simulate the fission process in detail more coupled effects are included. The angular correlation is more extreme at higher neutron energies and lower multiplicities [11,12]. The neutron multiplicity and energy are correlated [12,13]. Where data is available these effects have matched experimental measurements [14]. These correlations are most relevant for low multiplying samples. At higher multiplications the correlations tend to wash out through the averaging of many events in a fission chain [15]. The FREYA results of this work were generated with the RSICC release of MCNP6.2. CGMF results were generated with the RSICC release and occasionally with an internal build which gave identical results but allowed the use of a computing cluster for better statistics.

The standard safeguards model does not model each fission in detail, but instead independently samples from distributions to produce average quantities. The standard model is invoked by `method=3 data=3 shift=1` on the `FMULT` card to generate realistic fission multiplicities as opposed to the default MCNP options which only preserve average $\bar{\nu}$, and is further described in the MCNP manual [16]. In induced fission the average neutron multiplicity $\bar{\nu}$ is taken from the chosen nuclear data library. The multiplicity distribution is chosen by sampling a Gaussian distribution to preserve $\bar{\nu}$ without sampling negative numbers of neutrons. Spontaneous fission multiplicity comes from measured data referred to in the MCNP manual. Neutron energies use Watt spectra parameters from the data library for induced fission or from the manual for spontaneous fission, which were generated by the Madland–Nix model [17]. All properties are sampled independently, meaning there are no neutron angular correlations and all neutrons are emitted isotropically. The standard model in the RSICC release of MCNP6.2 was used.

MCNPX-PoliMi includes some correlations. The spontaneous fissions come from a model and the neutron spectrum depends on multiplicity, and the neutrons have an angular correlation. For induced fission an option is given for the source of multiplicity data, and in this work Holden and Zucker was used [18]. MCNPX-PoliMi is based on the faster MCNPX but cannot take advantage of new features in MCNP6 versions. MCNPX-PoliMi RSICC release version 2.0.0 was used in this study.

The isotopes of interest in this work were Cf-252, U-235, U-238, Pu-238, Pu-239, Pu-240, Pu-241, and Pu-242. The fissile isotopes U-235, Pu-239, and Pu-241 were studied as thermal induced fission which is the most common neutron production mechanism in thermal neutron counters. The remaining isotopes were studied for spontaneous fission. The standard model includes data for all of these isotopes. MCNPX-PoliMi has data for all but Pu-238, one of the least common isotopes in safeguards applications. FREYA handles all of the isotopes in this study. CGMF lacks data for U-238, Pu-238, and Pu-241 and uses the LLNL fission model when these isotopes are called.

Even with increasingly economical and fast computers, computing time is still a concern in some applications. In a typical safeguards simulation, interrogation of 1-kg of uranium in an AWCC, FREYA took 40% more, CGMF took 1200 times more, and MCNPX-PoliMi took 10% less, time than the standard model. CGMF's factor of 1000 slowdown is prohibitive for regular use.

The structure of the paper is as follows. First, the properties of common safeguards isotopes as given by the different models are shown. Consensus values of measured data are included for the multiplicity distributions. Then, hypothetical simulations are used to isolate the effects of individual differences in the codes. Highly simplified coincidence counters were designed to be sensitive to only one property at a time. The doubles rates are compared. For example, to study differences in the fission spectrum, the thickness of 4π detectors was varied. The results indicate what detector designs are affected by the differences in fission models and to what magnitude. Then the models are compared in simulations of measurements taken with two safeguards detectors, the AWCC and AEFC. Finally, PTRAC, which generates a list of events which occurred in the simulation, is used to explain in more detail how the models affect the probabilities of different correlated events which lead to the change in doubles rate.

2. Nuclear data

2.1. Average multiplicity, average energy, and angular correlation

The neutron emission properties of spontaneous and induced fission vary in the different fission models. The average neutron multiplicity and energy were found for each of the four models. The angular, multiplicity, and energy distributions were also found. For induced fission the incident neutron energy was 0.0253 eV. The results were compared to published values and their uncertainties, where available. Spontaneous fission neutron multiplicity values were compared to the data accumulated in Santi and Miller [19] and induced fission data comes from Holden and Zucker [18]. Both are consensus of published measured values with uncertainties and are thus expected to be 'true'. With the exception of Cf-252, neutron spectra results were not compared to reference values because a consensus of experimental energy distribution data rarely exists, and instead models are commonly used. The fission model data have negligible statistical uncertainty which is plotted in each multiplicity figure.

The multiplicity values are prompt for FREYA, CGMF, MCNPX-PoliMi, and the published results. The MCNP standard model spontaneous fission multiplicity values are also prompt, are tabulated in the MCNP output file, and closely match the values of Santi and Miller. The induced fission multiplicity values for the standard model are generated by sampling from a Gaussian distribution based on $\bar{\nu}$. Total $\bar{\nu}$ is used and taken from the specified nuclear data library for the incident neutron energy. Prompt $\bar{\nu}$ can be specified by the `TOTNU` card, which adjusts the Gaussian distribution. The difference in multiplicities from utilizing prompt and total $\bar{\nu}$ is small, and neither multiplicity distribution is based on measurements. The `TOTNU` card is often ignored in simulations of safeguards detectors, and so it was not used in this work.

The average neutron multiplicity is shown in Fig. 1. All but four multiplicities agree within 3 $\sigma_{measured}$. The FREYA value for Pu-240 differs by 0.08 neutrons per fission and 17 $\sigma_{measured}$. The FREYA value of Pu-241 differs from the reference value by 0.07 neutrons per fission and 6 $\sigma_{measured}$. The standard model and MCNPX-PoliMi U-235 $\bar{\nu}$ differ from measurements by slightly more than 3 $\sigma_{measured}$.