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Comparison of Geant4 and MCNP6 for use in delayed fission radiation simulation

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ABSTRACT

Neutron induced fission fragment distributions and delayed fission radiation are extremely important with reactor applications in fission cross sections and heating. Data on the fragment distributions are sparse so simulations use models or interpolations between known neutron energies. Different simulations perform different treatments of the distributions, and have different capabilities and flexibility in use. MCNP is a typical workhorse for fission simulations and coupled with burn-up codes such as CINDER can provide delayed radiation from fission. Geant4 is an extremely flexible physics based Monte Carlo simulation framework, but is not typically used for fission research. In this work the applicability of Geant4 for delayed fission radiation simulations is examined, with comparison to MCNP6 coupled with the CINDER2008 burn-up code. The Fisher and Engle fission experiment with the Godiva II subcritical assembly as a fission neutron source is used as a test case. Both simulations are adapted from that experiment and simulation results are compared with that experiment. Following Fisher and Engle, photons/fission/sec, MeV/fission/sec, and MeV/photon are examined. For the first two quantities results from both simulation codes are similar and are lower than experimental values, with Geant4 giving a higher value for earlier time bins and MCNP6/CINDER giving a higher value for the later time bins. For the last quantity both simulations are usually within uncertainty of the experimental values, with MCNP6/CINDER values consistently higher than both experimental and Geant4 values.

1. Introduction

Fission fragment distributions and the delayed radiation from the fragments are extremely important to many fields, including for delayed signals from active interrogation (Hall et al., 2007) and delayed heating in reactors (Blanchet et al., 2008). Unfortunately data are sparse on fission fragment distributions and delayed radiation. Fragment yield data are only available for some actinides and even then only available for thermal, 0.5 MeV, or 14 MeV incident neutrons (Romano et al., 2010). Therefore models or interpolating calculations are used. Simulations are performed to try to understand delayed radiation from different situations, especially with complex geometries, shielding, and timing. Different simulations, though, apply different approaches to particle transport, tracking, fission, and the delayed radiation.

The MCNP Monte Carlo codes (Pelowitz, 2013) can be used for simulating neutron-induced fission (e.g., (Hashemi-Nezhad et al., 2008)). MCNP tracks the neutrons to the fissionable material and produces secondary neutrons through the fission, which add to the total neutron flux. To move one step forward and examine the fragment decay radiation, MCNP can be coupled with a burn-up code such as CINDER (Wilson et al., 1995; Holloway et al., 2011), which takes the neutron flux as an input to determine reaction rates and outputs transmutation products and delayed radiation. A variant of this specific coupling was added in MCNPX 2.6 by the addition of an internal interface routine to link MCNPX with routines from CINDER'90 for fission calculations (Durkee et al., 2009a). This feature of MCNPX was transitioned into MCNP6 (Pelowitz, 2013) still using CINDER'90 routines.

The simulations produce neutron and gamma rays from individual fission events by statistical sampling of distributions based on a combination of measured data and analytic models (Verbeke et al., 2010). In the external coupling examined, the neutron flux is passed from MCNP6 to CINDER2008 in a multigroup fashion, limiting fineness of neutron energies used. Using the internal coupling of MCNP6 and CINDER'90, the reaction rates are calculated using continuous energy in MCNP6, and then CINDER'90 is only used for decay path information. If the problem of interest involves any sort of attenuation due to a shielded source, the fragment

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and gamma inventory generated by CINDER needs to be re-coupled with MCNP to accommodate the attenuation and transport.

The Geant4 Monte Carlo toolkit (Allison et al., 2006; Agostinelli et al., 2003) provides a contrasting approach to simulations to compare with MCNP6/CINDER. The Geant4 toolkit is a physics based set of programming objects based on C++, and allows for the full transport of all particles, creation of fission products, fission product decay via specific transitions, as well as the consequent transport of the gamma radiation from the decay event within a single application. Rather than taking bulk fluxes and using condensed histories, Geant4 allows event-by-event simulations, from the incident neutron through fission to the fission fragment decays. There is also a continuous change of the fission fragment distribution as a function of energy, between the low-energy asymmetric mass peak distribution to the high-energy more symmetric distribution, rather than sampling from distributions for discrete energy bins. The flexibility in programming the open source code, and the variety of existing programming objects, makes Geant4 a powerful simulation framework.

In this work we explore the applicability of the Geant4 Monte Carlo simulation toolkit, version 9.6.1, to problems involving creation and decay of fission fragments. For comparison, simulations are also performed with MCNP6 externally coupled to CINDER2008. The Fisher and Engle fission experiment (Fisher and Engle, 1964) is used as a framework for the simulation comparisons, and both simulations are compared with Fisher and Engle results.

Geant4 and MCNP codes have been compared before for a variety of non-fission applications (e.g., (Colonna and Altieri, 2002; Maigne et al., 2011; Shirin et al., 2006)). MCNPX internally coupled with CINDER'90 has been compared with Fisher and Engle data by Durkee et al. (2009b) and comparative results were presented for 17 bin energy sets for several discrete time periods. In that work they refer to the comparison not as a validation due to the many experimental details missing for a high fidelity simulation, but as a demonstration of the introduced MCNPX functionality. We take a similar approach to Durkee et al. (2009b), making comparisons using the framework of the Fisher and Engle experiment in demonstrating the usability of Geant4 for problems involving fission fragments. One of the authors (Blakeley) performed similar comparisons with previous versions of MCNP, CINDER, and Geant4 within a larger master's thesis work (that non-refereed work is available at Blakeley (2013)).

2. Methods

Two Monte Carlo simulations of delayed gamma-ray radiation following fission are presented in this work, MCNP6 coupled with CINDER2008, and Geant4 version 9.6.1. The Fisher and Engle study, after which the simulations are modeled, examined the energy and time dependence of the delayed gamma emission of the fissionable nuclides ^{232}Th, ^{233}U, ^{235}U, ^{238}U, and ^{239}Pu. The fission targets consisted of metal discs 0.105 in. in diameter and varied thicknesses irradiated by the GODIVA II ^{235}U prompt critical fission burst assembly as a neutron source (Wimett and Orndoff, 1958). The subsequent delayed gamma radiation from the fission sample went through a 1.072 in. diameter collimator and a 3.1 in. thick CH_2 absorber and was incident in a $4'' \times 4''$ NaI total absorption spectrometer.

^{235}U is of particular interest for energy and nonproliferation, so simulations were compared with the results obtained from the experiment on a 99.90 atomic% ^{235}U and 0.10 atomic% ^{238}U fission target. In the experiment, the fission target was of variable thickness, and the large self-attenuation of soft gamma rays was corrected in the reported values. The simulated fission target was modeled as a small sphere, with a radius of 0.01975 cm, to reduce the self-shielding attenuation in ^{235}U of the delayed gamma signal, following Durkee et al. (2009b).

Experiments were performed with a fission neutron source, which Durkee models using a Watt fission spectrum. For simplicity and ease of simulation comparison, simulations were run at 2 MeV, near the average Watt fission neutron energy. The results in the current work are the cumulative photon emissions as a function of time following the time dependent Fisher and Engle results: photons/fission/sec, Mev/fission/sec, and MeV/photon. Both Geant4 and MCNP6/CINDER2008 simulations used identical geometries, but methods varied.

MCNP6 was run using ENDF/B-VII.1 cross-section data (Conlin et al., 2013) and 3 million neutron histories. Forced collisions were implemented to improve fission statistics within the small sphere. A volume averaged cell flux tally was employed to get a 63-group neutron flux for the region in question. This 63-group neutron flux was then supplied to CINDER2008, along with the CINDER'90 63-group data library, in order to perform the activation and depletion analysis. The neutron flux in CINDER2008 was active for 0.043 s, mirroring the experimental beam pulse. For the time dependent signal, the nuclide inventory and emission data were requested at time ranges 0.2–0.5, 1.0–2.0, 4.0–5.5, 10.0–13.0, and 35.0–45.0 s, with 6 time sub-bins in each range to capture the within bin trends more accurately.

A limitation of external coupling of MCNP6 and CINDER2008 is the disparity between neutron cross section data, and therefore also between the calculated reaction rates in either code. The library from CINDER'90 was preserved in this work to ensure consistent decay data when compared to the previous work by Durkee et al. (2009b). Codes such as the Serpent Monte Carlo reactor physics code (Leppänen, 2013) and MCNP6 (Pelowitz, 2013) avoid this data discrepancy with a single data set but currently lack the ability to exploit the full range of transport and burn-up methods available in external coupling.

Geant4 was run with identical geometries as used for MCNP6, with a planar beam of 2 MeV neutrons incident on the sphere of HEU, and statistics on gamma rays produced within the sphere were recorded. The same time bins were used as in the MCNP6 calculations, and energies were summed directly without binning. Geant4 did not use forced collisions so 1 billion incident neutrons were used to produce 5 million fission events.

Simulations carried out within this work were performed with an application written for Geant4 version 9.6.1 using the Geant4 ParaFission model. Geant4 handles all processes within the same program, from transport of the neutrons to the target, fission, production and transport of fission fragments, and decay of the fission fragments and the accompanying gamma ray emissions. The specific programming objects can be activated for different physics processes, and modified where the need arises. Geant4 was originally developed for high-energy physics but has been modified extensively for lower energy applications. It has not been optimized for fission, but as it handles processes in a different manner than MCNP/CINDER and is open to programming modifications it has great potential.

3. Results and discussion

From the Fisher and Engle experiments, several easily reproducible quantities of interest regarding delayed gamma emission were obtained as a function of time. Results are presented for the Fisher and Engle experiment, MCNP6/CINDER2008 simulations, and Geant4 simulations for photons/fission/sec in Fig. 1, MeV/fission/sec in Fig. 2, and MeV/photon in Fig. 3. Time bins are 0.2–0.5, 1.0–2.0, 4.0–5.5, 10.0–13.0, and 35.0–45.0 s. The energy range is

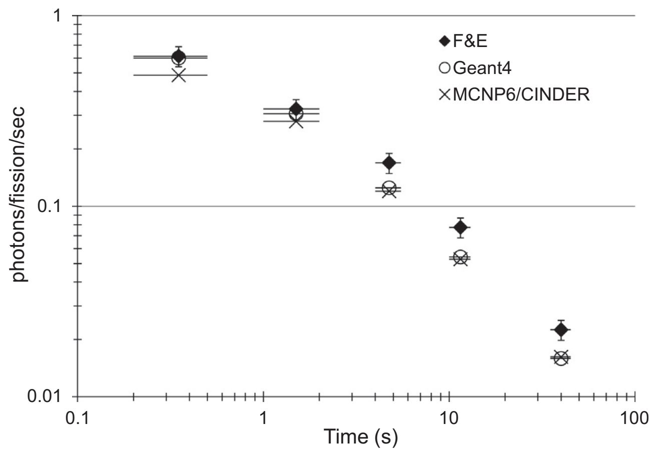

Fig. 1. Average rates of photons per fission for the Fisher and Engle experiment (Fisher and Engle, 1964), and simulations in the current work using MCNP6/CINDER2008 and Geant4. Time bins and values are given in Table 1.

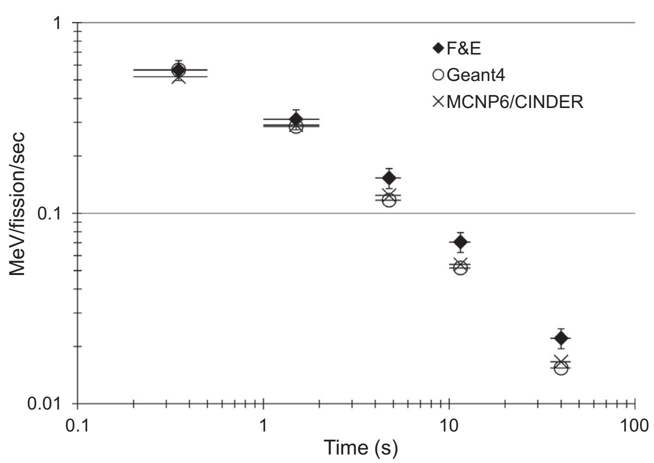

Fig. 2. Average rates of photon energy released per fission for the Fisher and Engle experiment (Fisher and Engle, 1964), and simulations in the current work using MCNP6/CINDER2008 and Geant4. Time bins and values are given in Table 1.

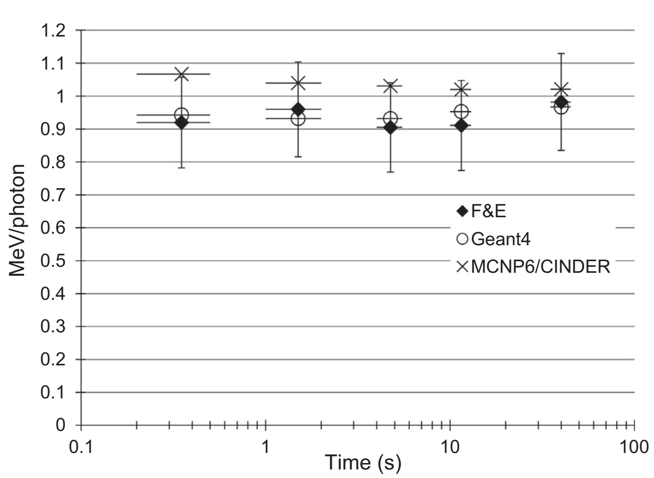

Fig. 3. Average energies per photon for the Fisher and Engle experiment (Fisher and Engle, 1964), and simulations in the current work using MCNP6/CINDER2008 and Geant4. Time bins and values are given in Table 1.

constrained to 120 keV–6.5 MeV photons. The metrics presented in Fisher and Engle provide an experimental basis for comparison. Results are summarized in Table 1. The nominal uncertainty given by Fisher and Engle is 12% for these time quantities from n+ ^{235}U fission, 15% for average MeV/photon, and 0.46 uncertainty for photons/fission. Fisher and Engle used a polynomial fit to the five photons/fission data points and summed the fit from 0.2 to 45.0 s to estimate photons/fission over the full time range. For all values calculated with Geant4 the photons were directly summed in their respective time bins following fission as they were produced. For CINDER2008, the beta-delayed photons were binned in a 25 energy bin multi-group fashion from 0 to 25 MeV.

The simulation result shows close agreement for many of the values, coming within experimental uncertainty for most simulated values for the 0.2–0.5 and 1.0–2.0 second time bins for photons/fission/sec, Fig. 1, and MeV/fission/sec, Fig. 2. Except for one point that is just above the experimental value (the Geant4 value for photons/fission/sec for the 0.2–0.5 s bin) all the simulated values for photons/fission/sec and MeV/fission/sec are below the experimental values, with the difference increasing with increasing time values. In general, both simulations are closer together for these quantities than they are to experiment. Comparing between the simulations for these quantities, Geant4 gives a higher value for earlier time bins and MCNP6/CINDER gives a higher value for the later time bins.

The values of MeV/photon, Fig. 3, are the ratios of the previous quantities for each time range, and fairly constant values are found for each method, though they differ between the methods with MCNP6/CINDER2008 giving the highest values. Almost all simulation values for MeV/photon agree with Fisher and Engle values within experimental uncertainty. Geant4 and experimental values are very close for all time bins, with a smaller variation in Geant4 values than experimental values. The Geant4 results are entirely reasonable, but the differences should still be examined.

One source of differences may be the handling of low energy photons. The photons/fission values in Table 1 for both MCNP6/CINDER2008 and Geant4 are lower than experiment, with MCNP6/CINDER2008 slightly lower than Geant4. CINDER2008 outputs a full 0–25 MeV energy range, which was reduced by consid-

Table 1
Results from the Fisher and Engle experiment (Fisher and Engle, 1964), and Geant4 and MCNP6/CINDER2008 simulations from the current work. Nominal experimental error was given as 12% for photons/fission/sec and MeV/fission/sec, as 15% for MeV/photon, and as 0.46 for photons/fission, with corresponding numerical values presented in parentheses.

Interval (s)	Fisher and Engle Photons/fiss/sec	Geant4 Photons/fiss/sec	MCNP6/CINDER Photons/fiss/sec
0.2–0.5	0.613(74)	0.600	0.487
1.0–2.0	0.324(39)	0.306	0.279
4.0–5.5	0.169(20)	0.125	0.120
10.0–13.0	0.0775(93)	0.0542	0.0528
35.0–45.0	0.0225(27)	0.0159	0.0162
Interval (s)	MeV/fiss/sec	MeV/fiss/sec	MeV/fiss/sec
0.2–0.5	0.564(68)	0.565	0.520
1.0–2.0	0.311(37)	0.285	0.290
4.0–5.5	0.153(18)	0.117	0.124
10.0–13.0	0.0706(85)	0.0516	0.0539
35.0–45.0	0.0221(27)	0.0154	0.0166
Interval (s)	MeV/photon	MeV/photon	MeV/photon
0.2–0.5	0.920(138)	0.943	1.067
1.0–2.0	0.960(144)	0.932	1.040
4.0–5.5	0.905(136)	0.932	1.031
10.0–13.0	0.911(137)	0.953	1.020
35.0–45.0	0.982(147)	0.967	1.021
Full time (s)	Photons/fission	Photons/fission	Photons/fission
0.2–45.0	3.31(46)	2.58	2.40

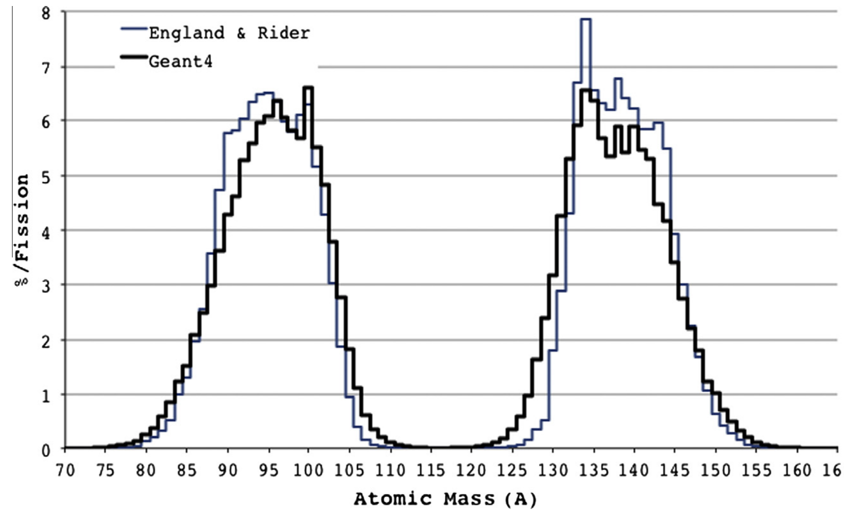

Fig. 4. Comparison of fission product mass for thermal neutrons calculated using Geant4 and from data from England and Rider (England and Rider, 1993).

ering the proportions in each energy bin; thus uncertainties may have come in. As there are many low energy photons produced, nearly exponentially higher at low energies, a mis-cut at low energies can change the number of low energy photons counted, moving the photon numbers down and the energy per photon values up.

Geant4, meanwhile, uses cut lengths on the photons tracked. If it is determined that a photon will not travel that length in the material, regardless of the actual simulated geometry, the photon is not tracked. This biases against low energy photons but does not give a sharp energy cut-off, and may affect the low energy photon numbers counted.

Another factor in the differences may be that MCNP6/CINDER2008 and Geant4 use different initial fission fragment distributions. MCNP6/CINDER2008 results are based on data tables. MCNP uses interpolated and modeled values for fission fragments distributions over a range of neutron energies, using only those discrete listed values. CINDER uses a selected fission yield data set from thermal, 0.5 MeV, or 14 MeV neutron energies. Then, rather than just sampling, CINDER uses that full yield set and follows every single isotope's decay. Geant4 uses a continuous energy distribution based on asymmetric and symmetric fission distributions for low and high energy neutron induced fission, respectively, with an energy based scaling function between the two, $F(A_f) = F_{sym}(A_f) + F_{asym}(A_f)$. The Geant4 Physics Reference Manual presents detailed information on the parameterizations (CERN, 2013). The continuous energy function can be advantageous, but the distributions themselves may not be ideal. A comparison of the Geant4 fission fragment distribution with England and Rider data, both for thermal energy neutrons, is shown in Fig. 4. The England and Rider values represent data used by MCNP6 and CINDER2008, though the simulation yields are not directly accessible.

A forced fission fragment distribution in Geant4, using the fragment distribution from data as the starting point for fragment decays and thus for the delayed gamma-ray emissions, may be the subject of future investigation. In the current work, though, the focus is on examining Geant4 for its suitability for fission simulations using the unmodified programming objects from the CERN program distributions.

4. Conclusions

Investigations were focused on using Geant4 for fission simulations for delayed radiation, following the process from neutron induced fission through the fission fragment decay chains and photon emissions. The flexibility of the Geant4 simulations makes this a highly desirable tool to use. The Fisher and Engle experiment on neutron induced fission of ^{235}U was used as a standard. The quantities MeV/fission/sec, gamma/fission/sec, and MeV/photon were used for comparison with experiment, and for comparison with MCNP6/CINDER2008 simulation. Simulation results for both MCNP6/CINDER2008 and Geant4 were slightly lower than experiment, with the difference increasing with greater times. The simulations themselves were typically closer together than to the experimental values, Geant4 slightly closer to experiment for short times and MCNP6/CINDER2008 closer to experiment for later time bins. Geant4 results were reasonable compared with MCNP6/CINDER2008. Geant4 can be modified so fragments match data to improve delayed radiation results, though the current study was on Geant4 output without modifications. This preliminary comparison suggests Geant4 as a useful simulation tool for delayed radiation from fission, and higher fidelity simulations may be possible with modifications. This is significant as Geant4 offers an exceptional set of programming tools that allow for expansion into a wide variety of simulated experimental settings.

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