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Calculation of photon pulse height distribution using deterministic and Monte Carlo methods

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HIGHLIGHTS

- Generation of new multi-group gamma cross section library using Klein–Nishina relation.
- Benchmarking of the new generated multi-group gamma cross section library using ANISN and MCNP codes.
- Calculation of pulse height distribution using deterministic method: ANISN code and collided component program.
- Calculation of pulse height distribution using Monte Carlo method: MCNP and FLUKA codes.

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ABSTRACT

Radiation transport techniques which are used in radiation detection systems comprise one of two categories namely probabilistic and deterministic. However, probabilistic methods are typically used in pulse height distribution simulation by recreating the behavior of each individual particle, the deterministic approach, which approximates the macroscopic behavior of particles by solution of Boltzmann transport equation, is being developed because of its potential advantages in computational efficiency for complex radiation detection problems. In current work linear transport equation is solved using two methods including collided components of the scalar flux algorithm which is applied by iterating on the scattering source and ANISN deterministic computer code. This approach is presented in one dimension with anisotropic scattering orders up to P8 and angular quadrature orders up to S16. Also, multi-group gamma cross-section library required for this numerical transport simulation is generated in a discrete appropriate form. Finally, photon pulse height distributions are indirectly calculated by deterministic methods that approvingly compare with those from Monte Carlo based codes namely MCNPX and FLUKA.

1. Introduction

Identification of a radiation source is typically done by measurement of radiation fields and analysis of Gamma ray spectroscopy. Pulse height distribution data which is defined as the distribution of the energy deposited in detector volume gives some information about the profiles of emitting radiation source. This non-Boltzmann quantity can be calculated by numerical simulation of the radiation interactions in the detector and its environment. Radiation transport simulation is broadly categorized as stochastic, deterministic and hybrid methods. Historically, this quantity has been calculated by Monte Carlo method, because it simulates the physics of problems on a particle-by-particle basis leading to easy access to the details of interactions and produces the results with arbitrary accuracy. Since, individual particles must be tracked through each event; Monte Carlo codes are very slow for large scale with high scatterings or attenuations such as large-volume or highly shielded sources. While deterministic method that solves linear transport equation offers several advantages for applying them in some special detection problems. The first advantage of this method is global solution; it means the flux quantity is calculated in individual point. Furthermore, there are no statistical errors, and the greatest is that deterministic methods are extremely computational efficient compared to Monte Carlo methods for scattering and attenuation dominated problems (Smith et al., 2008). In deterministic approach, which has been recently considered, transport equation is solved using discretizing in space, angle, and energy based on source iteration procedure (Benz and Palmer, 2010).

In current paper, we want to calculate pulse height distribution

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by the deterministic methods and compare it with the Monte Carlo results. A brief history of two methods in calculation of pulse height distribution is represented in Section 2. Also, we generate multi-group gamma cross section library which are required for numerical solution of transport equation. In Section 3 the results of defined test problem are reported, and finally a discussion of the results is presented in the last section.

2. Methods discussion

In Monte Carlo radiation transport, history of each particle is individually tracked from birth to death, including every interaction, for uncharged particles. This method has been a standard and precise model in the detection problems for over 20 years because of direct simulation of the particle physics, geometric flexibility, well-tested cross section libraries, high accuracy and straightforward calculation of pulse height distribution. This non Boltzmann quantity is simply determined by subtracting the final energy of each particle from its initial energy. The worst disadvantage of Monte Carlo methods is its extremely long run times to achieve a good statistical precision, particularly for deep penetration, high degree of self-attenuation, or large physical scale problems, although variance reduction techniques are employed to optimize the Monte Carlo method (Benz and Palmer, 2010).

Before the Monte Carlo techniques became common in radiation transport simulation, deterministic methods were frequently used in this area. Inasmuch as energy deposition is inherently a stochastic process, pulse height distribution could not be calculated by solving single Boltzmann transport equation. For this reason, deterministic solution is rarely used for generation of pulse height distribution.

In deterministic method, we have utilized three discretized variables including space, angle and energy to calculate the angular flux. By calculating the collided components of the angular flux at each step, scattering source would be generated for the next step. Collided components of the flux are defined as photons escaping from the detector without any interaction form the uncollided or zero component and particles which once scatter in the detector form the 1st-collided component of the flux and so on. In this method, convergence of the scalar flux determines the degree of collided components.

One dimensional transport equation in steady state with anisotropic scattering in energy group g and direction cosine μ_n is represented by Eq. (1). In this equation, the angular variable is discretized using discrete-ordinate (S_N) method with level symmetric quadrature (Stammler and Abbate, 1983). The scattering source is described by Legendre polynomial expansion of angular flux and angular moments of the scattering cross section. The components of the scalar flux and partial current are represented by Eqs. (2) and (3), respectively.

$$\mu_n \frac{\partial \psi_g\left(\vec{x}, \mu_n\right)}{\partial x} + \sigma_{t,g}\psi_g\left(\vec{x}, \mu_n\right) = \sum_{l=0}^{L} \frac{2l+1}{2} \sum_{g=1}^{G} \sigma_{s,l,g'\to g}(x)\varphi_{l,g'}(\mathrm{x})P_l\left(\mu_n\right) + S_g\left(\vec{x}, \mu_n\right) \tag{1}$$

where

$$\varphi_{l,g}(x) = \sum_{n=1}^{N} w_n \psi_{g,n}(\mathrm{x}) P_l(\mu_n) \tag{2}$$

$$J_g = \sum_{n=1}^{N} w_n \psi_{g,n} \mu_n \tag{3}$$

Here, $\sigma_{s,l,g'\to g}$ represents the probability of scattering per unit path length of a particle from group g' into group g, for a given Legendre polynomial expansion of order l, and $\sigma_{t,g}$ is the total cross section in group g, and $S_g(\vec{x}, \mu_n)$ is definition of source in group g and direction μ_n. $P_l(\mu_n)$ is Legendre polynomial of order l in the angular variable. Because the transport equation is an integro-differential equation, iteration on the scattering source is often employed to compute the solution. In general, photon transport equation in slab geometry with discrete direction μ_n using collided components method is written by Eq. (4).

$$\mu_n \frac{\partial \psi_{g,n}{}^{(j+1)}(x)}{\partial x} + \sigma_t \psi_{g,n}{}^{(j+1)}(x) = Q_{g,n}{}^{j}(x) \qquad n = 1 \ldots\ldots N \tag{4}$$

where

$$Q^j(x) = \sigma_s(E' \to E, \mu' \to \mu)\phi^j(x) + S^j(x) \tag{5}$$

$$\phi_g^j(x) = \sum_{i=1}^{N} W_i \psi_{g,n}^j(x) \tag{6}$$

In equations above, the superscript "j" indicates degree of collided components, parameter Q_n is a definition of scattering source, ψ_n is the angular flux in the nth angular ordinate and ϕ is the scalar flux.

The solution of transport equation by determination of boundary condition is specified. Typically, there are no internal sources in detection problems and the external source is introduced into the system as a boundary condition. The source iterations begin with the 0th component of the first energy group by definition of external source, and subsequent iterations calculates the remaining scattered components of the flux. The external source boundary condition is set to zero for the remaining iterations, because higher scattered components of the flux depend only on previously calculated flux components which are determined as scattering source (Benz and Palmer, 2010).

In radiation detection systems, three fundamental interactions which are important in energy deposition are considered: photoelectric absorption, Compton scattering, and pair production. The fourth interaction, coherent scattering, is ignored here, because it is not significant for energy deposition analysis (Knoll, 2000). In the test problem photon energy is defined below the pair production threshold to skip energy loss by annihilation photons. So, photoelectric is considered as an absorption interaction and Compton effect as a scattering interaction. In Compton collision, it is assumed that the energy received by the target electron is totally deposited in the slab. This assumption is a good approximation for the centimeter-scale detectors, in which the maximum range of scattered electrons of a few MeV is in order of a few millimeters.

Photons could interact with detector material via absorption or scattering. In scattering interaction of photon through the detector volume, only direction and energy of scattered photon change and no extra photons are generated. Therefore, by simplifying the photon interactions, it can be concluded that the number of initial photons that incident to the slab is balanced to the number of absorbed photons plus the escaped ones.

A mono-energetic photon beam at energy E_0, which incident on the face of the slab in a direction close to the normal, is defined as the external source. Fraction of the photons, which are absorbed in the detector volume, deposit their total energy, there. The remains escaping from detector at energy E_g, deposit amount of energy equal to $(E_0 - E_g)$ in the detector volume.

The incident partial current is defined as the number of photons crossing the front face of the detector in the $+\mu$ direction. We can calculate partial current of photons leaving the slab in each direction and energy group using Eq. (3). The outgoing partial current for the sth collided component of the flux, represents the number of particles which leave the system in energy group g after s collisions. Chain interactions in energy deposition are shown in