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New Results for Pulse Height Tally Verification in MCNP5

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INTRODUCTION

Code verification is the link between the mathematical equations and computational algorithms. One method of code verification includes comparison of calculated results with analytic solutions. For radiation transport, exact solutions to the particle transport equations in three-dimensional space as a function of energy, angle, and time are complex and often impossible. One technique to provide analytic solutions is to simplify or eliminate terms in the transport equation (eg. one dimension, single energy group, isotropic scattering, ...). An alternative approach to generating analytic solutions is to simplify the nuclear data, leaving the mathematical equations and computer code unaltered. This approach allows code verification independent of solution technique (eg. deterministic, Monte Carlo) [1]. In this work, we improve on an existing approach that simplifies the physical data to verify the non-Boltzmann pulse-height tally (PHT) in the Monte Carlo code, MCNP 5 [2].

The pulse height tally is unique among the various tallies in MCNP. Unlike other tallies which are calculated as soon as the particle exits or collides in the cell, the PHT requires the entire set of tracks for a history must be completed. The PHT requires detailed bookkeeping by a Monte Carlo code when variance reduction is used to determine the history pulse. Variance reduction with photon and electron pulse height tallies is a feature being implemented for the next release of MCNP [3]. In this work, we present previously unpublished details to the analytic solution of the PHT distribution and report new MCNP 5 verification results using fictitious nuclides [4].

PROBLEM DEFINITION

Shuttleworth [5] has cleverly devised a set of fictitious nuclides with simplified physical interaction mechanisms for the verification of MCBEND [6]. His verification approach uses fictitious nuclides with a simple geometry that is continuous in space and discrete in energy and angle. The cross sections are constant and allow for threshold reactions with particle progeny. Shuttleworth has followed only a few collisions and reported a few analytic results [7]. We extend the use of these fictitious nuclides by calculating all possible collisional probabilities.

The verification problem defined by Shuttleworth consists of a cylinder made with three fictitious elements, each with the total macroscopic cross section of 1.0 cm^{-1}. The elements and their physical interaction mechanisms are defined as:

1. Moron, atom fraction 0.2. At all energies, a collision with this nuclide absorbs the incident particle.
2. Odium, atom fraction 0.3. At all energies, a collision with this nuclide produces one secondary particle that has half the energy of the incident particle. The secondary particle is not deflected.
3. Kneeon, atom fraction 0.5. At all energies, a collision with this nuclide produces two secondary particles, each having one quarter of the energy of the incident particle. At, or above an incident energy of 1.0 MeV, one particle is scattered forwards and one particle is scattered through 90°. Below 1.0 MeV, both particles are scattered forwards.

These three nuclides represent the photon physical interactions of photoelectric absorption (Moron), Compton scatter (Odium), and pair production (Kneeon).

The cylinder is divided into an insensitive region followed by an active region. Each region is a cylinder of length ln(2) and radius ln(2). The source particles start along the cylinder axis at 0 and have an initial energy of 3.2 MeV. All particles are instantaneously absorbed at 0.15 MeV or below. With this simplified problem, we can analytically determine the probability of each possible pulse height for 1, 2, or any combination of regions. The particle tracks are terminated by absorption, escape, or energy cutoff. The probabilities for axial and radial escape, binned by energy as well as the number of collisions that occurred in the cell, are also easily calculated.

DESCRIPTION OF THE ACTUAL WORK

Figure 1 depicts the 161 possible interactions for a single region. Radial scattering is a subset of this tree.

Assuming an absorption free media where each track continues until the particle exits, the probability of entering a detector of length Δx, total cross section of unity can be evaluated exactly as:

$$p_{exit}(n) = \frac{(\Delta x)^n \exp(-\Delta x)}{n!}$$

where n is the number of collisions. We can extend p_{exit} to include tracks that do not exit the detector. The probability, $p_{abs}(n)$, that a particle entering the detector undergoes (n-1) scattering collisions and is absorbed on the n'th collision is given by:

$$p_{abs}(n) = \frac{e^{(-\Delta x)}\left[(n-1)!e^{\Delta x} - (\Delta x)^{n-1} - (n-1)(\Delta x)^{n-2} - (n-1)(n-2)(\Delta x)^{n-3}\ldots\right]}{(n-1)!}$$

The relationships for p_{exit} and p_{abs} do not include the individual cross sections for each of the n collisions and therefore must be multiplied by the cross section for the appropriate number of odium, kneeon, or moron collisions.

Equations 1 and 2 account for all possible odium, moron collisions and *some* kneeon collisions. These equations are not general enough to account for the correlated particles produced by kneeon collisions and require special treatment.

A computer code was developed to generate high-precision numerical results for all possible collisions. Verification of this code was done by comparing code results with known analytic probabilities at several points in figure 1. New MCNP 5 analog and splitting/russian roulette results are compared to the analytic solution in Table I.

RESULTS

TABLE I. New Pulse Height Distribution Results for Region 1

Energy (MeV)	Analytic	MCNP 5 (R.E.)	Number of SD away	Spl/RR 2:1(R.E.)	Number of SD away
3.2	1.149854E-01	1.14974E-01 (0.0001)	0.99	1.14974E-01 (0.0001)	0.99
3.0	5.745194E-03	5.74715E-03 (0.0006)	-0.57	5.74534E-03 (0.0006)	-0.04
2.8	2.417574E-02	2.41788E-02 (0.0003)	-0.42	2.41759E-02 (0.0003)	-0.02
2.6	1.000594E-02	1.00001E-02 (0.0004)	1.46	1.00022E-02 (0.0005)	0.75
2.4	6.859668E-02	6.85896E-02 (0.0002)	0.52	6.85925E-02 (0.0002)	0.30
2.2	2.511753E-02	2.51163E-02 (0.0003)	0.16	2.51164E-02 (0.0003)	0.15
2.0	6.075803E-02	6.07621E-02 (0.0002)	-0.33	6.07642E-02 (0.0002)	-0.51
1.6	1.906155E-01	1.90630E-01 (0.0001)	-0.76	1.90640E-01 (0.0001)	-1.29
0.0	5.000000E-01	5.00002E-01 (0.0000)	---	4.99997E-01 (0.0000)	---
sum	**1.000000**	**1.00000**		**1.00001**	

REFERENCES

1. A. SOOD, R. A. FORSTER, D.K. PARSONS, Prog. Nucl. Ener. **42**, 1, pp. 55-106 (2003).
2. MCNP, Version 5, Vol. 1 LA-UR-03-1987 (2003).
3. T.E. BOOTH, LA-12433, (1992).
4. A. SOOD, R.A. FORSTER, B.J. ADAMS, M. C. WHITE, Fifth Int. Indust. Radiat. and Radioiso. Meas. Appl., Bologna, Italy (June 2002).
5. T. SHUTTLEWORTH, Proc. of the Eighth Int Conf. Radiat. Shielding, Arlington, Texas (1994).
6. MCBEND/MONK, Answers Software Service (UK).
7. T. SHUTTLEWORTH private communication (June 2002).

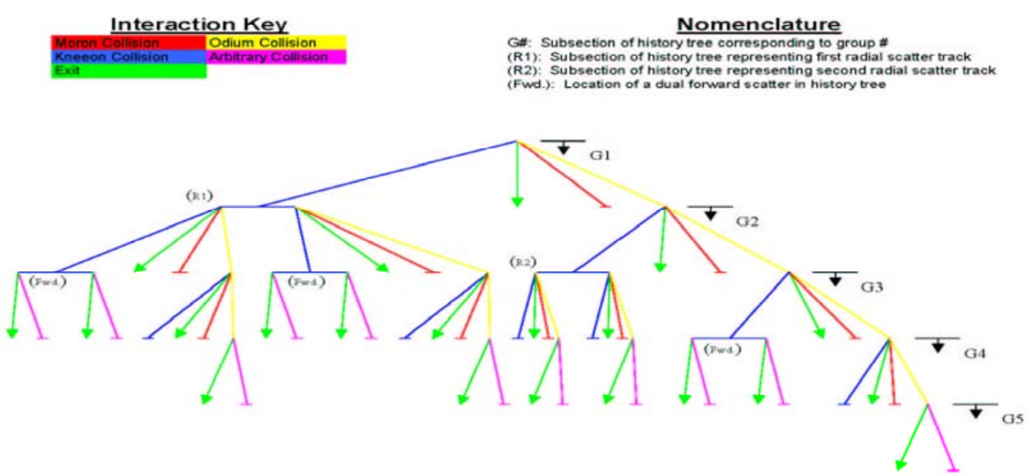

Fig. 1. Scenario Tree