Title: Workshop on Radiation Detection and Simulation with MCNP

Author(s): Avneet Sood (X-3, LANL)

Submitted to: 14th Biennial Topical Meeting of the Radiation Protection and Shielding Division of the American Nuclear Society Carlsbad, NM April 6, 2006
Workshop on Basic Radiation Detection and Simulation with MCNP

Avneet Sood

MCNP Code Development Team, X-3
Applied Physics (X) Division
Los Alamos National Laboratory

ANS RPSD Conference,
Carlsbad, NM
6 April 2006
Outline

Introduction

Radiation Detection Physics
   Sources of electromagnetic (gamma-ray) radiation
   Interaction mechanisms of gamma-rays
   Pulse-height spectra

Monte Carlo Simulation of Radiation Detectors

MCNP Features useful in radiation detection
   MCNP F8 Tally
   MCNP Photon, Electron Physics

Comparisons of Calculations and Experiment
   Deviations from ideal response
   Benchmark measurements
   Comparison of Experimental Results with MCNP
   Benchmark HPGe Detector Measurements
This introductory workshop on basic radiation detection and simulation will cover the following topics:

1. Review the basic physics involved with gamma-ray radiation detection and discuss the limits of the simulation physics.

2. Review MCNP features useful in comparing typical calculations (e.g., efficiency, spectroscopy) with experimental measurements for both active and passive gamma-rays.

3. Discuss comparisons with MCNP calculations and benchmark experiments for NaI and HPGe detectors.
Common gamma-ray sources
- Na-22: 1.274 MeV, annihilation, + Ne X-rays
- Cs-137: 0.662 MeV + Ba X-rays
- Co-60: 1.173, 1.332 MeV

Γ-ray following beta decay

Na-22: 1.274 MeV, annihilation, + Ne X-rays
Cs-137: 0.662 MeV + Ba X-rays
Co-60: 1.173, 1.332 MeV

Common gamma-ray sources
- Na-22: 1.274 MeV, annihilation, + Ne X-rays
- Cs-137: 0.662 MeV + Ba X-rays
- Co-60: 1.173, 1.332 MeV

30.07(3) yr. $^{137}$Cs Decay Scheme [C]

5.2714(5) yr. $^{60}$Co Decay Scheme [C]

Gamma rays following beta decay
Gamma rays following beta decay (continued)

- Common gamma-ray sources: Well defined energies
  - Nearly Monoenergetic
  - Photon energy distribution small compared to detector resolution
- Usually limited to $E_\gamma \leq 3.0$ MeV
- Often used for detector calibration
Annihilation radiation

- Positron and electron emission, and subsequent absorption to produce two oppositely directed 0.511 MeV photons
- eg. Na-22 produces both 0.511 and 1.274 MeV photons

2.6019 Yr. $^{22}\text{Na}$ [C]

GAMMA-RAY ENERGIES AND INTENSITIES

<table>
<thead>
<tr>
<th>$E_{\gamma}$ (KeV)</th>
<th>$\Delta E_{\gamma}$</th>
<th>$I_{\gamma}$ (rel)</th>
<th>$I_{\gamma}$ (%)</th>
<th>$\Delta I_{\gamma}$</th>
<th>$S$</th>
</tr>
</thead>
<tbody>
<tr>
<td>511.006</td>
<td>± 0.008</td>
<td>100</td>
<td>170</td>
<td>± 1.0</td>
<td>1</td>
</tr>
<tr>
<td>1274.537</td>
<td>± 0.008</td>
<td>62.2</td>
<td>99.94</td>
<td>± 0.01</td>
<td>1</td>
</tr>
</tbody>
</table>
Bremsstrahlung

- Created by fast electrons interacting in matter
- Increases with electron energy and absorbing materials of high atomic number
- Used in conventional x-ray tubes
- Energy spectrum is a continuum of photon energies
- Normally, cannot be used directly to calibrate radiation detectors
Characteristic X-rays

- Disruption of orbital electrons can cause shift in electron structure
- X-ray released that is characteristic of element - photon energy is related to electron’s binding energy
- example: vacancy created in K shell of atom, will release a characteristic K x-ray when vacancy is filled.
  - If electron from L shell fills vacancy, $K_\alpha$ photon is produced.
  - If electron from M shell fills vacancy, $K_\beta$ photon is produced
- K series X-rays most practical. Energy increases with atomic number ranging from few keV to 100 keV.
- L series does not reach 1 keV until $Z=28$ and is 10 keV at $Z=74$. 
Characteristic X-rays (continued)

- Other nuclear process leading to characteristic X-rays
  - Electron capture by nucleus or internal conversion resulting in disruption of electron orbital structure
  - Auger electron competes with characteristic X-rays.

- Typical radioisotope sources:
  - Ca-41 3.69 keV (K_α_)
  - Ti-44 4.508 keV (K_α_)
  - Fe-55 5.895 keV (K_α_)

- Characteristic X-rays may be generated from external sources

- of ionizing radiation (X-rays, electrons, alpha particles, ... (eg. external source is X-rays – called x-ray fluorescence)
Detection of gamma-rays is dependent on causing interaction with matter that transfers all/part of photon energy to electron in absorbing material.

Each process leads to partial/complete transfer of gamma-ray photon energy to electron energy.

Electron energy deposited is the value collected/tabulated in gamma-ray radiation detection.
Interaction mechanisms of gamma-rays (continued)

- Three major types of photon interactions are dominant in radiation measurements

- 1. Photoelectric absorption
  - absorption where incident gamm-ray photon disappears.
  - photo electron produced from electron shell (usually K) of absorber with energy = photon incident energy
  - Auger electrons or characteristic X-rays emitted to due to liberation of photoelectron
  - additional low-energy electrons may be created (from binding energy of photoelectron)
  - Predominant reaction for low energy photons (few keV)
  - Spectrometers would show single peak corresponding to incident gamma-ray energy
Interaction mechanisms of gamma-rays (continued)

2. Incoherent scatter
   - (Compton) scatter, a photon collides with an atomic electron in absorbing material.
   - Photon transfers portion of energy to electron.
   - Predominant reaction for typical gamma-rays from radioisotopes.
   - Simplest assumption is that electron is unbound
   - Electron binding effects taken into account using form factors for specific materials to correct photon scattering angles and Doppler energy broadening to correct distribution of scattered photon energy
3. Pair production
   ▶ If gamma-ray energy $\leq 1.02$ Mev (2\times\text{electron rest mass}), pair production is possible.
   ▶ Predominant reaction for high energy gamma rays
   ▶ Gamma-ray photon disappears; replaced by electron-positron pair
   ▶ Excess kinetic energy (above 1.02 MeV) carried away by electron-positron pair
   ▶ Positron subsequently annihilate after slowing down in medium, releasing two photons as secondary products of pair production.
Interaction mechanisms of gamma-rays (continued)

![Graph: Relative importance of the three photon interaction mechanisms as a function of photon energy and atomic number of the absorbing material.]

- Photoelectric effect dominant
- Compton effect dominant
- Pair production dominant

\[ h\nu \text{ in MeV} \]

\[ Z \text{ of absorber} \]
Pulse-height spectra

- Radiation detectors set up to record each individual quantum of radiation that interacts in detector.
- The time-integrated burst of current (i.e. charge) from collection of electrons created is recorded.
- Charge directly related to gamma-ray energy deposited in detector (i.e. transferred to electrons in absorbing media and then collected).
- Common problem of high rates of energy deposition if time between adjacent events (pulses) becomes too short to distinguish or if current pulses from successive events overlap (aka pulse-pileup).
- Amplitudes of pulses measured from mono-energetic radiation source will differ due to inherent response of radiation detector.
Energy resolution (continued)

- Response to monoenergetic radiation source differs according to materials used in radiation detector.
- Pulse amplitudes differ due to response of individual detector.
- Idealized pulse-height spectra never seen (see figure).
- Resolution measured as FWHM/E_0.
- Most of fluctuations are due to random fluctuations in collection of charge (Poisson statistics apply).
- Usually described as Gaussian:

\[
G(E) = \frac{A}{\sigma \sqrt{2\pi}} \exp\left(-\frac{(E - E_0)^2}{2\sigma^2}\right)
\]

\[
FWHM = 2.35\sigma
\]
Interaction mechanisms of gamma-rays (continued)

Photoelectric effect + Compton Scatter + Pair Production

\[ E_e + E_p = h\nu - 2m_0c^2 \]
Interaction mechanisms of gamma-rays (continued)

- Compton ‘edge’ ($\theta = \pi$)
- Photopeak
- Compton continuum

Energy distribution:
- $N(E)\,\text{d}E$
- $E=h\nu$
- Compton 'edge'

Energies:
- $h\nu \approx 2m_0c^2$
- "Double escape" peak
- "Photopeak, or full-energy peak"

Counts:
- $dN/dE$
Fig. 15. Detector Response Function Features of a Ge Detector for Gamma Rays: (1) flat continuum, (2) exponential tail, (3) Gaussian full energy peak, (4) Compton single scatter continuum and sum of all Compton scatters, (5) Compton double scatter and triple scatter and sum of all Compton scatters, (6) single annihilation photon escape peak, (7) double annihilation photon escape peak, and (8) Compton scatter continuum of one annihilation photon.
Gaussian Pulse-heights

\[ y_0 e^{-\frac{(x - x_0)^2}{b_0}} \]

![Graph showing Gaussian fit to experimental photopeak of Cs137 (0.662 MeV) showing deviation from functional.](image)
DETECTION EFFICIENCY

- Uncharged radiation must undergo significant interaction before detection.
- Large ranges compared to detector dimensions
- Must relate pulses counted to number of incident photons
- Detector with known efficiency can be used to measure absolute activity of radiation source
  - Absolute efficiency
  - defined as: \[ \frac{\text{number of pulses recorded}}{\text{number of particles emitted by source}} \]
Intrinsic efficiency

- defined as \( \frac{\text{number of pulses recorded}}{\text{number particles incident on detector}} \)
- depends on details of counting geometry (source-to-detector distance), detector material, source energy

\[ \epsilon_{\text{intrinsic}} = \epsilon_{\text{abs}} \times \left( \frac{4\pi}{\Omega} \right), \]
\( \Omega = \text{solid angle of detector seen from source.} \)

- Usually, experimenters require pulses larger than defined minimum.
- Peak efficiencies examine interactions that deposit full energy of incident radiation
Outline

Introduction

Radiation Detection Physics

Sources of electromagnetic (gamma-ray) radiation

Interaction mechanisms of gamma-rays

Pulse-height spectra

Monte Carlo Simulation of Radiation Detectors

MCNP Features useful in radiation detection

MCNP F8 Tally

Comparisons of Calculations and Experiment

Deviations from ideal response

Benchmark measurements

Comparison of Experimental Results with MCNP

Benchmark HPGe Detector Measurements

Illustration of Peak-to-total Ratio concept for NaI pulse-height spectrum.
Intrinsic efficiency

- Absolute source activity related to peak efficiency:
  - \( S = N4\pi/\varepsilon_ip\Omega \)
  - \( S \) = source intensity, \( N \) = number of events under full peak
  - \( \Omega \) = solid angle subtended by detector at source position
  - \( = \int (\cos(\alpha)/r^2dArea) \)
  - \( = 2\pi(1 - d/\sqrt{d^2 + a^2}) \) for point source
Workshop on Basic Radiation Detection and Simulation with MCNP
Avneet Sood

Outline
Introduction
Radiation Detection Physics
Sources of electromagnetic (gamma-ray) radiation
Interaction mechanisms of gamma-rays
Pulse-height spectra
Monte Carlo Simulation of Radiation Detectors
MCNP Features useful in radiation detection
MCNP F8 Tally
Comparisons of Calculations and Experiment
Deviations from ideal response
Benchmark measurements
Comparison of Experimental Results with MCNP
Benchmark HPGe Detector Measurements

Fig. 25 - Expression for calculation of detector efficiency for point source of radiation and cylindrical detector.

Fig. 26 - Expression for calculation of detector efficiency for disk source of radiation and cylindrical detector.
PART 2: Review useful MCNP features
Monte Carlo Simulation of Radiation Detectors

- Modeling radiation detectors requires simulating effect of a *collection* of particles - not an individual particle
- Monte Carlo simulation is ideal for simulating radiation detectors.
  - Continuous energy physics is critical to accurate simulation.
  - 3-D geometry modeling is important to simulate real-world radiation sources/detection
  - Description of almost any source of radiation
  - No approximation in modeling correct physics – if correct detail/level physics is used
  - Quantity recorded is energy deposited from primary source and all progeny during
  - Common sense approach...
Notes on MCNP

Outline

Introduction

Radiation Detection Physics
Sources of electromagnetic (gamma-ray) radiation
Interaction mechanisms of gamma-rays
Pulse-height spectra

Monte Carlo Simulation of Radiation Detectors

MCNP Features useful in radiation detection
MCNP F8 Tally

Comparisons of Calculations and Experiment
Deviations from ideal response
Benchmark measurements
Comparison of Experimental Results with MCNP
Benchmark HPGe Detector Measurements
Pulse Height Tally (F8)

- Energy distribution of pulses created in a cell models a physical detector
- Variance reduction should not be used when energy binning is used
- *F8 gives energy deposition tally (MeV)
- +F8 gives charge deposition tally (charge)
What is a Pulse Height Tally (PHT)?

Flux Tally: Each track scores a different $E$

PHT: Tally pulse energy from HISTORY

\[ E_{\text{in}_1} + E_{\text{in}_2} - E_{\text{out}_1} \]
Photon Physics

• Cross-Section Libraries
• PHYS:P
• Simple / Detailed Photon Physics
• Electron Production at Photon Collisions
• Photon Approximations
• Photonuclear Data and Physics
Photon Physics

- Storm and Israel, ENDF, EPDL
- Coherent (Thomson) scattering + Form Factors
- Incoherent (Compton) Scattering + Form Factors
- Pair Production
- Photoelectric Absorption and Fluorescence
- Thick-Target Bremsstrahlung
Four photon cross-section libraries are currently available for MCNP.

1. **MCPLIB**
   - based largely on ENDF/B-IV (supplemented by Storm and Israel)
   - ZAIDs end in .01p
   - photon energy ranges from 1 keV to 100 MeV (15 MeV for 7 elements)
   - data provided for Z=1 through Z=94

2. **MCPLIB02**
   - data from MCPLIB extended to 100 GeV based on EPDL
   - ZAIDs end in .02p
   - data provided for Z=1 through Z=94

MCNP will convert any isotopic ZAIDs found on material cards to elemental before searching for photoatomic cross-section tables. For example:

```
M1 92235.60c 1
```

will result in MCNP searching for ZAID=92000.xxp if photons are being transported.
Two new photon cross-section libraries are available in the new data release.

3. MCPLIB03
   - data from MCPLIB02 updated to include Compton Doppler energy broadening data
   - ZAIDs end in .03p
   - photon energy ranges from 1 keV to 100 GeV
   - data provided for Z=1 through Z=94

4. MCPLIB04
   - based on ENDF/B-VI Release 8 (EPDL97)
   - is current default
   - ZAIDs end in .04p
   - data provided for Z=1 through Z=100
   - includes new Compton Doppler energy broadening data
   - updated fluorescence data (MCNP uses K-shell and average L-shell fluorescence)

Future plans for photoatomic / electron data
   - update libraries with new shell-wise data
   - improve atomic relaxation sampling
PHYS:P  EMCPF IDES NOCOH PNINT NODOP

- **EMCPF** = simple physics if $E > \text{EMCPF}$
  
  Default: 100 MeV

- **IDES** = 0/1 = TTB or electron transport/turn off electron production

  Default: 0

- **NOCOH** = 0/1 = on/off coherent scatter

  Default: 0

- **PNINT** = -1/0/1 = analog photonuclear interactions turned on/photonuclear physics turned off/biased photonuclear interactions turned on

  Default: 0

- **NODOP** = 0/1 = on/off doppler energy broadening

  Default: 0
# Simple vs. Detailed Photon Physics

<table>
<thead>
<tr>
<th>Simple</th>
<th>Detailed</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ignores coherent scattering</td>
<td>Coherent scattering with form factors (ignored if NOCOH=1)</td>
</tr>
<tr>
<td>Compton scattering on free electron</td>
<td>Compton scattering with incoherent form factors</td>
</tr>
<tr>
<td>Photoelectric effect is pure absorption modeled by implicit capture</td>
<td>Photoelectric effect is analog absorption plus possible K and L-shell fluorescence</td>
</tr>
</tbody>
</table>

Pair production is modeled the same way in simple and detailed treatments

Detailed physics is recommended for most applications, particularly for high Z nuclides, low energy photons, and deep penetration problems.
## Electron Production at Photon Collisions

<table>
<thead>
<tr>
<th>Mode</th>
<th>Description</th>
<th>Mode P (w/o TTB)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Coherent</td>
<td>No electrons</td>
<td>No electrons</td>
</tr>
<tr>
<td>Incoherent</td>
<td>Electron produced and transported</td>
<td>Electron energy deposited</td>
</tr>
<tr>
<td>Photoelectric</td>
<td>Electron(s) produced and transported</td>
<td>Electron energy deposited</td>
</tr>
<tr>
<td>Pair Prod.</td>
<td>Electron and positron produced and transported</td>
<td>Electron energy deposited; two 0.511 MeV photons created and transported</td>
</tr>
</tbody>
</table>
Thick-Target Bremsstrahlung

- Electrons generated, then immediately generate bremsstrahlung photons without transporting electrons
- Eliminates expensive electron transport
- Is default, for mode p. Consider turning off TTB if bremsstrahlung unimportant; consider transporting electrons (mode p e) if bremsstrahlung is important
Comparison of Computer Times

(SGI 2000; Demo Problem, Ch. 5 MCNP Manual with NPS 104,000)

• MODE P, TTB off: 0.10 cpu minutes
• MODE P, TTB on: 0.14 cpu minutes
• MODE P E: 27.28 cpu minutes
## Electron Production at Photon Collisions

<table>
<thead>
<tr>
<th></th>
<th>MODE P E</th>
<th>MODE P (w/ TTB)</th>
<th>MODE P (w/o TTB)</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Coherent</strong></td>
<td>No electrons</td>
<td>No electrons</td>
<td>No electrons</td>
</tr>
<tr>
<td><strong>Incoherent</strong></td>
<td>Electron produced and</td>
<td>Electron produced; TTB photon(s)</td>
<td>Electron energy deposited</td>
</tr>
<tr>
<td></td>
<td>transported</td>
<td>transported</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>Electron energy deposited</td>
<td></td>
</tr>
<tr>
<td><strong>Photoelectric</strong></td>
<td>Electron(s) produced</td>
<td>Electron(s) produced; TTB photon(s)</td>
<td>Electron energy deposited</td>
</tr>
<tr>
<td></td>
<td>and transported</td>
<td>transported</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>Electron energy deposited</td>
<td></td>
</tr>
<tr>
<td><strong>Pair Prod.</strong></td>
<td>Electron and positron</td>
<td>Electron and positron produced</td>
<td>Electron energy deposited</td>
</tr>
<tr>
<td></td>
<td>produced and transported</td>
<td>produced; TTB photon(s) transported</td>
<td>two 0.511 MeV photons created and transported</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Major Photon Physics Approximations in MCNP

- Only K,L edges treated for photoelectric absorption
- Thick-target bremsstrahlung is the default
- No distinction between pair and triplet production
Doppler Energy Broadening for Photons

- Incoherent photon scattering can occur with a bound electron and generate a Compton electron and a scattered photon
  - The electron binding effect becomes increasingly important for incident photon energies less than 1 MeV
- The bound-electron effect on the angular distribution of the scattered photon appears as a reduction of the total scattering cross section in the forward direction
  - This effect has been accounted for in MCNP by modifying the Klein-Nishina cross section with a form factor
- The bound-electron effect on the energy distribution of the scattered photon appears as a broadening of the energy spectrum due to the pre-collision momentum of the electron
  - This second effect is the definition of Doppler energy broadening for incoherent photon scattering and is new in MCNP 5
Doppler Energy Broadening for Photons

![Graph showing Doppler broadening effects on a detector response to an 88 keV point source. The graph compares MCNP 5 and MCNP4C3 models. Notable features include the Doppler broadened Compton scattering peak.](image)
Cross Sections and Physics

- Introduction
- Neutron Physics
- Photon Physics
- Electron Physics
- Summary
Electron Physics

- Condensed History Algorithm
- Data Libraries
- PHYS:E and Electron Options
- Recent Electron Improvements
Condensed History Algorithm

An electron passing through matter will interact with each atom along its trajectory

- Energy loss from the electron to the media or to radiation
- Small deflections or scatterings along its path
- Production of secondary electrons or photons

The condensed history algorithm attempts to average the effect of all these interactions into aggregate quantities.

- The effect of many small deflections is a single scattering deflection in a substep due to the multiple-scattering theory of Goudsmit and Saunderson.
- The effect of energy loss is accounted for by a single energy loss modified for straggling in each step.
- A step is related to the average distance an electron traverses to lose a specified amount of energy.
$d_i$ = standard substep distance (a function of energy).

$\delta$ = partial substep distance. $\delta < d_i$.

$n$ = angular substeps per energy step (here $n = 2$).

$\Delta E_i$ from CSDA plus Landau straggling, for distance $n \times d_i$.

$\Delta \Omega_i$ from Goudsmit-Saunderson theory, for distance $d_i$. 

$\Delta E = (\Delta E_7/n)(\delta/d_7)$

Partial $\Delta \Omega$
Test Problem for new algorithm...

Three Equivalent Test Cases
10-MeV electrons on a 15-mm slab of water
No angular deflection. Substep = 1.364 mm

---

Diagram showing three equivalent test cases for a 10-MeV electron beam on a 15-mm slab of water, with no angular deflection. The substep size is 1.364 mm.
MCNP (bin-centered) Straggling Logic
10 MeV electrons after 15 mm water, no angular deflection

Number per MeV per Source Electron

Transmitted Electron Energy (MeV)
ITS (nearest-group-boundary) Straggling Logic
10 MeV electrons after 15 mm water, no angular deflection

Number per MeV per Source Electron

Transmitted Electron Energy (MeV)
Step-Specific Straggling Logic
10 MeV electrons after 15 mm water, no angular deflection

Number per MeV per Source Electron

Transmitted Electron Energy (MeV)

10^{-3}
10^{-2}
10^{-1}
10^{0}
10^{1}

15 mm cell
1 mm cells
0.1 mm cells
Electron Physics in MCNP

- Foundation is the condensed history method of Berger.
- Angular deflections from Goudsmit and Saunderson.
- Energy straggling from Landau, Blunck and Leisegang, Blunck and Westphal, and Seltzer. Model is equivalent to ITS 3.0.
- Density effect correction from prescription of Sternheimer, Berger, and Seltzer.
- Occupation numbers and atomic binding energies from Carlson.
- Bremsstrahlung cross sections from Berger and Seltzer.
- Riley cross sections and Mott / Rutherford cross sections.
- Moller cross sections for knock-on electrons.

(References provided in the MCNP5 manual)
Electron Data Libraries for MCNP

- Prior to MCNP4C, only one MCNP electron library has been available (EL1; ZAID’s ending in .01e).
- With MCNP4C, a second improved MCNP electron library is available (EL03; ZAID’s ending in .03e).
- Both contain elemental data for Z = 1 through Z = 94.
- Both contain data from E = 1 keV to E = 1 GeV.
- EL03 is part of the standard RSICC MCNP 4C cross-section distribution.
- Users cannot mix .01e and .03e sets in the same MCNP4C problem.
- Several MCNP4C electron physics improvements are only invoked when EL03 data are used.
- EL1 is roughly equivalent to the data used in ITS 1.0; EL03 is roughly equivalent to the data used in ITS 3.0.
Electron Data for MCNP

On libraries:

- energies
- radiative stopping power parameters
- bremsstrahlung production cross sections
- bremsstrahlung energy distributions (EL03 only)
- K-edge energies
- Auger electron production energies
- parameters for the evaluation of the Goudsmit-Saunderson theory for angular deflections
- atomic data of Carlson for density effect calculations (EL03 only)

Internally calculated:

- electron stopping powers and ranges
- K x-ray production probabilities
- knock-on probabilities
- bremsstrahlung angular distributions (EL1 only)
- data for Landau-Blunck-Leisegang theory of energy-loss fluctuations
PHYS:E   EMAX IDES IPHOT IBAD ISTRG BNUM XNUM RNOK ENUM

- EMAX = upper limit for electron energy (100 MeV)
- IDES = 0/1 = on/off electron production from photons
- IPHOT = 0/1 = on/off photon production from electrons
- IBAD = 0/1 = detailed/simple bremsstrahlung production
- ISTRG = 0/1 = straggling/expected-value electron energy loss
- BNUM ≥ 0; scaling of bremsstrahlung photons (1.0)
- XNUM ≥ 0; scaling of electron-induced x-rays (1.0)
- RNOK ≥ 0; scaling of knock-on electrons (1.0)
- ENUM ≥ 0; scaling of photon-induced electrons (1.0)
- NUMB = 0/1 = on/off substep bremsstrahlung production
Improvements in Electron Transport

Data-related improvements:

• Radiative stopping powers
• Density effect corrections
• Electron-induced X-rays
• Bremsstrahlung production
• Variance reduction

These improvements require the use of EL03 data libraries.

Detailed Landau Straggling logic:

• Selected by setting DBCN(18) = 2
PART 3: Comparisons with MCNP calculations and benchmark experiments
Theoretical electron energy distribution (single events) for Compton and photoelectric interaction in a NaI detector compared with an experimental pulse-height distribution obtained on a 3”x3” NaI detector (0.50 MeV).
Deviations from ideal response

- Low energy losses in detector
  - electron escape
  - bremmstrahlung escape
  - characteristic escape

- Non-ideal source
  - additional radiation created from source
  - Bremstrahlung - superimposes on gamma-ray spectrum
  - Annihilation
Deviations from ideal response (continued)

- **Surrounding materials**
  - Backscatter peak - Compton scattering first in surrounding material with subsequent detection
  - Characteristic X-ray - create in surrounding material
  - Annihilation peak - PP in surrounding materials create annihilation photons at 0.511 MeV that are subsequently detected

- **Summation effects**
  - Decay often produced two or more gamma-rays from same source (eg. Co-60)
  - Radioisotope often emits multiple cascades of gamma rays
  - Possible for both gamma-rays to interact and deposit all energy within resolving time of detector/electronics
  - Summation peak is observed if frequency is often enough
Possible events in NaI Detector

Illustration representing a NaI scintillation detector showing sequence of events producing output from electron multiplier and various processes which contribute to the response of a detector to a gamma-ray source.
Influence of surrounding materials

[Diagram showing radiation detection processes]

- Source
- Detector
- Photoelectric absorption
- Characteristic X-ray
- Compton scattering
- Pair prod.
- Annihilation photons

[Graph showing pulse-height spectra]

1. X-ray peak
2. Backscatter peak
3. Annihilation peak

Workshop on Basic Radiation Detection and Simulation with MCNP
Avneet Sood

Outline
Introduction
Radiation Detection Physics
Sources of electromagnetic (gamma-ray) radiation
Interaction mechanisms of gamma-rays
Pulse-height spectra
Monte Carlo Simulation of Radiation Detectors
MCNP Features useful in radiation detection
MCNP F8 Tally
Comparisons of Calculations and Experiment
Deviations from ideal response
Benchmark measurements
Comparison of Experimental Results with MCNP
Benchmark HPGe Detector Measurements
Gaussian Broadening

**Background**

Comparison of *calculated* and *measured* \(\gamma\)-ray spectra is complicated by finite resolution of real-world detector

- **Measurement:** mono-energetic source appears as Gaussian shaped peak at source energy
- **Calculation:** mono-energetic source appears as a point (without broadening) at source energy

**Lack of broadening continues for each energy bin of simulated spectra**
Comparison of Calculated and Measured Spectra

Comparison of Calculated and Experimental $\gamma$-Spectra for NaI3x3: Cs-137

Heath Original
MCNP

Normalized Yield

Energy (MeV)

Comparison of Calculated and Measured $\gamma$-Spectra for NaI3x3: Cs-137
Heath Original
MCNP

Deviations from ideal response
Benchmark measurements
Comparison of Experimental Results with MCNP
Benchmark HPGe Detector Measurements
Background (contd.)

- Spectrum broadening is attributed to scintillation process, detector nonlinearity, electronics, etc, and is characteristic to each detector system.
- Thus every detector’s resolution must be characterized using well-known sources.
- Spectrum broadening is *NOT* part of normal particle transport calculation, but can be included as part of the detector simulation.
MCNP Simulation of Gaussian Broadening

- Treated as a 'special tally treatment'. User requests this feature and provides input on shape of Gaussian:

\[
FWMH = a + b(E + cE^2)^{1/2}, \quad E \text{ in MeV}
\]

User supplies values for \(a\), \(b\), and \(c\). \(E\) is energy in MeV

- MCNP changes energy of incident particle (and all progeny) at end of particle history – just before it is tallied

- Randomly samples energy to be deposited from a Gaussian distribution centered on original particles’ energy

- Process is repeated for every history
MCNP Simulation of Gaussian Broadening

- Approach provides a more and more accurate pulse height distribution as number of histories increases
- Exact for an infinite number of histories
Benchmark measurements

- Gamma-ray spectrum catalogue by R.L. Heath (1964)
  - Benchmark quality experiments performed to minimize X-ray escape, scatter from surrounding material, annihilation, summation, etc
  - NaI Detectors and HPGe detectors
  - Not Widely known???
  - Experimental data not widely available...
Heath Detector Shield

Detector Shield used by Heath

Fig. 42 - Standard laboratory detector shield used for experimental measurement of all spectra in the Spectrum Catalogue.
Sample NaI spectra from Heath Catalogue

**Mn-54**

314 day Mn 54
3" x 3" - 2 No 1
1-26-62
ABSORBER 1.18 g/cm² Be
SOURCE DIST. 10 cm (r)
ENERGY SCALE 1 keV/PHU(Ch)
Sample NaI spectra from Heath Catalogue

Cs-137

30.07 yr. $^{137}\text{Cs}$ [C]

Be K X-Ray

30 yr. Cs$^{137}$

3" x 3" - 2 Na I

7 - 9 - 63

ABSORBER 1.19 g/cm$^2$ Be

SOURCE DIST. 10 cm (c)

ENERGY SCALE 1 KeV/PHU(Cs)

Backscatter

PULSE HEIGHT

NE $\times$ E/CHANNEL

10$^2$ 10$^3$ 10$^4$ 10$^5$
Sample NaI spectra from Heath Catalogue

Co-60

5.24 yr. Co$^{60}$
3''x3''-2 NaI
9-2-57
ABSORBER 200 mg/cm$^2$
SOURCE DIST.-0.3 cm
ENERGY SCALE 4 keV/PHU

Decay Data

Sum Peak

Pulse Height
Sample NaI spectra from Heath Catalogue

**Na-22**

- 2.6 yr. \( \text{Na}^{22} \)
- 3” x 3” - 2 No 1
- e - 3.63
- **ARShORBER** 1.1B g/cm² Be + 0.1B g/Sc Sandwich
- **SOURCE** DIT: 10 cm (c)
- **ENERGY SCALE** 1 keV/PHI/Ch

**Energy Peaks:**
- 1.274 keV
- Sum (0.51 + 1.27) keV
- Pulse Height
Comparison of Experimental Results with MCNP: NaI

NaI 3 x 3: CS-137

Comparison of MCNP Models of Heath Experiment for NaI3x3: CS137

MCNP Normalized Yield

Comparison of MCNP Models of Heath Experiment for NaI3x3: CS137
MCNP pe
MCNP p
Heath Original
Comparison of Experimental Results with MCNP: NaI

NaI 3 x 3: CO-60

Comparison of MCNP Model of Heath Experiment for NaI3x3: CO60

- MCNP pe
- Heath Original

Energy (MeV)

MCNP Normalized Yield
Comparison of Experimental Results with MCNP: NaI

**NaI 3 x 3: NA-22**

Comparison of MCNP Model of Heath Experiment for NaI3x3: NA22

- **MCNP Normalized Yield**

<table>
<thead>
<tr>
<th>Energy (MeV)</th>
<th>MCNP pe</th>
<th>Heath Original</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.5</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1.5</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2.5</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**MCNP pe**

**Heath Original**
Similar Benchmark experiments carried out for HPGe detectors
Sample HPGe spectra from Heath Catalogue

HPGe: MN-54

- Anomalous data point
- \(^{54}\text{Mn}\) (312 day)
- 10-16-71
- 55cm\(^3\) coaxial Ge(Li)
- No absorber
- 10 cm
- 25-54-1
Sample HPGe spectra from Heath Catalogue

HPGe: Cs-137

Table of Contents
Sample HPGe spectra from Heath Catalogue

**HPGe: Co-60**

- **Pb K x-rays**
- **DE 511-Ann.Rad.**
- **SE**

**Table of Contents**

- Introduction
- Radiation Detection Physics
  - Sources of electromagnetic (gamma-ray) radiation
  - Interaction mechanisms of gamma-rays
  - Pulse-height spectra
- Monte Carlo Simulation of Radiation Detectors
  - MCNP Features useful in radiation detection
  - MCNP F8 Tally
  - Comparisons of Calculations and Experiment
  - Deviations from ideal response
  - Benchmark measurements
  - Comparison of Experimental Results with MCNP
  - Benchmark HPGe Detector Measurements
Workshop on Basic Radiation Detection and Simulation with MCNP

Avneet Sood

Outline

Introduction

Radiation Detection Physics

Sources of electromagnetic (gamma-ray) radiation

Interaction mechanisms of gamma-rays

Pulse-height spectra

Monte Carlo Simulation of Radiation Detectors

MCNP Features useful in radiation detection

MCNP F8 Tally

Comparisons of Calculations and Experiment

Deviations from ideal response

Benchmark measurements

Comparison of Experimental Results with MCNP

Benchmark HPGe Detector Measurements

Sample NaI spectra from Heath Catalogue

HPGe: Na-22

Table of Contents
Comparison of Experimental Results with MCNP: HPGe

**HPGe: CS-137**

Comparison of MCNP Models for HPGe: Cs−137

![Graph showing comparison of MCNP Models for HPGe: Cs−137](chart.png)
Differences in Experimental and Calculated Results

- Many important detector characteristics are not known
- Many features of interest cannot be simulated correctly
- Includes:
  - detector crystal dead-layers (semi-conductors)
  - crystal imperfections
  - charge collection
Example of unknowns in HPGe

X-ray of HPGe to determine crystal length
Differences in Experimental and Calculated Results

- Effects are on:
  - Flat continuum
  - Standard deviation of Gaussian resolution
  - "Exponential tail" features on photopeak
  - Non-linear light-collection (scintillators)
Some effects of unknowns in NaI

Example of non-linear light collection


![Graph showing Monte Carlo non-linear spread spectrum (--) versus Heath experiment (---) for $^{24}$Na.](image)

Fig. 5. Monte Carlo non-linear spread spectrum (--) versus Heath experiment (---) for $^{24}$Na.
Some effects of unknowns in NaI

Example of non-linear light collection

Fig. 1. Experiment versus model data for NaI non-linearity with electron energy.
Gamma-ray Spectrometry Simulation

Summary

- Accurate simulation of gamma-ray spectra is needed for real-world applications
- Monte Carlo simulation needs additional help to model unknown parameters
- Precise characterization of real-world radiation detector required
- More at ANS Summer Meeting, Reno, NV 2006...
References:

- Knoll, G.F. Radiation Detection and Measurement,