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Comparison of Geant 4, MCNP Simulation Codes of Studying Attenuation of Gamma rays through Biological Materials with XCOM and Experimental Data

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Abstract

Monte Carlo simulations have been carried out for studying mass attenuation coefficients for some vital biological materials (Blood, Bones, and Muscle) at different photon energies (59.5, 81.0, 356.5, 661.6, 1173.2 and 1332.5 keV). Appreciable variations are noted for attenuation coefficients by changing the photon energy and the chemical composition of the samples. The numerical simulations attenuation coefficients were compared with experimental data wherever possible and the XCOM theoretical data. The simulations show that the simulated mass attenuation coefficient values are very close to experimental values better than the other obtained theoretical data base for the same samples. The results indicate that MCNP and Geant4 simulation codes can be applied to estimate mass attenuation for various biological materials at different energies. Monte Carlo method may be employed to make additional calculations on the photon attenuation characteristics of different biological sample for unknown experimental data.

Keywords: Attenuation coefficient; Monte Carlo; Biological materials

Introduction

The use of X- and gamma-rays in various fields such as in medicine, industry and agriculture is increasing; however the leakage and scattering of these rays can be harmful for human-beings. The leaked radiation may possibly interact with human being involve directly handling the nuclear facilities or public living nearby it. An understanding of how vital human organs such as blood (whole), bones and soft tissues interact with radiation is essential in the development of radiation protection and dosimetry. As such, a better understanding of X-ray interaction with human organs is necessary [1-4].

The mass attenuation coefficient (μ/ρ) is a measure of gamma ray absorption or scattering capability of element, compound or per unit mass. It is the fundamental parameter to derive many other parameters of radiation interaction, shielding and dosimetric interests. An extensive data is available in literatures relevant to mass attenuation coefficient and scattering cross–section for almost all elements, compounds as well as mixtures. Most of the obtained experimental data are compared with the theoretical tabulations used by XCOM program [5].

Geant4 code is based on object-oriented programming and allows user to derive classes to describe the detector geometry, primary particle generator and physics processes models along electromagnetic, hadronic, and decay physics based on theory, materials and elements, experimental data or parameterizations. Most of physics processes models include multiple scattering, ionization, Bremsstrahlung, positron annihilation, photo-electric effect, Compton and Rayleigh scattering, pair production, synchrotron and transition radiation, Cherenkov effect, refraction, reflection, absorption, scintillation, fluorescence, and Auger electrons emission [6,7]. The Geant4 simulation toolkit covers a wide energy range starting from 250 eV to the TeV. The Geant4 simulation is modeling of the photon attenuation through materials in computer environment gives flexibility and ease of use, instead of performing an experimental determination of mass attenuation coefficient of different composite materials. Recently one attempt has been used for simulation of attenuation coefficients [8].

Monte Carlo simulation is found an effective tool to calculate radiation interaction parameters in different types of compounds and mixtures for shielding and energy deposition in human organs and tissues. MCNP is a general purpose Monte Carlo code for transport of neutrons, photons and electrons. The user can apply up to second order surfaces (boxes, ellipsoids, cones, etc.) and fourth order torii to build a 3D geometry which can be filled with materials of arbitrary composition and density. Point, surface or volume sources of radiation can be defined, from which the mentioned particles are emitted with user specified probability distributions for energy and direction. The code then simulates the particle tracks and interactions with the materials, according to probability density distributions [9]. In the present study, the program used is based on Monte Carlo N Particle transport (MCNP-4C) code developed by the Los Alamos National Laboratory. The main objectives of the present study were to test the validity of MCNP and Geant4 based Monte Carlo simulations to demonstrate its success in studying radiation interactions through some vital biological materials (Blood, Bones, and Muscles). The two codes were applied in calculating mass attenuation and compared with their experimental measurements and the theoretical data obtained by XCOM program.

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Monte Carlo Model and Simulations

MCNP simulation code

Monte Carlo simulation is a general purpose tool for study of interaction of X-, gamma, neutron and electrons with matter. It is based on the Monte Carlo method to solve the transport equation; furthermore, it can work on different modes of delivery that are capable to consider neutrons, electrons and photons, alone, or in pairs all three together. MCNP is a general-purpose, continuous-energy, generalized geometry, time-dependent, coupled neutron-photon-electron Monte Carlo transport code system. The MCNP-4C uses physics models for particle interactions and nuclear cross section libraries [10-12].

The simulated geometry consisted of a cubic model of 10×10×1 cm^3, the beam. The environment except the mentioned phantom was filled with the air. Finally, the cubic model was centered in an air sphere for variance reduction. Anything outside the air cube was considered void into which MCNP did not perform particle transport. Tally F2 was used to obtain MCNP-4C simulation data. This tally calculates flux in the cube sides for every source.

The MCNP source was modeled as a directional plane source in a vacuum. This source located at 10 cm away from the entry plane of the mentioned cube. The initial direction of gamma source was parallel to the beam axis. Simulations were performed with 100000 histories. All simulation data obtained by MCNP code were reported with less than 2% error.

Geant4 *simulation* code

The physics of Geant4 simulation depends on narrow beam geometry with the various photon energies. The experimental set-up of the simulation, consisting of a mono-energetic photon beam impinging on a sample is similar to earlier report for scintillation detectors [8]. The mass attenuation coefficients of investigated biological samples were determined by the transmission method according to Beer Lambert's law ($I = I_o e^{-\mu} m^x$), where I_0 and I are the incident and attenuated photon intensity, respectively, μ_m ($cm^2.g^{-1}$) is the mass attenuation coefficient and x is the thickness of the slab. The thickness of the target is optimized according to the energy of the incident beam, to avoid that all the photons are absorbed in the target or traverse the slab without interacting. The primary photons emerging unperturbed from the slab are counted. The energy range of incident photons varied between 1 keV and 100 GeV. Attenuation of photons is calculated by simulating all relevant physical processes and interactions before and after inserting the samples under investigation. Photon interactions include photo-electric effect, Compton scattering, pair production, Rayleigh scattering, and electrons interactions include Bremsstrahlung, multiple scattering and ionization. Atomic effects after photo-electric effect, as X-rays emission and Auger effect are included. So it is possible to have a vertex from photoelectric effect [13]. A good agreement between Geant4 model for electromagnetic processes and National Institute of Standards and Technologies (NIST) reference data has been reported recently [13]. This statistical analysis estimated quantitatively the compatibility of Geant4 electromagnetic models with reference data and highlighted the respective strengths. The Geant4 models are found in good agreement with the NIST reference data.

XCOM Software

The μ/ρ values of biological samples were calculated by mixture rule ($(\mu/\rho)_{composite} = \sum_i^n w_i(\mu/\rho)_i$) where w_i is the proportion by weight and $(\mu/\rho)_i$ is mass attenuation coefficient of the i[th] element by using XCOM (5). The uncertainties in μ/ρ values is about 1% for low-Z (1<Z<8) in Compton region (30 keV to 100 MeV). It can generate cross-sections and attenuation coefficients for elements, compounds or mixtures in the energy range between 1 keV and 100 GeV, in the form of total cross-sections and attenuation coefficients as well as partial cross-sections of the following processes: incoherent scattering, coherent scattering, photoelectric absorption and pair production in the field of the atomic nucleus and in the field of the atomic electrons. Below 30 keV energy, the uncertainties are as much as 5-10% because of correction to experiments for high-Z impurities and departure of Compton cross section from Klein-Nishina theory. Also above 100 MeV photon energy, uncertainties in μ/ρ values may be 5-10%. Uncertainties in photon energy absorption coefficient may be slightly greater values [14]. The gamma sources of photon energies above 5 keV are being used in medical, biological, industrial, radioactive source transportation and other shielding applications. Hence uncertainty in the result may not have any impact for practical applications.

Materials and Method

Experimental setup

The gamma ray spectrometry system consists of HPGe detector (Canberra model) coupled with analog digital converter (ADC), high voltage 5000 V with negative polarity and relative efficiency of 70%. Genie 2000 software (Canberra Industries, Meriden, USA) with analyzer cart was used to record the intensity of the incident and the transmitted gamma rays. Energy calibration of the system was done initially with ^{241}Am, ^{57}Co, ^{137}Cs, and ^{60}Co gamma ray point sources. Resolution (FWHM) of the system was 2.3 keV at 1332.5 keV gamma peaks of ^{60}Co point source kept at a distance of 10 cm in front of the detector face.

The detected spectra can be translated to ASCII and processed with custom-made programs based on ROOT. Automatic pulse shaping and pole-zero correction settings were used and the energy scale was calibrated using point radioactive sources. Incident and transmitted photons for each detector material were measured for sufficiently large fixed preset time to reduce statistical uncertainty. The measuring time is ranged from 5 to 10 min depending upon the photon energy and background noise. The background was counted in the same manner of measuring intensity of attenuated photons in the samples [8].

Gamma source

The sources were considered as planar ones with uniform distribution of radioactive material that emit gamma rays perpendicular to the front face of the shields. The emitted gamma rays were 59.5, 81.0, 356.5, 661.6, 1173.2 and 1332.5 keV photons emitted by ^{241}Am (2.78 GBq), ^{133}Ba (2.92 GBq), ^{137}Cs (3.14 GBq), and ^{60}Co (3.7 GBq) radioactive point source.

Checking uniformity

The uniformity of the measurements was checked by exposing different parts of samples to the incident gamma-ray beam. Stability and reproducibility of the procedure was tested before and after each run. The errors are attributed to the evaluation of the area under peaks, in the determination of the thickness of sample, the weighing of the sample, geometric factor, and intensity of the source, the systematic errors and the counting statistics.

Specification of materials

For specification of material in simulation, the user has to obtain the elemental composition of blood, bones, and muscles on the base of their chemical composition and weight percent. The percentages by weight of the different elements for the investigated samples are presented in Table 1 [15,16]

Gamma ray transmission factor

The physics of simulation depends on narrow beam geometry with the various photon energies. The experimental set-up of the simulation, consisting of a mono-energetic photon beam impinging on a slab of one of the selected materials, the mass attenuation coefficients of investigated biological samples are determined by the transmission method according to Beer Lambert's law ($I = I_o e^{-\mu} m^x$), where I_0 and I are the incident and attenuated photon intensity, respectively, μ_m ($cm^2.g^{-1}$) is the mass attenuation coefficient and x is the thickness of the slab. The thickness of the target is optimized according to the energy of the incident beam, to avoid that all the photons are absorbed in the target or traverse the slab without interacting. The primary photons emerging unperturbed from the slab are counted. The mass attenuation of photons for selected samples is calculated by simulating all relevant physical processes and interactions before and after inserting the investigated sample.

Results and Discussion

The mass attenuation coefficients of the biological samples were determined at 59.5, 81.0, 356.5, 661.6, 1173.2 and 1332.5 keV photons by using gamma transmission method. The experimental error was estimated by combining errors for the product of linear attenuation coefficient and thickness, density and thickness measurements in

Sample	Elemental Concentrations (% weight)
Blood	H(0.102), C(0.11), N(0.033), O(0.745), Na(0.001), P(0.001), S(0.002), Cl(0.003), K(0.002), Fe(0.001)
Bone	H(0.064), C(0.278), N(0.027), O(0.41), Mg(0.002), P(0.07), S(0.002), Ca(0.147)
Muscle	H(0.102), C(0.123), N(0.035), O(0.729), Na(8×10^{-4}), Mg(2×10^{-4})

Table 1: Chemical compositions of the investigated biological materials [15,16].

Energy (keV)	Mass attenuation coefficients (cm^2g^{-1})											
	Blood				Bone				Muscle			
	Simulation		XCOM	Exp.	Simulation		XCOM	Exp.	Simulation		XCOM	Exp.
	Geant 4	MCNP			Geant 4	MCNP			Geant4	MCNP		
59.5	0.199	0.19	0.206	0.19	0.276	0.252	0.278	0.24	0.2	0.189	0.206	0.19
81	0.191	0.172	0.182	0.16	0.197	0.192	0.207	0.19	0.187	0.171	0.187	0.17
356.5	0.111	0.109	0.11	0.1	0.1	0.105	0.107	0.09	0.098	0.109	0.11	0.09
661.6	0.088	0.084	0.085	0.08	0.081	0.081	0.082	0.07	0.081	0.084	0.085	0.08
1173.3	0.061	0.064	0.065	0.06	0.057	0.061	0.062	0.04	0.075	0.064	0.065	0.05
1332.5	0.057	0.06	0.066	0.06	0.061	0.057	0.058	0.05	0.055	0.06	0.061	0.05

Table 2: Calculated and measured mass attenuation coefficients of the some biological materials.

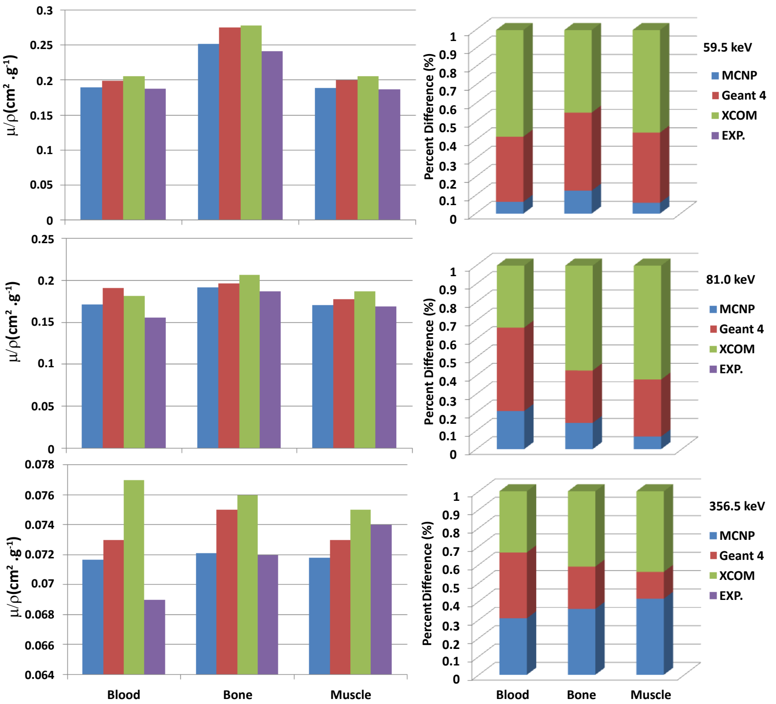

Figure 1: Mass attenuation calculated by MCNP, Geant4 and XCOM with respect to experiment according to relative deviation at 59.5, 81.0 and 356.5 keV in biological samples.

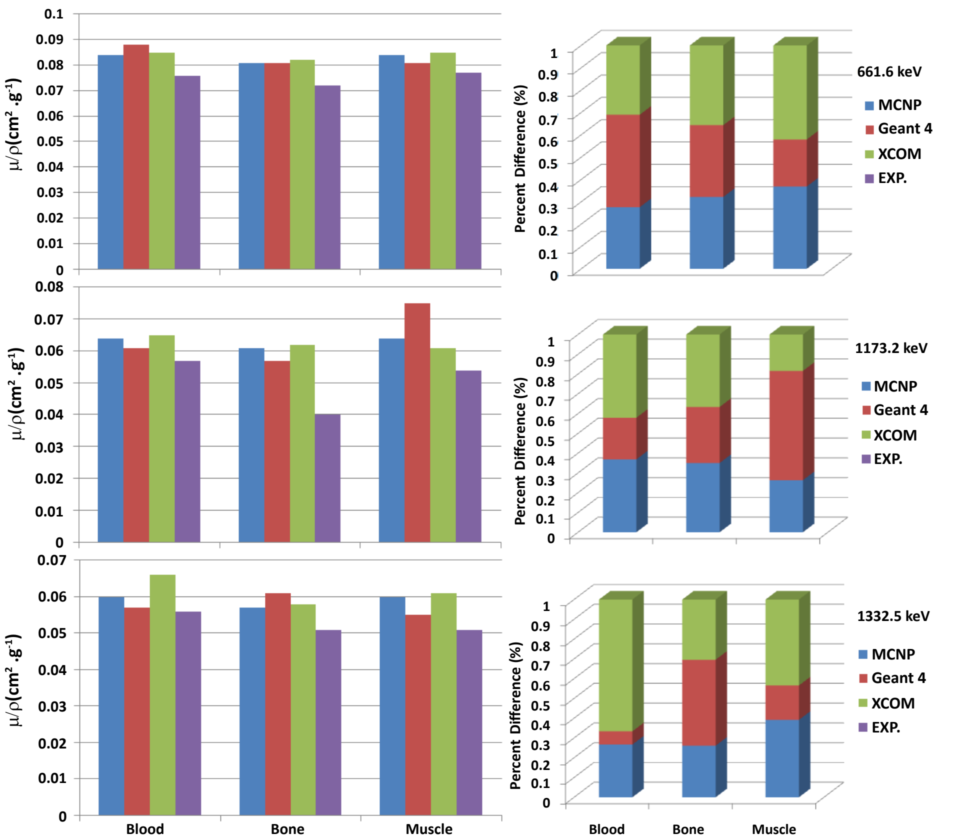

Figure 2: Mass attenuation calculated by MCNP, Geant4 and XCOM with respect to experiment according to relative deviation at 661.6, 1173.2 and 1332.5 keV in biological samples.

quadrature. Calculations of the mass attenuation coefficients of all investigated biological samples were carried out by the XCOM program.

The results of our presented Geant 4 and MCNP simulation were compared with the theoretical values obtained using XCOM database and the obtained experimental results are shown in Table 2.

It is clear that there is satisfactory agreement between experiment and theory, although the experimental values tend to be lower than the theoretical estimation. Discrepancy in the values of the calculated and the experimental mass attenuation coefficients could be due to deviations from narrow beam geometry in the source-detector arrangements. The percent difference parameter between the experimental and theoretical values are lower than the corresponding values of XCOM program at different photon energies as shown in Figures 1 and 2. It is clear from this figures that percent difference values of MCNP and Geant4 are lower than the corresponding values of XCOM for the different photon energies. The high values of XCOM return to the effect of chemical composition of biological samples and mixture rule. It is clear that the representative plot of the Monte Carlo generated data for mass attenuation coefficients as a function of incident photon energy and chemical composition. This trend was observed for each sample and this signifies that if we increase the energy of the incident photons we would obtain smaller attenuation, and therefore more penetration of the photons in the attenuator.

Conclusion

Monte Carlo simulation is a powerful tool in studying interaction of photons in materials. The applicability of this method is greatly dependent on the accuracy of geometry model, composition and density distribution of the sample matrix. The MCNP and Geant4 simulation were used to calculate mass attenuation coefficients of different wide types of materials in the 59.5-1332.5 keV photon energy range. The simulations show that the calculated values of mass attenuation coefficients of biological samples are close to experimental values better than the values obtained by XCOM data base. These results conclude that MCNP and Geant4 Monte Carlo simulations can be applied to estimate mass attenuation coefficients for various attenuator and energies for which experimental results are not available.

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