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Impact of photon cross section uncertainties on Monte Carlo-determined depth-dose distributions

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ABSTRACT

This work studies the impact of systematic uncertainties associated to interaction cross sections on depth dose curves determined by Monte Carlo simulations. The corresponding sensitivity factors are quantified by changing cross sections by a given amount and determining the variation in the dose. The influence of total and partial photon cross sections is addressed. Partial cross sections for Compton and Rayleigh scattering, photo-electric effect, and pair production have been accounted for. The PENELOPE code was used in all simulations. It was found that photon cross section sensitivity factors depend on depth. In addition, they are positive and negative for depths below and above an equilibrium depth, respectively. At this depth, sensitivity factors are null. The equilibrium depths found in this work agree very well with the mean free path of the corresponding incident photon energy. Using the sensitivity factors reported here, it is possible to estimate the impact of photon cross section uncertainties on the uncertainty of Monte Carlo-determined depth dose curves.

1. Introduction

MC simulations have been widely used in Medical Physics during the last two decades [1–3]. This method has been even used to calculate physical quantities that are very difficult to determine experimentally [4,5]. Based on the fact that this approach is used to simulate stochastic phenomena, quantities determined in these simulations have an intrinsic statistic uncertainty. This uncertainty is the only one reported in the vast majority of scientific articles in which MC simulations were used. Several works have addressed the impact of cross section uncertainties in the results of MC simulations, yet not all in a systematic way. Demarco et al. [6] used the MCNP4C MC code [7] to study the impact of different photon cross section sets on absorbed dose in water in the 10–1000 keV energy range. They compared the cross section libraries DLC-015 [8], DLC-146 [9] and DLC-200 (default of MCNP4C) to the XCOM compilation from the National Institute of Standard and Technology (NIST) [10]. The DLC-200 tabulation departs the most from the XCOM set. At 40 keV, there is an extreme underestimation of the absorbed dose at 1 cm from a point source determined with the DLC-200 set when compared to that obtained with the XCOM compilation. This seems to be caused by a corresponding underestimation of the photoelectric cross section (DLC-200.vs.XCOM), which is around 10%. Below 10 keV, the ratio between the DLC-200 and XCOM absorbed doses results in a diverging overestimation. A year later, Bohm et al. [11] benchmarked the MCNP/MCNPX MC code (see Ref. [12] and references there in) for the characterization of low energy brachytherapy sources (also ^{125}I and ^{103}Pd). They performed calculations using two cross section sets and reported on the consequent impact on the corresponding dose rate constants and radial dose functions. According to their results, differences of about 10% and 6% in the photoelectric and total cross sections in this energy range, respectively, lead to changes in the dose rate constant of 3% and 5%, and of 18% and 20% in the radial dose function for the ^{125}I and ^{103}Pd sources, respectively. Williamson and Rivard [13] carried out a more systematic work on uncertainty propagation during the determination of dosimetric parameters of brachytherapy sources by using Monte Carlo simulations. They proposed the following formula to account for systematic and statistical uncertainties of a given quantity (Y):

$$\%\sigma_Y = \sqrt{\%\sigma^2_{Y|\mu} + \%\sigma^2_{Y|geo} + \%\sigma^2_{Y|s}} \quad (1)$$

$$= \sqrt{\left(\%\frac{\partial Y}{\partial \mu}\right)^2 \%\sigma^2_{\mu} + \left(\%\frac{\partial Y}{\partial geo}\right)^2 \%\sigma^2_{geo} + \left(\%\frac{\partial Y}{\partial s}\right)^2 \%\sigma^2_{s}}, \quad (2)$$

where μ is the total attenuation coefficient, *geo* is a geometrical parameter and *s* is the statistical uncertainty associated to the MC

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simulation. Y can be any of the quantities of interest, such as the dose rate constant (Λ) and the radial dose function ($g(r)$). They used two cross section sets to estimate the corresponding sensitivity factor and obtained, for instance, $\%\partial\Lambda/\partial\mu = 0.68$.

Rogers and Kawrakow [14] published a work tackling the systematic uncertainty problem in MC simulations in a more consistent way. Specifically, they studied the sensitivity of several correction factors used in the Canadian air-kerma primary standard, to some influence parameters. These parameters were the MC code and transport algorithm, the ^{60}Co spectrum, the source diameter, and the source-chamber distance. More recently, Wulff et al. [15] studied the systematic uncertainties of ionization chamber quality correction factors (k_Q) determined by MC simulations. Various uncertainty sources were investigated, including geometrical factors and interaction cross sections. For photons, they scaled the corresponding cross section whereas for electrons, the mean excitation energy was varied as it is the main source of uncertainty for stopping powers. This way, sensitivity factors were found and combined with the corresponding estimated uncertainty to know how cross section uncertainties propagate to k_Q. In a similar work, Muir and Rogers [16] carried out a very detailed analysis on systematic uncertainty sources when determining the beam quality correction factors for ionization chambers (k_Q). They included items such as photon cross sections, electron stopping power, chamber dimensions, and photon spectra.

Recently, Ali et al. [17] used a very sophisticated statistical method to derive uncertainties of photon cross sections. This method was firstly applied to experimental and Monte Carlo simulated transmission factors for several megavoltage beams. Secondly, the approach was directly applied to experimental and theoretical (XCOM+IAEA set) photon interaction cross sections. Only graphite and lead materials were included in this study. Unfortunately, this method was not sensitive enough to resolve the energy dependence of the uncertainties in question. Thus, the authors reported energy-independent photon cross section uncertainties of 0.6% and 0.2% for graphite and lead, respectively (68% confidence), obtained from the comparison between experimental and simulated transmission curves. These uncertainties were 0.2% and 0.9% (68% confidence) for graphite and lead, respectively, when the method was directly applied to experimental and theoretical cross sections. For practical reasons, the authors recommend using an overall CS uncertainty of 0.5% (68% confidence) for photons with energies from 100 keV up to 40 MeV.

The uncertainties reported by Ali et al. [17] are lower than those previously estimated by the seminal compilation of Hubbell [19]. According to this review, photoeffect cross section uncertainties can be estimated as 2% and 1%–2% (68% confidence) for photons with energies of 5 keV–100 keV and 100 keV–10 MeV, respectively. In addition, Hubbell recommends an overall uncertainty for the total mass attenuation coefficient (μ/ρ) of the order of 1%–2% (68% confidence) for photon energies from 5 keV up to a few MeV.

One of the most important source of systematic uncertainty in MC simulations is interaction cross section. Besides the approach followed by Ali et al. [17], there are two other approaches for evaluating the impact of systematic uncertainties on a quantity determined by MC simulations. The first one varies the input quantity during simulation according to a given distribution and the corresponding variance. Namely, this quantity can be sampled during each MC step. A second simulation can be done by choosing the expected value of the same quantity, or its reference value, during each MC step. Then, the two corresponding final uncertainties can be compared and the influence of the systematic uncertainty on the quantity in question can be deconvoluted. This method could be regarded as a statistical or Type A evaluation of the uncertainty associated to a systematic effect. That is, the systematic effect of this quantity is converted into a random effect during its evaluation (see §3.3.3 of [18]). The second method is simpler. The input quantity is artificially scaled, let's say in ±5%. A long MC simulation would give back a negligible statistical uncertainty, then the sensitivity factor $\partial F/\partial X_i$ can be determined, where F is the quantity of interest and X_i is the influence variable. This factor can be used in conjunction with the known systematic uncertainty of X_i to calculate the contribution of this variable to the uncertainty of the quantity F. The latter approach was followed in current work.

A complete study of systematic uncertainties in MC simulations for the determination of absorbed dose distributions would involve several parameters, such as both differential and total interaction cross sections, material composition and density, geometrical factors, and so forth. The systematic study of electron CS must include all the transport parameters related to the history condensation algorithm. This algorithm and the associated controlling parameters are specific for each MC code. For these reasons, electron CS uncertainties were left out of the scope of this work. In this study, only the influence of total and partial photon cross sections on the central depth dose distribution of a primary photon beam is investigated. This influence is quantified trough the determination of the dose-to-CS sensitivity factors. The methodology used in current work is able to account for energy dependency of the dose-to-CS sensitivity factors. That is, the impact of photon CS uncertainty on dose uncertainty can be energy-resolved. The sensitivity factors reported here can be used in conjunction with CS uncertainties to quantify the corresponding systematic uncertainty of MC-determined absorbed dose. The basic geometry in our work is a photon beam impinging on a water phantom. Broad scattering conditions, as found in brachytherapy applications, are out of the scope of this work.

2. Methods

2.1. The PENELOPE code

PENELOPE is a Monte Carlo code for simulating coupled photon-electron transport in virtually any medium [20]. This code can handle the transport of photon, electrons, and positrons from about 1 GeV down to 50 eV. A mixed simulation strategy can be used to simulate electron and positron transport, in which part of the history of the charged particle is condensed and the other is treated in detail. In addition, the user can decide to follow every charged particle step-by-step, namely, in an analog simulation. PENELOPE is a well documented MC code with a relatively simple structure, which makes it suitable for our purposes in this study. On the one hand, C_1 and C_2 parameters control the mean free path between hard or catastrophic interactions in the mixed simulation algorithm. On the other hand, W_{cr} and W_{cc} represent the threshold energy for the creation of a secondary particle through radiative and collisional events, respectively. As in all MC code, photon (P_{abs}) and electron (E_{abs}) cutoff transport energies have to be defined.

2.2. Simulations settings

The user code PENMAIN was used in our simulations. In this case, the geometry is defined through an input file with extension .geo. The simulation geometry consists of a homogeneous water phantom with density of 1.0 g/cm^3. The front face of the phantom is covered with an air slab. Photons were the primary particles in all simulations, with energies of 20 keV, 100 keV, 1.25 MeV, 2 MeV, and 5.0 MeV. Pencil beams were used for all photon energies. In addition, 3×3 cm^2 normal and divergent beams were simulated only for ^{60}Co photons in order to explore possible effects of

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