A study of Type B uncertainties associated with the photoelectric effect in low-energy Monte Carlo simulations

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Abstract

Purpose. To estimate Type B uncertainties in absorbed-dose calculations arising from the different implementations in current state-of-the-art Monte Carlo (MC) codes of low-energy photon cross-sections (<200 keV). Methods. MC simulations are carried out using three codes widely used in the low-energy domain: PENELLOPE-2018, EGSnrc, and MCNP. Three dosimetry-relevant quantities are considered: mass energy-absorption coefficients for water, air, graphite, and their respective ratios; absorbed dose; and photon-fluence spectra. The absorbed dose and the photon-fluence spectra are scored in a spherical water phantom of 15 cm radius. Benchmark simulations using similar cross-sections have been performed. The differences observed between these quantities when different cross-sections are considered are taken to be a good estimator for the corresponding Type B uncertainties. Results. A conservative Type B uncertainty for the absorbed dose ($k = 2$) of 1.2%–1.7% (<50 keV), 0.6%–1.2% (50–100 keV), and 0.3% (100–200 keV) is estimated. The photon-fluence spectrum does not present clinically relevant differences that merit considering additional Type B uncertainties except for energies below 25 keV, where a Type B uncertainty of 0.5% is obtained. Below 30 keV, mass energy-absorption coefficients show Type B uncertainties ($k = 2$) of about 1.5% (water and air), and 2% (graphite), diminishing in all materials for larger energies and reaching values about 1% (40–50 keV) and 0.5% (50–75 keV). With respect to their ratios, the only significant Type B uncertainties are observed in the case of the water-to-graphite ratio for energies below 30 keV, being about 0.7% ($k = 2$). Conclusions. In contrast with the intermediate (about 300 keV) or high (about 1 MeV) energy domains, Type B uncertainties due to the different cross-sections implementation cannot be considered subdominant with respect to Type A uncertainties or even to other sources of Type B uncertainties (tally volume averaging, manufacturing tolerances, etc). Therefore, the values reported here should be accommodated within the uncertainty budget in low-energy photon dosimetry studies.

1. Introduction

Advanced algorithms for brachytherapy absorbed dose calculations in commercial treatment planning systems (TPSs) are becoming common. This situation opens an interesting and challenging scenario, where accuracy
improvements may be accompanied by departures from inter-clinic uniformity. In this context, a joint Working Group on Model-Based Dose Calculation Algorithms in Brachytherapy (WGDCAB) was created by the American Association of Physicists in Medicine (AAPM), the European Society for Radiotherapy and Oncology (ESTRO), and the Australasian Brachytherapy Group (ABG) to develop new methods and tools for standardized clinical commissioning. Specifically, the WGDCAB is charged with developing test case plans and engaging vendors to promote uniformity of clinical practices, building on the recommendations of the joint AAPM/ESTRO/ABG Task Group 186 report (Beaulieu et al 2012).

The first test cases delivered were made for $^{192}\text{Ir}$-based TPSs, a radionuclide with an average photon energy of about 350 keV (Perez-Calatayud et al 2012), where typical Type B uncertainties in the Monte Carlo (MC) simulations of less than 0.5% (Ballester et al 2015, Ma et al 2017) were reported. Since 2015, TPSs for brachytherapy applications in the energy range below 50 keV have been developed, e.g. electronic brachytherapy (Valdivieso–Casique et al 2015) and COMS eye plaques (Morrison et al 2018). Therefore, the WGDCAB has endeavored to generate test cases for these clinical sites using state-of-the-art MC simulations. Unfortunately, the relatively large uncertainties affecting some of the cross-sections involved below 100 keV may play a relevant, even dominant, role in the Type B uncertainty budget (Andreò et al 2012). At low photon energies, the photoelectric effect is the most important interaction in terms of the energy transferred to secondary electrons. For that reason, it is hardly surprising that different implementations of the photoelectric libraries in MC systems account for most of the differences observed between MC codes (Andreò et al 2012). In this regard, the possible use of Pratt’s renormalization screening approximation (PRSA) (Pratt 1960, Pratt et al 1973) has been extensively discussed in the literature (Selzer et al 2014, Sabattucci and Salvat 2016).

To explore these issues, Ye et al (2004) simulated the absorbed dose to water delivered by an isotropic point-like source emitting mono-energetic photon beams between 10 and 200 keV. The source was at the center of a cylindrical water phantom of 15 cm radius and 20 cm height. The simulations were performed with PENELOE-2001 and MCNP4 MC codes. MCNP4 used two different photon cross-section libraries, the DLC-200 and the DLC-146. These results were compared with those obtained with EG54 in Luxton and Jozsef (1999). The authors concluded that PENELOE-2001 presented a better agreement with MCNP4/DLC-146 (within Type A uncertainties of about 5%) than EG54, while MCNP4/DLC-200 showed significant differences between 10 keV and 60 keV and depths smaller than 6 cm.

Andreò et al (2012) carried out a systematic analysis of mass energy-absorption coefficients and their ratios for air, graphite, and water for photon energies between 1 keV and 2 MeV. Possible differences between NIST-XCOM (Hubbell and Seltzer 2004) and a modified PENELOE-2011 version incorporating PRSA in the photoelectric cross-sections were explored, reporting expanded uncertainties on the mass-absorption coefficients of about 2.5% for energies up to 30 keV, decreasing gradually to tenths of a percent for 100 keV. With respect to the water- to- air mass energy-absorption coefficient ratios, the uncertainties reported were almost negligible except in the energy region below 4 keV where they reach values up to 1%.

However, the use of the PRSA has been controversial due to inconclusive evidence regarding the agreement between calculated and measured cross-sections. The ICRU Report 90 (Selzer et al 2014) made a detailed technical and historical review of the photoelectric cross-sections calculations and their effect on the mass energy-transfer and mass energy-absorption coefficients. One of the main issues addressed is the use of PRSA. Although this correction was already included in the early 80s in some physical libraries, e.g. Hubbell and Gimmi (1980), it was deprecated shortly after because of worse agreement with experimental data for photon energies lower than 1 keV. PRSA libraries were also removed for energies above 1 keV despite the fact that there was no experimental evidence supporting it at that time. More recently, Buhr et al (2012) performed measurements of the mass energy-absorption coefficients in air, for energies between 3 and 60 keV, with uncertainties within 1% ($k = 2$). A better agreement between the experimental data and the calculated values was found when PRSA was considered. However, Kato et al (2010) carried out measurements of the mass attenuation coefficient in air for photons between 2 and 4 keV. The data reported in this publication, with uncertainties within 1% ($k = 2$), presents better agreement without PRSA. The ICRU Report 90 refrains from issuing any official recommendations in this regard.

Mainegra-Hing (2019) compared half-value layer (HVL) and air attenuation correction ($A_{att}$) of a free-air chamber measurements with their simulated values for beams between 10 and 80 kV. The simulations were performed with EGSnrc (Kawrakow et al 2019) using different physical libraries, including photoelectric cross-sections with and without PRSA. Without PRSA, maximum differences of 0.75% in $A_{att}$ (corresponding to a 25% difference in the air attenuation cross-section) and 35% in the HVL are reported. On the other hand, when PRSA is applied, the maximum differences reported are reduced to 0.3% and 8% for $A_{att}$ and HVL, respectively.

Basaglia et al (2020) took a different approach based on using different statistical metrics on the photoelectric cross-sections evaluated using different models. No dosimetry calculations were performed. The experimental data include elements up to $Z = 92$ and photon energies between 100 eV and 1 MeV. According to their analysis, EPDL97 (Cullen et al 1997) cross-section tabulations, based on Scofield calculations (Scofield 1973)
without PRSA, gave better agreement with respect to total and K-shell photoelectric experimental cross-sections. According to the authors, modern photoelectric libraries incorporating PRSA present statistically significant differences with respect to the experimental data. Therefore, there is a lack of consensus regarding the proper description of the photoelectric effect in MC simulations for medical physics. Hence, until this issue is resolved, any possible difference arising from them should be included in the Type B budget uncertainty. For this reason, the present work estimates these Type B uncertainties in absorbed dose, mass energy absorption coefficients, and fluence spectra. To do so, MC simulations are carried out using three state-of-the-art MC codes: PENELOPE, EGSnrc, and MCNP6 for a selected set of energies below 200 keV using a simple geometry commonly used in brachytherapy studies.

2. Material and methods

2.1. MC study

The simulations performed consist of the transport of ten mono-energetic photon beams (5, 10, 15, 35, 45, 55, 75, 100, 150, and 200 keV) emitted isotropically from a point-like source located at the center of a sphere of 15 cm in radius. Water has been recommended by the IAEA Code of Practice TRS-398 (Andreo et al. 2000) and AAPM TG-253 (Fulkerson et al. 2020) as the reference medium for low energy kV photon beams. Therefore, liquid water with the composition recommended by ICRU Report 37 (Berger et al. 1984) and the updated mean excitation energies (78 eV) and mass density (0.998 g cm$^{-3}$) given by ICRU Report 90 (Seltzer et al. 2014) is considered as the transport medium. The mean free path (MFP) in water for all the energies studied is shown in figure 1; therefore, full scatter conditions are expected for all energies at radii less than 10 cm (Perez-Calatayud et al. 2004).

The following observables are evaluated:

i. Mass energy-absorption coefficients in three different materials of interest in clinical dosimetry: water (same composition as the water phantom defined above), graphite (Seltzer et al. 2014), and standard dry air (Berger et al. 1984).

ii. Absorbed depth dose using spherical shells from $r = 0$ to $r = 5$ cm with a $\Delta r = 0.1$ cm grid. Due to the energies considered, charged particle equilibrium is guaranteed. Additionally, radiation yield is negligible, and therefore collisional kerma is scored as a surrogate for absorbed dose. For PEN18 this has been done by performing event-by-event analog simulations where electron transport has not been considered and its energy assumed to be deposited on the spot, i.e. an infinite energy cutoff for electrons is considered while retaining a 1 keV energy cutoff for photons. MCNP and EGSnrc consider the same energy cutoffs but collisional kerma is scored using a track-length estimator (Williamson 1987).
iii.Photon-fluence spectrum is obtained for 15 keV, 45 keV, 100 keV, and 200 keV at ¼, ½, and ¾ of their corresponding MFP depths (between 0.2 and 5.5 cm). They are scored in spherical shells with a thickness of \( \Delta r = 0.1 \text{ cm} \).

During the last decades, the standard for MC codes was the independent electron model based on the Dirac–Hartree–Fock–Slater (DHFS) self-consistent potential. This approximation considers a single electron in a central potential, interacting with a photon without taking into account the influence of the electrons in other orbitals. This approach facilitates the calculations, but it is expected to deliver less accurate results than a more elaborate atomic model such as multi-configuration Dirac–Fock (MCDF), which involves a non-local potential, different for each sub-shell. Those considerations complicate the calculations needed, making them unavailable for a MC simulation of a realistic experimental setup (Sabbatucci and Salvat 2016). To solve this problem, Pratt’s renormalization screening approximation is considered. This method corrects the DHFS cross-sections by the ratio of the electronic densities calculated with MCDF and DHFS at the limit when the radius tends to zero. All the MC systems discussed in this work use the independent electron model corrected or not by PRSA. For this reason, we adopt the following terminology: ‘DHFS’ is used to refer to all data obtained without the PRSA; ‘MCDF’ is used to refer to all data obtained using the PRSA. Results obtained with (MCDF) and without (DHFS) considering the PRSA are compared to illustrate the effect in the three quantities mentioned above of the photoelectric cross-section implementation. For that purpose, EGSnrc (DHFS), EGSnrc (MCDF), MCNP (DHFS), PENELOPE-2018 (DHFS), and PENELOPE-2018 (MCDF) simulations have been performed for all energies and observables.

2.2. MC codes

Three different MC codes have been used: (i) the PENELOPE-2018 MC system (henceforth denoted PEN18) (Salvat 2019) together with the penEasy v. 2019-09-21 code (Sempau et al. 2011), (ii) EGSnrc-2017 (Kawrakow et al. 2019) with egs_brachy-2017.10.02 (Chamberland et al. 2016) (EGSnrc in the following), and (iii) MCNP6 (version 1.0) henceforth denoted as MCNP (Goorley et al. 2012).

PENELOPE simulates electron and photon transport from 50 eV to 1 GeV, having been extensively used in the description of low energy phenomena. PEN18 obtains the photoelectric libraries from PHOTACS (Sabbatucci and Salvat 2016), a Fortran program that calculates subshell cross-section for arbitrary atomic potentials. PHOTACS uses the DHFS self-consistent potential supplemented by the Pratt’s renormalization screening approximation. The user can choose to exclude this correction (Salvat 2019).

The Rayleigh scattering cross-sections are calculated using non-relativistic perturbation theory, obtaining the atomic form factors from EPDL97 (Cullen et al. 1997). Compton interactions use the relativistic impulse approximation, which takes into account both binding effects and Doppler broadening (Ribberfors 1983). Furthermore, PEN18 explicitly simulates the emission of characteristic x-rays, Auger and Coster–Kronig electrons that result from vacancies produced in K, L, M, and N shells, using transition probabilities extracted from the Evaluated Atomic Data Library (EADL) (Perkins et al. 1991). The energy of the x-rays published in the EADL was updated, when available, with the K and L shell transitions from Deslattes et al. (2003), and the M shell transitions from Bearden (1967). Other transition energies are calculated from the energy eigenvalues of the DHFS equations for neutral atoms (Perkins et al. 1991).

EGSnrc is an MC toolkit for the simulation of the coupled transport of charged particles (\( e^- \) and \( e^+ \)) and photons in the energy range below 1 keV and 100 GeV in arbitrary media and geometries. Although a set of default transport and interaction parameters have been judiciously selected, users have great flexibility in choosing the physical models from different EGSnrc options or user-supplied data. Cross-sections from the NIST library XCOM (Berger et al. 2010) are used by default for photon interactions in the energy range of interest for brachytherapy, except for incoherent scattering which, to account for binding effects and Doppler broadening, is modeled according to the relativistic impulse approximation (Ribberfors 1975, Ribberfors and Berggren 1982) using shell-wise Hartree–Fock Compton profiles (Biggs et al. 1975). However, the use of total Compton cross-sections from the XCOM library or any user-supplied compilation can be requested via the input file. In its current default implementation, EGSnrc models the atomic photoelectric effect using unnormalized photoelectric cross-sections (Scofield 1973) by sampling interactions with the K and L shells followed by atomic relaxations using transition probabilities from the EADL library (Perkins et al. 1991). Initial vacancies beyond the LIII shell are not explicitly modeled, and the photo-electron receives the entire incident photon energy. This approach partially accounts for spreading out the binding energy of outer shells around the interaction point. EGSnrc has the option to use photoelectric cross-sections incorporating PRSA (Sabbatucci and Salvat 2016). If this option is selected, photoelectric interactions are sampled from any shell with binding energies above 1 keV. This effectively translates into interactions with all atomic shells out to NiV for Einsteinium (\( Z = 99 \)) for which the binding energy is around 1 keV. The user can also use the legacy
Timing

Dose to water, photon-fluence spectra, and \(\mu_{\text{eff}}/\rho\) values: on average 2 \times 10^{11} histories, 412 h (CPU time) per simulation.

Scored quantities

Absorbed dose calculated using collision kerma approximation, fluence, and energy spectrum calculations (Goorley et al. 2012; Chamberland et al. 2016)

Statistical uncertainties

History-by-history calculation of statistical uncertainties. \(\leq 0.1\% (k = 2)\)

Post-processing

None

implementation in which interactions with the K and L shells are sampled explicitly while interactions with the N and M shells are accounted for in an average manner (Kawrakow et al. 2019). Simulation of coherent scattering is based on the independent atom approximation whereby form factors for molecules are obtained from atomic form factors (Hubbell and Gimm 1980). The user can supply their custom atomic or molecular form factors for determining Rayleigh cross-sections. Users can switch from the default photon cross-sections to using the photon cross-sections from the EPDL97 library (Cullen et al. 1997) as well as from any other photon cross-section library as long as it follows the proper format and naming convention.

The MCNP6 radiation transport code (version 1.0) is a general purpose MC radiation transport code that tracks nearly all particles as well as photons and electrons at energies between 1 keV and 1 GeV for electrons, and 1 eV to 100 GeV for photons. Photon cross sections, form factors, and fluorescence data are all derived from the ENDF/B-VI.8 data library for photon energies down to 1 eV (Brown et al. 2015). In addition to extending some pre-existing data to lower energies, the ENDF/B-VI.8 databases also include subshell photoelectric cross sections. The photoelectron directions are obtained by means of an algorithm (Seltzer 1988) relying on precomputed tables based on work by Fischer and by Sauter (Fischer 1931, Sauter 1931).
Table 1 summarizes the details of the MC simulations performed in this work following the recommendation of AAPM TG-268 (Sechopoulos et al 2018).

2.3. Uncertainty evaluation

The standard protocol for evaluating uncertainties is the Guide to the expression of Uncertainties in Measurements (GUM) (Joint committee for guides in measurements 2008). This protocol supersedes the outdated terms of random and systematic errors (ill-defined and prone to confusions) in favor of Types A and B uncertainties. Type A uncertainties are those evaluated by the users by performing statistical analysis of their measurements. Type B uncertainties are those evaluated by any other means. Whichever the type of uncertainty, its evaluation is based on statistical distributions and, therefore, they should be quantified, if possible, in terms of their respective variances. For the former, MC simulations leading to mean values for dose to water and photon-fluence spectra allow us to obtain Type A uncertainties below 0.1% ($k = 2$) using standard history-by-history techniques (Walters et al 2002). For the second type of uncertainty, the GUM does not specify a unique protocol to determine it, offering to the user different possibilities for a given dataset based on its range of variation.

Different assumptions can be made depending on the amount of information available. If there is no specific knowledge about the possible values within an interval, one can only assume that it is equally probable for the true value to lie anywhere within it. That corresponds to a uniform or rectangular distribution described by the highest ($a_+$) and lowest ($a_-$) values obtained. In this case, the GUM gives the standard uncertainty ($k = 1$) as

$$
\sigma_B = \left| \frac{a_+ - a_-}{2} \right| \frac{1}{\sqrt{3}}. \tag{1}
$$

If more information regarding the true value location is known, other less restrictive alternatives, Gaussian, triangular, trapezoidal, etc, may be used. In this particular case, and due to the absence of further information on the distribution, we have preferred to use the more conservative option, i.e. larger uncertainties, namely to assume a uniform distribution limited by the results obtained using different MC physical libraries and equation (1) as a good estimator for Type B uncertainties (Andreo et al 2012).

3. Results

In the following, we present results for mass energy-absorption coefficients, absorbed dose, and photon fluence with (MCDF data) and without (DHFS data) PRSA. Type A uncertainties are less than 0.06% for all cases (the largest value for the range considered).
3.1. Mass energy-absorption coefficients

DHFS and MCDF mass energy-absorption coefficients have been evaluated using PEN18 for three materials of interest in clinical dosimetry (water, air, and graphite). The DHFS to MCDF ratios for PEN18 are shown in figure 2 (left). Differences between DHFS and MCDF mass energy-absorption coefficients exceeding Type A uncertainties can be observed in all three materials for energies lower than about 100 keV. The maximum differences observed are about 2.7% for air or water and about 4% for graphite. A detailed review of these differences can be found in table SM4 as supplementary material (available online at stacks.iop.org/PMB/66/105014/mmedia). For energies below 30 keV, Type B uncertainties about 1.5% \((k = 2)\) for water and air and 2% for graphite have been found. For energies between 40 and 50 keV, these uncertainties are reduced up to 1% \((k = 2)\), diminishing even further, less than 0.5% \((k = 2)\), for energies larger than 75 keV. In figure 2 (right), we show DHFS versus MCDF differences in the mass energy-absorption coefficients water-to-air and water-to-graphite ratios. Differences beyond Type A uncertainties are only observed for the mass energy-absorption coefficients water-to-graphite ratio. In the case of water-to-graphite ratio (see additional information in table SM5 in supplementary material), the only significant Type B uncertainties are observed for energies lower than 30 keV, being about 0.6%–0.9% \((k = 2)\).

3.2. Absorbed dose comparisons using similar photoelectric cross-sections implementations

Figure 3 shows the absorbed dose and their differences calculated with EGSnrc and PEN2018, using the DHFS photoelectric library, for monenergetic beams of 10, 45, 75, and 150 keV. The light yellow, green, and blue zones represent 1, 2, and 3 mean free paths, respectively. The dashed black lines represent the percentage differences found between both codes. Type A uncertainties are \(\leq 0.1\% (k = 2)\). Error bars are removed for clarity.
energies. Similar results (included in the supplementary material, table SM2) have been observed when comparing EGSnrc (MCDF) and PEN18 (MCDF) implementations. A complete discussion on maximum absorbed-dose differences with respect to PEN18 for each energy and depth is given as supplementary material.

3.3. Absorbed dose comparisons using different photoelectric cross-sections implementations

Figure 4 shows the absorbed dose simulated with different photoelectric cross-section implementations, DHFS versus MCDF, together with the differences observed. For energies below 15 keV, differences about 20%, 10%, and 5% can be observed at 10, 5, and 3 MFP, respectively. At depths smaller than 2 MFP, energies between 15 and 45 keV present maximum differences between 2% and 3%. Energies between 50 and 75 keV present maximum differences between 1% and 2% for all depths. Considering depths smaller than 2 MFP and the range of energies between 15 and 55 keV, the maximum difference is at 1 mm depth (see figure 4 for 45 keV). Finally, energies larger than 100 keV present differences lower than 0.5%. A complete report, including all energies and depths considered in this work, is included as supplementary material.

3.4. Photon-fluence spectra comparisons using similar photoelectric cross-sections implementations

Photon-fluence spectra for selected energies and MFP values are shown in figure 5 for MC codes implementing PRSA in their photoelectric cross-sections (MCDF). Differences have been evaluated as a weighted average, obtaining 0.2% (15 keV), 0.5% (45 keV), 0.3% (100 keV), and 0.1% (200 keV), hence mostly compatible with Type A uncertainties. Larger differences appear in the lowest energy regions and a set of discrete energies about 110, 75, 50, 35, and 12 keV. The latter might present maximum differences up to 15%. In both cases the photon-fluence spectra values are about four orders of magnitudes smaller than their maximum values; hence, these discrepancies are not expected to play any significant role in the determination of the absorbed dose.
3.5. Photon-fluence spectra comparisons using different photoelectric cross-section implementations

We compare in figure 6 photon-fluence spectra for some representative MFP values for MC codes implementing different photoelectric cross-sections, EGSnrc (DHFS) and PEN (MCDF). Differences have also been evaluated as a weighted average, being 0.9%, 0.7%, 0.3%, and 0.2% for initial photon energies of 15 keV, 45 keV, 100 keV, and 200 keV respectively. Differences larger than 5% arise for photon-fluence spectra values two orders of magnitude smaller than their maximum values, hence higher energies than in section 3.4. The same discrepancies at about 110, 75, 50, 35, and 12 keV are also present.

4. Discussion

As shown above, the maximum differences observed in the mass energy-absorption coefficients are about 2.7% for air or water and 4% for graphite. It would be expected that such differences translate into similar discrepancies when evaluating the absorbed dose. However, in low-energy x-ray beams dosimetry based on ionization chamber calibrations in terms of air kerma, the absorbed dose to water is determined from measurements made free-in-air (Ma et al 2001, Andreo 2019). To do such air-to-water transformation, the most relevant photon-related quantities are not the mass energy-transfer coefficients for air or graphite and water, but their ratio. In turn, in this energy range, these can be replaced without any approximation by the corresponding mass energy-absorption coefficients (Andreo 2019). The general trend observed is that differences are considerably reduced when ratios are considered. It can be observed in figure 2 (right) how, in the case of water-to-air mass energy-transfer coefficients ratio, no significant differences larger than Type A uncertainties are found. This is not the case for the water-to-graphite ratio, where differences of the order of 0.5% can still be observed for energies lower than 35 keV, reaching maximum differences of the order of 1%–1.5% for energies ≤20 keV. Therefore, only for ionization chamber dosimetry involving water-to-graphite corrections below, or...
Figure 6. Comparison of the Photon-fluence spectra simulated with EGSnrc (DHFS) and PENELOPE-2018 (MCDF) for monoenergetic beams of 15, 45, 100, and 200 keV. The dashed black lines represent the differences (code/PEN18–1, %) between both codes.

Figure 7. Comparison of the Photon-fluence spectra simulated with EGSnrc (MCDF) and PENELOPE-2018 (MCDF) for a monoenergetic beam of 200 keV at a depth of 0.25 × MFP. The dashed black lines represent the differences (code/PEN18–1, %) between both codes.
about, 35 keV a conservative 0.6%–0.9% value should be considered as Type B ($k = 2$) uncertainty for cross-sections.

When evaluating the photon-fluence spectra, type B uncertainties for initial photon energies lower than 25 keV can be estimated at 0.5% due to the maximum differences observed. The only discrepancies above 25 keV are observed at a set of discrete photon energies regardless of the cross-section used. We show in figure 7, an inset showing an example of these differences. They appear in all cases at the energies produced by Compton backscatter; namely, given an initial photon energy of 200 keV, a backscattered photon with an energy of 112.2 keV is produced. This one creates a backscattered photon with an energy of 77.9 keV, and iterating one end up with similar photons at 59.7 keV, 48.4 keV, 40.7 keV, etc. As expected, the relevance of such contributions diminishes both with depth (smaller differences at ½ MFP than at ¾ MFP) due to the reduced amount of backscatter material and with the number of interactions (the effect at 77.9 keV is more reduced than at 112.2 keV). As can be seen in figure 7, they are caused by a small redistribution of the fluence in a region of about 2–3 keV around the backscattered photon energies. These differences can be traced back to different approximations in the numerical implementation of the Compton scattering (Kawrakow et al 2019, Salvat 2019).

As discussed in section 2.1, collisional kerma is scored as a surrogate for absorbed dose. In doing so, the role played by the fluence spectra and the mass energy-absorption coefficients in the absorbed dose can be evaluated separately. With that purpose, we have evaluated the absorbed dose at 4 mm depth for a 15 keV beam (worst-case scenario), using the fluence-spectra simulated with EGSnrc (DHFS) and PEN18 (DHFS) and the same mass energy-absorption coefficient library from PEN18 (DHFS). The calculated absorbed doses differ by less than 0.04%. Therefore, the observed differences in the fluence spectra do not play any relevant clinical role. By repeating the same procedure but using different mass energy-absorption coefficient libraries, PEN18 (DHFS) and PEN18 (MCDF), the absorbed dose difference reaches a value of 2.6%, consistent with those reported in section 3.3.

Clinically relevant regions for photon-emitting sources below 200 keV can be restricted to distances closer than 1–3 cm. Hence, for the energy range studied here, these typically correspond to depths within 1–2 MFPs. For radionuclide based brachytherapy, Task Group 43 Report (Rivard et al 2004) established a reference distance, 1 cm from the center of the active source along its transverse plane, located within this region. In the case of electronic brachytherapy, the typical clinical prescription depth is about 0.3–0.5 cm (Ouhib et al 2015, Fulkerson et al 2020). Therefore, such distances are a fundamental location where any significant uncertainty is bound to have a global effect on a clinical plan. Absorbed dose benchmarking calculations using similar cross-sections show that differences below 3 MFP depths are mostly compatible with Type A uncertainties. When different implementations are considered (see tables SM3 and SM4 in supplementary material), energies

![Figure 8. Predicted Type B ($k = 2$) uncertainties (%) for $^{125}$I as a function of depth obtained with equation (2) and parameters showed in table 2.](image-url)
between 15 and 45 keV present maximum differences below 2 MFP of about 2%–3% in the absorbed dose, diminishing up to 1%–2% for 50–75 keV and 0.5% or less for 100 keV upwards. These differences are consistent with those observed for the mass energy-absorption coefficients discussed above, considering that no additional significant differences in the photon-fluence spectra above 25 keV, other than those already observed at the Compton backscattered energies, have been observed. Therefore, using the above-mentioned differences and equation (1), a conservative global maximum Type B uncertainty corresponding to the cross-section used of 1.2%–1.7% (<50 keV), 0.6%–1.2% (50–100 keV), and 0.3% (100–200 keV) should be considered in dosimetric calculations.

To help the clinical user in establishing a more detailed Type B uncertainty for the particular low energy photon spectra used, the Type B uncertainties reported in this work are fitted using an empirical functional form (see supplementary material for more details):

\[
u_eta(E, r) = |a \cdot E^b r^c + u_0|,\]

where energies are given in keV and depths in cm. The fit parameters \(a, b, c,\) and \(u_0\) are given in Table 2. This fit is valid for depths within 10 MFPs. As an illustrative example, we show in Figure 8 Type B \((k = 2)\) uncertainties as a function of depth for a typical \(^{125}\text{I}\) spectrum, a low-energy photon-emitting radionuclide widely used in clinical brachytherapy practice.

### Table 2. Parameters \(a, b, c,\) and \(u_0\) obtained from the fit using equation (2); energies in keV and distances in cm. The uncertainty estimates obtained from this fit should not be used beyond the range of fitted data.

| Parameter | Value | Range of energies (keV) |
|-----------|-------|------------------------|
| \(a\)     | \(-4.9227 \times 10^4\) | \(5 \leq E \leq 40\) |
| \(b\)     | \(-2.8559\) |                        |
| \(c\)     | \(0.90255\) |                        |
| \(u_0\)   | \(1.1725\) |                        |
| \(a\)     | \(-2.5808 \times 10^4\) | \(40 < E \leq 200\) |
| \(b\)     | \(1.8780 \times 10^{-4}\) |            |
| \(c\)     | \(2.7182 \times 10^{-5}\) |            |
| \(u_0\)   | \(2.5845 \times 10^4\) |            |

5. Conclusions

Type B \((k = 2)\) uncertainties of about 1.5% (air and water) and 2% (graphite) have been observed for the mass energy-absorption coefficients of dosimetrically relevant materials. However, such uncertainty becomes severely reduced in the case of the mass energy-absorption water-to-air ratio. Only in the case of ionization chamber dosimetry involving water-to-graphite corrections below 35 keV a conservative Type B \((k = 2)\) 0.6%–0.9% uncertainty should be considered. The differences observed in the photon-fluence spectra are either within Type A uncertainties or not clinically relevant; hence no additional Type B uncertainty is recommended in this case with the exception of energies below 25 keV, where a Type B uncertainty of 0.5% has been estimated. With respect to the absorbed dose, a Type B \((k = 2)\) uncertainty of 1.2%–1.7% (<50 keV), 0.6%–1.2% (50–100 keV), and 0.3% (100–200 keV) should be considered in dosimetric calculations.

Opposite to what happens in the intermediate (about 500 keV) or high (about 1 MeV) energy domains, Type B uncertainties due to the different cross-sections implementation cannot be considered subdominant with respect to Type A uncertainties or even to other sources of Type B uncertainties (tally volume averaging, manufacturing tolerances, etc.). Therefore, the values reported here should be accommodated within the uncertainty budget in low-energy dosimetry studies.

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