Uncertainties in Monte Carlo-based absorbed dose calculations for an experimental benchmark

F Renner¹, J Wulff², R-P Kapsch¹ and K Zink²

¹ Physikalisch-Technische Bundesanstalt Braunschweig, Bundesallee 100, 38116 Braunschweig, Germany
² Institut für Medizinische Physik und Strahlenschutz, Technische Hochschule Mittelhessen, Gießen, Germany

E-mail: franziska.renner@ptb.de

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Abstract
There is a need to verify the accuracy of general purpose Monte Carlo codes like EGSnrc, which are commonly employed for investigations of dosimetric problems in radiation therapy. A number of experimental benchmarks have been published to compare calculated values of absorbed dose to experimentally determined values. However, there is a lack of absolute benchmarks, i.e. benchmarks without involved normalization which may cause some quantities to be cancelled. Therefore, at the Physikalisch-Technische Bundesanstalt a benchmark experiment was performed, which aimed at the absolute verification of radiation transport calculations for dosimetry in radiation therapy. A thimble-type ionization chamber in a solid phantom was irradiated by high-energy bremsstrahlung and the mean absorbed dose in the sensitive volume was measured per incident electron of the target. The characteristics of the accelerator and experimental setup were precisely determined and the results of a corresponding Monte Carlo simulation with EGSnrc are presented within this study. For a meaningful comparison, an analysis of the uncertainty of the Monte Carlo simulation is necessary. In this study uncertainties with regard to the simulation geometry, the radiation source, transport options of the Monte Carlo code and specific interaction cross sections are investigated, applying the general methodology of the Guide to the expression of uncertainty in measurement. Besides studying the general influence of changes in transport options of the EGSnrc code, uncertainties are analyzed.
by estimating the sensitivity coefficients of various input quantities in a first step. Secondly, standard uncertainties are assigned to each quantity which are known from the experiment, e.g. uncertainties for geometric dimensions. Data for more fundamental quantities such as photon cross sections and the \textit{I}-value of electron stopping powers are taken from literature. The significant uncertainty contributions are identified as the energy of the radiation source and the underlying photon cross sections as well as the \textit{I}-value of media involved in the simulation. The combined standard uncertainty of the Monte Carlo calculation yields 0.78% as a conservative estimation. The result of the calculation is close to the experimental result and with each combined standard uncertainty <1%, the accuracy of EGSnrc is confirmed. The setup and methodology of this study can be employed to benchmark other Monte Carlo codes for the calculation of absorbed dose in radiotherapy.

Keywords: radiotherapy, Monte Carlo calculation, benchmark, uncertainty evaluation

(Some figures may appear in colour only in the online journal)

1. Introduction

Monte Carlo (MC) techniques have many fields of application in radiation therapy (Seco and Verhaegen 2013) and well-known general-purpose MC codes are available, such as EGSnrc (Kawrakow \textit{et al} 2013), FLUKA (Ferrari \textit{et al} 2011), GEANT4 (Agostinelli \textit{et al} 2003), MCNP (X-5 2008) and PENELOPE (Salvat \textit{et al} 2011). An accepted method to assess the accuracy of these codes is a comparison with experimental data to benchmark the calculations, e.g. as shown by Chibani and Li (2002) and Faddegon \textit{et al} (2008). For the EGS code system which was of special interest in the present work, further benchmarks were published, e.g. by Rogers and Bielajew (1988) and Ali \textit{et al} (2012). A small number of publications deal with benchmarks of MC-calculated values without a previous normalization. Especially in connection with benchmarks of dosimetry in radiation therapy, the majority of publications considers relative comparisons and, consequently, no information is provided regarding the absolute accuracy of the MC-calculated absorbed doses. The main reason for performing relative comparisons is the stochastic nature of the MC radiation transport calculations. An MC-calculated quantity, e.g. absorbed dose, is a mean value per incident particle of the radiation source. In an experiment which is performed with a usual radiation source, the number of source particles is usually not directly accessible based on measurements and under this condition a direct (absolute) comparison with the MC calculation result is not possible. Alternatively, the resultant doses are normalized to a dose which is adequate as a reference and the corresponding ratios and their standard uncertainties are used for the comparison. With regard to the standard uncertainty of the MC-calculated dose, relative benchmarks are not as stringent verifications as are absolute comparisons. Due to the dose ratios, some of the contributions to the standard uncertainty of the dose can cancel out. This has already been remarked, e.g. in the investigation of uncertainties in MC-calculated beam quality correction factors with EGSnrc (Wulff \textit{et al} 2010), with the beam quality correction factors being the result of dose ratios. Hence, the normalization has a distinct influence on the result of a comparison between experimentally measured and correspondingly MC-calculated results.

With this in mind, a benchmark experiment for the absolute verification of MC radiation transport simulations for dosimetry in radiation therapy was established. At the national
metrology institute of Germany, the Physikalisch-Technische Bundesanstalt (PTB), an electron linear accelerator for research purposes is in operation (Derikum 2009). This accelerator is adequate for the needs of an absolute experimental benchmark, since a direct evaluation of the number of electrons of the beam is possible. This evaluation is based on measurements of the beam pulse charge with a calibrated beam current monitor and a division of the beam pulse charge by the elementary charge. In radiation therapy, predominantly high-energy photon radiation is utilized. Therefore, the accelerator was equipped with an x-ray target and the benchmark experiment was performed for primary photon radiation with nominal electron energy of about 27 MeV. The resultant photon radiation covers the maximum energy range used in clinical radiation therapy. During the experiment, an absorbed dose was measured by means of ionization chamber dosimetry. The latter can be considered as the method of choice for various dosimetric tasks in radiation therapy and is recommended by all current dosimetry protocols (Almond et al 1999, Andreo et al 2000, DIN 2008). The result of the benchmark experiment $D_{\text{Exp}}$ is the ratio of the mean absorbed dose to air in the cavity of the ionization chamber $D_{\text{cav}}$ and the number of electrons of the accelerator beam hitting the target $N_e$. It can be described in more detail by

$$D_{\text{Exp}} = \frac{D_{\text{cav}}}{N_e} = \frac{(W/\rho)_{\text{air}} \cdot Q}{m_{\text{air}} \cdot N_e} = \frac{(W/\rho)_{\text{air}} \cdot Q}{\rho_{\text{air}} \cdot V_{\text{cav}} \cdot N_e}.$$  

(1)

According to equation (1), the evaluation of the dose $D_{\text{cav}}$ was based on the ionization charge $Q$, the mass of the air in the cavity $m_{\text{air}}$, as well as the ratio of the mean energy expended in air per ion pair $W_{\text{air}}$ and the elementary charge $e$. The charge $Q$ equals the measured ionization charge corrected by factors to account for the following conditions: reference values of air pressure and temperature as well as dry air in the chamber cavity. Additionally, $Q$ was corrected for recombination loss and polarity effect. With regard to the comparison with a MC simulation it was also necessary to correct $Q$ for effects which result from discrepancies between the real radiation field distribution in the experiment and the ideal field distribution in the MC simulation. The mass of the air in the cavity $m_{\text{air}}$ was calculated by the product of the air density $\rho_{\text{air}}$ and the cavity volume $V_{\text{cav}}$. The latter was accurately determined on the basis of measurements with a coordinate measuring machine (Büermann and Burns 2009). The value of the ratio of $W_{\text{air}}$ and $e$ was taken from literature (Boutillon and Perroche-Roux 1987). Ultimately, for the benchmark experiment a mean dose per incident electron of 2.830 fGy was evaluated (Renner 2014).

A simulation model representing the experimental setup was created and the dose to the air in the cavity of the ionization chamber was calculated with EGSnrc (Kawrakow et al 2013). The experimentally evaluated absorbed dose and the MC-calculated dose were compared to verify the MC calculation. For a reliable and meaningful comparison between the two results, the assigned uncertainties had to be considered. For the benchmark experiment it was possible to use a straightforward method to calculate the uncertainty based on the methods given in the guide to the expression of uncertainty in measurement (GUM) (JCGM 2008): a mathematical model of the experiment was established according to equation (1) with the uncertainties evaluated for the input quantities. It results in a relative standard uncertainty of 0.66% (Renner 2014). For an MC calculation this method is not appropriate since generally no mathematical relationship for the MC result in dependence on the input quantities can be formulated in advance. Nevertheless, several sources of uncertainty exist in an MC calculation and need to be considered. These include influences of the simulation geometry, the radiation source, transport options of the MC code and specific interaction cross sections (Muir and Rogers 2010, Wulff et al 2010). The focus of the present work is the detailed evaluation of the resulting uncertainty in the MC calculation due to the aforementioned influences.
2. Methods

2.1. Monte Carlo simulation of the benchmark experiment

Figure 1 shows the MC simulation geometry representing the experimental setup. The main components of the setup which had to be included in the MC simulation were the accelerator’s electron beam, the x-ray target and the ionization chamber within the phantom. The cavity of the ionization chamber was defined as the dose scoring region. The electron beam represents the radiation source in the simulation. It impinged perpendicularly on an x-ray target which was a disc made of a tungsten-copper alloy (W/Cu) and fixed by a stainless steel flange at the end of the beamline. The particles which left the target behind traversed 207 cm of air before they struck a phantom made of polymethyl methacrylate (PMMA) that centrally held the cylindrical-type ionization chamber used as a dose detector. Since this ionization chamber is not waterproof a solid phantom was used. Apart from the electron beam, all the setup components are shown in figure 1 with relevant dimensions as determined by measurement.

The ionization chamber in the experiment was a copy of one of the primary standard measuring devices of PTB for the realization of the unit of air kerma for $^{137}$Cs and $^{60}$Co gamma radiation. This air-filled graphite-walled Bragg–Gray chamber, which is usually denoted by PTB-HRK2, is described, e.g. in the publications by Allisy et al. (2005) or by Buermann and Burns (2009). The model of the chamber used in the MC calculation is based on detailed information found in the original engineering drawings available at PTB. The chamber model matches the original chamber to a large degree (see figure 2). One difference can be recognized with regard to the central electrode. Contrary to the original chamber which has a central electrode with a rounded end, the modeled chamber has a cylindrical electrode, but an equal electrode volume in comparison to the original chamber. Further differences are obvious regarding the chamber stem which is modeled in a simplified form without details.

The characteristics of the accelerator’s electron beam in terms of its spatial and energy distribution were evaluated in connection with the benchmark experiment by means of beam profile monitors and a magnetic spectrometer (Renner et al. 2014a). The profiler measurements...
show an elliptical cross section of the beam with a semi-axis width of 0.25 cm \((x\text{-direction in figure 1})\) and 0.24 cm \((y\text{-direction in figure 1})\), i.e. the cross section lies in a plane perpendicular to the direction of the beam and parallel to the x-ray target disk. In the simulation the cross section was defined as a circle with a radius of 0.25 cm. By the method of magnetic spectrometry (Renner et al. (2014b)), a Gaussian-shaped energy spectrum with a mean energy of 27.125 MeV and a full width at half maximum (FWHM) of 180 keV was evaluated. The variation of the spectrum itself was characterized by a standard deviation of the mean energy of 35 keV.

All MC calculations were based on the EGSnrc system (Kawrakow et al. 2013) in its version V4-r2-4-0 (2013). The radiation transport in EGSnrc is controlled according to transport options which define, e.g. the photon and electron cross-section databases and transport threshold energies. Except otherwise stated, default transport parameter settings of the EGSnrc system were used, which have been demonstrated to yield accurate results within the 0.1\% level normalized to cross sections (Kawrakow 2000). The transport cut-off energies \(ECUT\) and \(PCUT\) were set to the lowest possible values of 512 keV and 1 keV, respectively, in all investigations. The transport of particles is performed in a user-defined simulation geometry and the egsp C++ class library (Kawrakow et al. 2009) was used to create a realistic model of the experimental setup. The transformation of the primary electron beam to the photon radiation in the target and the transport through air between target and phantom were implemented in BEAMnrc (Rogers et al. 2009). The absorbed dose to air detected by the sensitive volume of the ionization chamber was calculated with the user code egs_chamber (Wulff et al. 2008). BEAMnrc as well as egs_chamber provide techniques for variance reduction which were selected for maximal efficiency. The data sets (cross-section data) for the materials of the geometry were prepared by the PEGS4 data preprocessing code with material characteristics according to table 1. EGSnrc provides a number of density correction files for collisional electron stopping powers of various elements and compounds according to ICRU.

Figure 2. A scheme of the ionization chamber model used in the simulation in comparison to the real chamber. For the simulation model, the dimensions of the graphite walls and the central electrode are given which determine the air cavity of the chamber. Radii are marked with R. The reference point to position the chamber in the phantom lies on the central axis and 12 mm beyond the outer (circular) top surface of the graphite hollow cylinder.
2.2. Uncertainty evaluation in the Monte Carlo calculations

The GUM (JCGM 2008) introduces a general method to evaluate the combined standard uncertainty $u_c(y)$ of a measurand $y$. In general, the measurand $y$ can be expressed by a mathematical equation $f$ which contains input quantities $x_i$ which influence the value of $y$. In case there are $N_i$ uncorrelated quantities $x_i$, the combined standard uncertainty $u_c(y)$ of the measurand $y$ is given by

$$ u_c(y) = \sqrt{\sum_{i=1}^{N_i} \left( \frac{\partial f}{\partial x_i} \right)^2 u^2(x_i)} = \sqrt{\sum_{i=1}^{N_i} \left[ c_i \cdot u(x_i) \right]^2} \, . $$

In the above equation $u(x_i)$ represents the standard uncertainties of the input quantities. The weighting of the uncertainty of each input quantity, called sensitivity coefficient $c_i$, is determined by the partial derivative of a mathematical model function $f$ with respect to the quantity $x_i$. The standard uncertainty of the input quantity $u(x_i)$ has to be evaluated by statistical methods (type A evaluation of standard uncertainty) or by methods other than statistical ones (type B evaluation of standard uncertainty).

A type A evaluation is best estimated by the arithmetic mean of a number of observations. The standard uncertainty results from the experimental standard deviation of the mean in that case. MC codes calculate results which are assigned with a statistical uncertainty. This uncertainty component can be reduced to a negligible amount by the simulation of a sufficient number of primary histories and with the help of variance reduction techniques. With regard to dose values a negligible uncertainty is less than 0.1% (Affonseca et al 2005).

Regarding the type B evaluation of standard uncertainty, the task is to use available information to select an appropriate probability distribution which describes the input quantity. The estimate of the input quantity and its standard uncertainty result from this distribution.

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Table 1. Characteristics of the materials used in the simulation with EGSnrc.

| Material              | Density in g cm$^{-3}$ | Elemental composition (as fraction by weight) | Remark                                      |
|-----------------------|------------------------|-----------------------------------------------|---------------------------------------------|
| Air (dry air)         | $1.2048 \times 10^{-3}$| 0.000124 C, 0.755267 N, 0.231781 O, 0.012827 Ar | Air_dry_nearsealevel\(a\); in the experiment the absorbed dose was also evaluated for dry air performing a humidity correction\(a\) |
| Aluminum              | 2.698 9                | Pure element                                   | Aluminum\(a\)                               |
| Graphite              | 1.775                  | Pure element                                   | With mean ionization energy of 78 eV        |
| Polycarbonate         | 1.2                    | 0.055491 H, 0.755751 C, 0.188758 O             | Polycarbonate\(^a\)                          |
| PMMA                  | 1.19                   | 0.080538 H, 0.599848 C, 0.319614 O             | Polymethylmethacrylate\(^a\)                |
| Stainless steel       | 8.06                   | 0.001 C, 0.007 Si, 0.180 Cr, 0.010 Mn, 0.712 Fe, 0.090 Ni | Steel_stainless_type 302\(^a\)              |
| Tungsten copper       | 14.425                 | 0.72 W, 0.28 Cu                                |                                             |

\(a\) Material is available by PEGS4.

Report No. 37 (ICRU 1984). Density correction data were calculated by ESTAR (Berger et al 2005), reproducing the ICRU37 values.
Two typical distributions relevant to this work are the normal (or Gaussian) distribution and the rectangular distribution. The latter represents a uniform probability within a specified interval. The standard uncertainty of the rectangular distribution with boundaries $a$ and $b$ is calculated as $u = (b-a)/\sqrt{12}$, and in the case of a rectangular distribution with a half width $w$ it is $u = w/\sqrt{3}$. The standard uncertainty of a normal distribution is given by the standard deviation of the quantity: $u = \sigma$. The input quantities and the complete result are often stated as $x_i \pm k \cdot u(x_i)$ and $y \pm k \cdot u(y)$, respectively, with $k$ being a coverage factor which defines the confidence interval for the corresponding distribution. An assortment of typically used factors $k$ and their relative coverage of the confidence interval is given in table 2.

Type B uncertainties of an MC simulation can be characterized regarding their origin as outlined in the subsequent sections. The influence of various input quantities was investigated and either the sensitivity coefficient $c_i$ was determined and later multiplied with a known uncertainty $u(x_i)$ or the product of both was derived directly from the MC simulation. Finally, the result of equation (2) was evaluated for the complete MC simulation of the benchmark experiment.

### 2.2.1. Geometry variations.

The simulation model represents an idealized geometry and considers neither any variability in the manufacturing process of, e.g. the ionization chamber and x-ray target, nor uncertainties in positioning the whole experimental setup. While the latter was included in the experimental uncertainty budget, the other variations had to be considered explicitly. Furthermore, some simplifications in the geometry of the ionization chamber model regarding its stem and central electrode were introduced (see figure 2).

The simulation geometry was varied regarding possible variations in the mentioned details to investigate their influence on dose. In most cases, dimensions were available with an assigned standard deviation $\sigma$. It was assumed that almost 100% of the possible values for these dimensions lie within the interval of $+3 \cdot \sigma$ with regard to the mean value (see table 2), and the interval limits were treated as minimum and maximum values to investigate if there is a significant effect on dose caused by such large changes at all.

The target thickness (see figure 1) was evaluated by repeated experimental measurements before the target was installed in the experimental setup, resulting in a standard deviation of 0.001 mm used for the analysis in the MC simulation.

The measured dimensions and uncertainties of the ionization chamber’s cavity were available from internal documents. The uncertainty of the air cavity volume has already had to be considered in the uncertainty budget of the experiment, since it is an input quantity in equation (1). However, this does not take into account that the changed cavity volume is a result of the variation in the dimensions of the chamber wall and central electrode. To investigate this aspect further, simulations with a minimum and maximum possible cavity volume were performed, the changed cavity volume being a result of the variation of the dimensions of the

| $k$ | Relative coverage in % |
|-----|-------------------------|
| 1   | 68.27                   |
| 2   | 95.45                   |
| 3   | 99.73                   |
| $\geq 1.73$ | 100                  |

Two typical distributions relevant to this work are the normal (or Gaussian) distribution and the rectangular distribution. The latter represents a uniform probability within a specified interval. The standard uncertainty of the rectangular distribution with boundaries $a$ and $b$ is calculated as $u = (b-a)/\sqrt{12}$, and in the case of a rectangular distribution with a half width $w$ it is $u = w/\sqrt{3}$. The standard uncertainty of a normal distribution is given by the standard deviation of the quantity: $u = \sigma$. The input quantities and the complete result are often stated as $x_i \pm k \cdot u(x_i)$ and $y \pm k \cdot u(y)$, respectively, with $k$ being a coverage factor which defines the confidence interval for the corresponding distribution. An assortment of typically used factors $k$ and their relative coverage of the confidence interval is given in table 2.

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chamber wall and central electrode by $\pm 3 \cdot \sigma$ each. An additional investigation was performed by varying the radial chamber wall in the model by $\pm 0.05$ mm. These changes are limits generously covering the manufacturing precision of the lathe in radial direction. The influence of the construction of the chamber stem was based on a simulation without a chamber stem, i.e. the stem completely replaced by PMMA.

### 2.2.2. Variations of radiation source modeling.

The spectral fluence of the electrons used as primary radiation in the simulation was described by a mean energy $E_{\text{mean}}$, its standard deviation $\sigma_E$, and the FWHM of the Gaussian-shaped spectrum (see section 2.1). The probable minimal and maximal shift of the energy spectrum is realized by a decrease and an increase of the mean energy according to $E_{\text{mean}} \pm 3 \cdot \sigma_E$.

The geometrical cross section of the beam model was reduced by a factor of 2 to investigate a possible influence of the cross-sectional dimension on the calculated dose. This investigation also proved whether the representation of the cross section as a circle or an ellipse (see section 2.1) makes a significant difference for the dose calculation.

### 2.2.3. Different transport options.

In an MC code, usually different implementations of interaction processes are available that underlie the complete transport simulation. In EGSnrc the user has the choice to change, e.g. underlying cross-section databases, to explicitly neglect certain interaction channels, or to change values for transport cut-offs (for details see Kawrakow et al. 2013). This can be useful in terms of calculation efficiency if in the energy range under consideration a certain interaction has an expected negligible effect on the result. However, on the other hand, the result must not be biased. In fact, EGSnrc does not model all possible effects and, for example, only recently the handling of photonuclear attenuation was added (Ali and Rogers 2012).

Particularly the choice of cross-section databases might have an influence on the calculated result, but the choice is to some degree arbitrary. Hence, the influence of a changed transport option might be related to a general uncertainty of the MC calculation. Various options were changed from their defaults as is explained in table 3.

### 2.2.4. Cross section variation.

In addition to the general change in cross-section databases as outlined in the previous section, a more detailed investigation was performed for the two most important cross-section types in the scope of this work: the photon cross sections and the electron collisional stopping powers. This investigation followed a method used by Wulff et al. (2010) and Muir and Rogers (2010) and was originally introduced by de Carlan et al. (2008). This method is based on a replacement of the partial derivative of the mathematical model function $f$ with respect to the quantity $x_i$ (see equation (2)) by the ratio of the change $\Delta f$ resulting from a large change in $\Delta x_i$. The partial derivative was approximated by a linear slope for values of $\Delta f$ significantly larger (at least by a factor of 10) than the statistical uncertainty. A linear approximation is not necessarily reflecting the functional form of the underlying sensitivity. It was however shown to be appropriate within $\pm 5\%$ for the photon cross-section uncertainties and further slightly overestimating the effect of the mean ionization energy on electron stopping powers (see figure 2 in Wulff et al. 2010). In case $\Delta f$ is not significantly larger than the statistical uncertainty, the slope can be calculated by the sum of the statistical uncertainty and the change $\Delta f$.

For the photon mass attenuation coefficients of each interaction channel (Rayleigh scattering, photoelectric effect, Compton scattering and pair production) a change was achieved by multiplication with the factor 1.05, which ensures a significant and linear variation in the results. The scale was applied to each interaction channel and all materials one at a time.
assuming a correlation between the cross section of the same interaction type for different materials. For the Compton scattering which is the dominant process in the energy range of radiotherapy, the uncorrelated case was also considered and the photon cross section for Compton scattering was changed individually for each material of the chamber. Values for the standard uncertainties of the interaction channels of photons with matter for energies greater than 1.0 keV were taken from Cullen et al (1997).

Table 3. Possible transport option settings. The default option is the first one mentioned in the 2nd column. The abbreviations in brackets in the 1st column are of importance in section 3.3. For more details on transport options, see Kawrakow et al (2013) and references therein.

| Transport option                        | Possible options | Explanation |
|-----------------------------------------|------------------|-------------|
| Photon cross sections                   | XCOM, SI, EPDL   | XCOM: XCOM data from Berger and Hubbell; SI: photon cross-section data by Storm and Israel; EPDL: evaluated photon data library |
| Pair cross sections (pair cs)           | BH, NRC          | BH: extreme relativistic first Born approximation differential cross sections; NRC: differential pair cross sections by NRC |
| Pair angular sampling (pair ang)        | Simple, KM, Off  | Simple: leading term of angular distribution is used; KM: angular distribution according to Koch and Motz; Off: fixed pair angle |
| Triplet production (triplet)            | Off, On          | Off: approximation of triplet production; On: explicit simulation of triplet production events according to the first Born approximation result |
| Radiative Compton corrections (rad compt) | Off, On         | Off: no corrections; On: inclusion of radiative corrections for Compton scattering in a one-loop approximation |
| Rayleigh scattering (Rayleigh)          | Off, On          | Off: consideration of Rayleigh scattering in a simple way; On: explicit modeling of the scattering processes |
| Brems cross sections (brems cs)         | BH, NIST, NRC    | BH: first born approximation Bethe–Heitler cross sections; NIST: NIST bremsstrahlung cross-section database; NRC: NRC brems cross-section data |
| Electron impact ionization (eii)        | Off or Kawrakow, Penelope, e.g. | Off: no electron impact ionization; Kawrakow, Penelope: explicit simulation of electron impact ionization according to different theories (e.g. by Kawrakow) to derive the cross sections; note: there are more options than Kawrakow and Penelope |
| Photonuclear attenuation (photonuclear) | Off, On          | Off: no photonuclear attenuation; On: consideration of photonuclear attenuation (Ali and Rogers 2012) |
3. Results

3.1. Geometry variation

All investigated geometry variations resulted in a change of dose of less than 0.1% (see figure 3) and were considered to be negligible.

3.2. Variation of radiation source modeling

The energy increase or decrease, respectively, by shifting the Gaussian energy distribution of the source electrons, changes the calculated dose by about ±1% on average. This change was used to estimate the sensitivity coefficient for the influence of the energy uncertainty on dose according to the method described in section 2.2.4. With the standard deviation of the energy of 35 keV, this results in a contribution to the combined uncertainty of 0.37%.

The reduction of the geometrical cross section of the electron beam model did not influence the dose. This also served as proof that the geometrical description of the cross section as a circle or an ellipse has only a negligible effect on the dose calculation.

3.3. Different transport options

The ratio of the dose of different transport parameter settings relative to the dose calculated with default settings is shown in figure 4. In the majority of cases, a change in the transport parameter setting causes a change in dose of less than 0.1%, and that is negligible. An effect larger than 0.1% is only observed for changed settings of the photon and total bremsstrahlung cross sections. The largest effect is caused by the photon cross sections evaluated according to Storm and Israel (‘SI’). This causes a difference of about +0.29% to the default case of settings used for the calculations in this work. It has to be mentioned that in previous versions of EGSnrc ‘SI’ was the default setting for photon cross sections, e.g. in EGSnrc version...
V4-r2-3-1. The second largest effect is caused by the use of the NIST Brems cross-section database. It decreases the dose to about 99.78% of the default case.

To sum it up, all dose variations lie within an interval \([-0.22\%, +0.29\%]\) that forms a slightly asymmetric rectangular distribution with a standard uncertainty of 0.15%.

3.4. Cross-section variation

The resulting uncertainty contribution to the uncertainty of the MC calculated dose due to cross-section variations is given in the last row of table 4. It is the combined uncertainty without Rayleigh scattering, photoelectric effect, the contribution of aluminum and polycarbonate (PC) to Compton scattering, and the contribution of aluminum, PMMA, PC and tungsten copper to the stopping power uncertainty. The mentioned contributions were assessed as insignificant, since their uncertainty contribution is smaller than 0.1%. The uncertainty contribution of the photon cross sections is 0.43% altogether, and the overall contribution of the electron cross sections is 0.53%. The uncertainty contribution of the photon cross sections is dominated by Compton scattering with 0.41%, in combination with the single uncertainties of graphite and PMMA. The calculation is based on the assumption of uncorrelated uncertainties of Compton cross sections for all materials. A simulation assuming a correlation increased the uncertainty contribution of Compton scattering to 0.46%, resulting in a combined uncertainty of 0.72%. That makes just a slight difference which is not given further consideration. Anyway, the combined uncertainty is influenced in an almost equivalent manner by the uncertainty contribution of photon cross sections as well as the uncertainty contribution of stopping powers, which are dominated by the \(J\)-value of graphite. The second largest uncertainty contribution is caused by air due to the large sensitivity coefficient. This is not surprising as the detection material in the cavity is air.
3.5. Combination of the calculation results and comparison with the experimental result

Figure 5 shows the resultant dose of the MC simulation as it was calculated for the default case, i.e. the simulation geometry and radiation source parameters, as described in section 2.1, and usage of the default transport option settings of the mentioned EGSnrc version. The value of the mean dose per electron is 2.825 fGy or 17.634 eV g\(^{-1}\), respectively.

The relevant uncertainty contributions to the combined (standard) uncertainty of the MC simulation which were evaluated in this work are represented as error bars of the dose in figure 5. In the case of the uncertainty of the cross sections, a contribution of 0.69% was assumed to be a conservative value (see section 3.4). The cross-section uncertainty is the dominant contribution to the uncertainty of the MC calculation. The second largest contribution results from the uncertainty due to the source definition which is, however, only half of the uncertainty contribution owing to the uncertainty of the cross sections and which is, in fact, just an uncertainty of the energy of the source. The uncertainty of the transport options is rather small (0.15%) and, moreover, it should be taken into account that it also includes some influence of cross-section databases which were investigated separately in more detail. Therefore, the uncertainty of the transport options was assumed to be negligible. The statistical uncertainty of the MC simulation was also neglected since it was smaller than 0.1%. As a final result, for the MC simulation the dose value is obtained with a combined uncertainty of 0.78%, which is the combination of the uncertainty of the cross sections and the source modeling. In comparison to the result of the MC simulation, the corresponding result of the benchmark experiment and its combined uncertainty as stated in section 1 are shown in figure 5. The mean dose per electron of the experiment and the MC calculation differ by 0.19%. Nevertheless the results are in agreement, taking the uncertainties of both results into account.

### Table 4. The uncertainty budget regarding the uncertainty contribution due to cross-section data.

| Variation parameter                      | Medium | Sensitivity coefficient \(c_i\) | \(\sigma(x_i)/x_i\) in % | \(\Delta D/D\) in % |
|------------------------------------------|--------|--------------------------------|--------------------------|---------------------|
| Variations in photon cross sections      |        |                                |                          |                     |
| Rayleigh scattering                      | All    | 0.023                          | 2                        | (0.05)              |
| Photoelectric effect                     | All    | 0.033                          | 2                        | (0.07)              |
| Compton scattering                       | C      | 0.312                          | 1                        | 0.31                |
|                                          | PMMA   | 0.263                          | 1                        | 0.26                |
|                                          | PC     | 0.040                          | 1                        | (0.04)              |
|                                          | All    | 0.069                          | 2                        | 0.14                |
| Variations in stopping powers (mean excitation energy) |         |                                |                          |                     |
|                                          | Al     | 0.004                          | 0.8                      | (0.003)             |
|                                          | C      | 0.079                          | 6.1                      | 0.48                |
|                                          | PMMA   | 0.021                          | 1.4                      | (0.03)              |
|                                          | PC     | 0.005                          | 10                       | (0.05)              |
|                                          | W/Cu   | 0.006                          | 15                       | (0.09)              |
|                                          | Air    | 0.176                          | 1.3                      | 0.23                |

Combined uncertainty due to cross section variations: 0.69
4. Discussion

The analysis reveals that only some of the investigated uncertainty sources lead to significant contributions. Uncertainties of the geometry are insignificant, since all dimensions for the simulation are known with sufficient precision by experimental evaluation. Additionally, the investigations allow the conclusion that variations in the transport parameters can be considered as negligible for this setup as long as the default settings of EGSnrc are used. The statistical uncertainty of the simulation can be neglected since it is less than 0.1% and could, in principle, be decreased even further. Two relevant contributions are left: uncertainty of the radiation source modeling and cross-section uncertainties. The contribution of the radiation source is due to the uncertainty in the experimental evaluation of the energy of the electrons impinging on the x-ray target. This fact demonstrates the necessity to carefully evaluate the energy of the source during this type of an absolute benchmark experiment.

The major contribution to the combined uncertainty of the MC calculation is made by the cross-section data which is divided into photon cross sections and electron collision stopping powers in this study. Compton scattering is the most relevant interaction channel in the high-energy range of radiotherapy and, therefore, it has the strongest influence on the uncertainty of the photon cross sections. The strength of the influence is almost the same, regardless of whether the Compton scattering is assumed to be correlated or uncorrelated. On the other hand, it was already discussed by Wulff et al (2010) that the influence of Compton cross-section...
uncertainties is more realistically considered by comparing the simulation results with and without binding and radiative corrections. The assumed 1% uncertainty of the Compton cross section is due to the missing consideration of radiative corrections. Binding corrections for electrons are turned on by default in EGSnrc (see Kawrakow et al 2013 for details). It was checked that turning them off has a negligible effect on the calculated dose (result not explicitly shown). The effect of the consideration of radiative and binding corrections is negligible according to figure 4. Hence, in this case the contribution by photon cross sections would be reduced to the contribution of 0.14% due to pair production. A recent publication by Ali et al (2015) suggests a photon cross section uncertainty for the external radiotherapy energy range of 0.5% in contrast to 1% or 2%, respectively, as used in this work. This supports the tendency towards a smaller uncertainty contribution due to photon cross sections of about $\leq 0.20\%$ rather than $> 0.40\%$ as mentioned in section 3.4.

Electron collision stopping powers are assumed to be influenced only by the uncertainty of the mean ionization energy. Graphite is almost air equivalent and therefore often used in the construction of ionization chambers. Being directly adjacent to the sensitive air volume of the ionization chamber, the contribution to the overall result is large. The correct value of the mean excitation energy of graphite has been the subject of various investigations, e.g. in connection with the evaluation of the collision stopping powers for primary measurement standards in radiation dosimetry. For this application field, a mean excitation energy of graphite with an uncertainty of about 2.5% was proposed by Burns (2012) and Andreo et al (2013). Burns et al (2014) recently updated this value to 2.2%. Nevertheless, it was mentioned by Andreo et al (2013) that the mean excitation energy (and density) for graphite given in their publication is not directly applicable to the simulation of graphite bodies for MC calculations. As a conservative approach, the more than doubled uncertainty of ICRU37 was used in this work. If, in contrast, the value of Burns et al (2014) was applied, the uncertainty by electron stopping powers would yield only 0.29%. In combination with an uncertainty of the photon data of 0.14% and taking the uncertainty of the source modeling into account, a combined uncertainty for the MC simulation would result in 0.49%, which is even smaller than the experimental value. The alternative assumption of an uncertainty contribution of the photon data of $\leq 0.20\%$ following the analysis of Ali et al (2015) would result in a combined uncertainty for the MC simulation of 0.51%, which is also smaller than the experimental uncertainty. Hence, the value of 0.78% represents a conservative estimation.

In principle, one could extend the methodology for the systematic investigation of cross-section uncertainties also to bremsstrahlung or electron elastic scattering. The influence of bremsstrahlung cross section was studied by varying the underlying database (figure 4) and is thus generally included in the overall estimation. A preliminary test by changing elastic scattering cross sections according to the approach of Faddegon et al (2009) was conducted with a scaling by up to 10%. It is per se not clear, how large a realistic uncertainty for the elastic scattering cross section is, but taking the value of 10% is expected to be rather large. This scaling yielded a non-linear change of the absorbed dose by maximum 4 times the statistical uncertainty, which is not significantly large. Therefore, a significant uncertainty contribution by electron elastic scattering cross sections is not expected.

5. Conclusion

Benchmark experiments play an important role in the verification of MC calculations. At PTB, a benchmark experiment was performed to verify an MC-calculated absorbed dose for the application field of high-energy radiotherapy. The experiment stood out due to the fact that
its result could be directly compared to the MC-calculated absorbed dose, i.e. there was no normalization of dose involved.

The investigation of a number of different uncertainty contributions regarding the MC-calculated dose was presented and a combined uncertainty of 0.78% was determined as a conservative estimate. The most problematic uncertainty contribution results from cross-section uncertainty. Thereby, this study concentrates on photon cross sections and collision stopping powers of electrons. It is debatable how to correctly evaluate uncertainties of the photon cross sections, especially of the Compton cross section, and electron stopping powers of graphite. The latter requires a more accurate value of the mean ionization energy of graphite applicable for use with MC calculations. Indeed, the value of the combined uncertainty differs significantly, depending on the uncertainty contribution of the cross sections, and this changes the interpretation of the final results. In a conservative approach, the cross-section uncertainty is already slightly larger than the combined uncertainty of the benchmark experiment. Accordingly, the MC simulation does not reach the accuracy of a carefully evaluated experimental absorbed dose. On the other hand and as explained in section 4, alternative approaches which involve reduced photon cross section uncertainties and a reduced uncertainty of the mean excitation energy of graphite lead to the statement that the combined uncertainty of the MC-calculated absorbed dose is smaller than the experimental combined uncertainty. In that case, the MC calculation is more accurate than the experiment.

Nevertheless, the uncertainties related to both absorbed doses are less than 1% and the result of the MC calculation and the experimental result are in agreement. Hence, the dose calculated by the MC code EGSnrc for a specific radiotherapeutic setup is verified by the benchmark experiment. This verification is valid on an absolute basis. Furthermore, with the publication of the information about the setup and the result of the benchmark experiment, it becomes possible to also verify other MC codes for absorbed dose calculation in radiation therapy.

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