

Consistency in reference radiotherapy dosimetry: resolution of a conundrum when ^{60}Co is the reference quality for charged-particle and photon beams

Pedro Andreo¹, Jörg Wulff^{2,3}, David T. Burns⁴, Hugo Palmans⁵

¹ Medical Radiation Physics, Stockholm University at Karolinska University Hospital and Karolinska Institutet, Stockholm, Sweden

² Institut für Medizinische Physik und Strahlenschutz-IMPS, University of Appl. Sciences, Gießen, Germany

³ Varian Medical Systems, Particle Therapy GmbH, Bergisch-Gladbach, Germany

⁴ Ionizing Radiation, Bureau International des Poids et Mesures, Sèvres, France

⁵ Acoustics and Ionizing Radiation, National Physical Laboratory, Teddington, United Kingdom

Abstract

Substantial changes in ion chamber perturbation correction factors in ^{60}Co γ -rays, suggested by recent Monte Carlo (MC) calculations, would cause a decrease of about 1.5% in the reference dosimetry of all types of charged particles (electrons, protons and heavier ions) based on calculated k_Q values. It has been ignored so far that the ratio of calibration coefficients $N_{D,w,\text{Co60}}$ and $N_{K,\text{air},\text{Co60}}$ yields an experimental value of $F_{\text{ch},\text{Co60}} = (s_{w-\text{air}} p_{\text{ch}})_{\text{Co60}}$ through $N_{D,\text{air},\text{Co60}}$. Coefficients provided by the IAEA and traceable to the BIPM for 91 NE-2571 chambers result in an average $F_{\text{ch},\text{Co60}}$ which is compared with published (and new) MC simulations and with the value in IAEA TRS-398. It is shown that TRS-398 agrees within 0.12% with the experimental $F_{\text{ch},\text{Co60}}$. The 1.5% difference resulting from MC calculations (1.1% for the new simulations) cannot be justified using current fundamental data and BIPM standards if consistency in the entire dosimetry chain is sought. For photons, MC k_Q factors are compared with TRS-398. Using the same uncertainty for W_{air} , the two sets of data overlap considerably. Experimental k_Q values from standards laboratories lie between the two sets of calculated values, showing no preference for one set over the other. Observed chamber-to-chamber differences (also seen for ^{60}Co) justify the recommendation in TRS-398 for k_Q values specifically measured for the user chamber. Current developments on I -values for the stopping powers of water and graphite are presented. A weighted average $I_{\text{water}} = 78 \pm 2 \text{ eV}$ is obtained from published experimental and DRF -based values; this would decrease $s_{w-\text{air}}$ for all types of radiotherapy beams between 0.3% and 0.6%, and would consequently decrease the MC derived $F_{\text{ch},\text{Co60}}$. The implications of a recent proposal for $I_{\text{graphite}} = 81 \text{ eV}$ are analysed, resulting in a potential decrease of 0.7% in $N_{K,\text{air},\text{Co60}}$ which would raise the experimental $F_{\text{ch},\text{Co60}}$; this would result in an increase of about 0.8% in the current TRS-398 value when referred to the BIPM standards. MC derived $F_{\text{ch},\text{Co60}}$ using new stopping powers would then agree at a level of 0.1% with the experimental value, confirming the need for consistency in the dosimetry chain data. Should world average standards be used as reference, the figures would become +0.4% for TRS-398 and -0.3% for the Monte Carlo calculation. $F_{\text{ch},Q}$ calculated for megavoltage photons using new stopping powers would decrease by between 0.2% and 0.5%. When they enter as a ratios in k_Q , differences with MC values based on current key data would be within 0.2% but their discrepancy with k_Q experimental photon values remains unresolved. For protons the new data would require an increase in $W_{\text{air},Q}$ of about 0.6%, as this is inferred from a combination of calorimetry and ionometry. This consistent scenario would leave unchanged the current TRS-398 k_Q (NE-2571) data for protons, as well as for ions heavier than protons unless new independent $W_{\text{air},Q}$ values become available. Also in advanced radiotherapy modalities, the need for maintaining data consistency in an analysis that unavoidably must include the complete dosimetry chain is demonstrated.

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1 Introduction

A key step in the radiotherapy process is the requirement for consistent reference dosimetry traceable to metrological primary standards, and to enable reliable dosimetry comparisons common procedures within a country, or even worldwide, need to be followed for reference dosimetry. Many countries in Europe and elsewhere base their reference dosimetry for external beams, from ^{60}Co γ -rays to protons and heavier charged particle beams, on the IAEA TRS-398 Code of Practice (Andreo *et al.* (2000)) or use its data and/or similar procedures. The increased availability of standards laboratories providing calibrations of ionization chambers in terms of absorbed dose to water, N_{D,w,Q_0} , at high energy photon beam qualities (Allisy-Roberts *et al.* (2009)) has expanded the number of users following the recommendation in TRS-398 to use whenever possible experimentally determined k_{Q,Q_0} beam quality correction factors specifically measured for the user chamber. In the case of protons and heavier ions, although calorimetry-based primary standards will in the near future allow the use of heavy charged particle reference qualities and measured k_{Q,Q_0} factors, current reference dosimetry is still based on the use of ^{60}Co as reference quality. It is emphasized that comparisons of data and references to TRS-398 based solely on calculated beam quality correction factors often do not consider that their use is the third option in the international Code of Practice and that the mean energy required to produce an ion pair in dry air at a given beam quality (ICRU (1979)), $W_{\text{air},Q}$, still is one of the largest sources of uncertainty in ionization chamber dosimetry based on air-kerma or absorbed dose to water standards.

For reference dosimetry in any type of high-energy radiotherapy beam based on calculated beam quality factors k_Q (i.e. k_{Q,Q_0} normalized to the reference quality of ^{60}Co γ -rays), advanced Monte Carlo calculations used to derive ionization chamber perturbation correction factors, $p_{\text{ch},Q}$, have improved the accuracy of the data entering into the calculation of k_Q values. These include ratios of the perturbation correction factors mentioned and of other dosimetric quantities. In the case of megavoltage photon and electron beams, the factors $F_{\text{ch},Q} = s_{w\text{-air},Q} p_{\text{ch},Q}$, where $s_{w\text{-air},Q}$ is the Spencer-Attix water-to-air stopping-power ratio for the beam quality Q , play a key role, k_Q being equal to the ratio $F_{\text{ch},Q}/F_{\text{ch},\text{Co60}}$. For protons and heavier ions k_Q includes in addition the ratio $W_{\text{air},Q}/W_{\text{air},\text{Co60}}$. In certain cases it has been shown that some of the $p_{\text{ch},Q}$ correction factors previously used, derived using analytical expressions and measurements developed or made 30 years ago, were incorrect.

In the case of cylindrical ionization chambers of the Farmer-type, where the NE-2571 continues to be one of the most common reference instruments, various Monte Carlo calculations (e.g. Buckley and Rogers (2006); Wang and Rogers (2008); Wulff *et al.* (2008a)) have resulted in a considerable increase of $p_{\text{ch},\text{Co60}}$ for ^{60}Co which would raise the value of $F_{\text{ch},\text{Co60}}$. If directly applied at the clinic while keeping other basic data unchanged, it would decrease the reference absorbed dose to water, $D_{w,Q}(z_{\text{ref}})$, for all types of charged particles (electrons, protons and heavier ions) by up to 1.5%; the effect would be smaller for megavoltage photon beam dosimetry. Such a considerable change in the dosimetry of the most common reference beam quality raises an apparent conundrum for ^{60}Co . The increase in $F_{\text{ch},\text{Co60}}$ and subsequent decrease in $D_{w,Q}(z_{\text{ref}})$ was already questioned by Benmakhlouf and Andreo (2011) on the grounds of “a considerable discrepancy with current evidence”, and Andreo (2010, 2012) emphasized the need for finding a solution providing a consistent reference dose determination in the entire range of radiotherapy beams, irrespective of the procedure used for deriving the necessary data, as a major priority in their dosimetry.

This work aims first at resolving the ^{60}Co conundrum by considering data on ionization chamber calibrations traceable to the standards of the Bureau International des Poids et Mesures (BIPM); the analysis is supported by new Monte Carlo simulations of the NE-2571 chamber. Considering the agreement between different standards laboratories worldwide (c.f. Allisy-Roberts *et al.*

(2009)), the findings can be considered of general applicability. It will also analyze k_Q values for megavoltage photon beams, comparing calculated values with new simulations and with experimentally derived data measured at standard laboratories (electron k_Q values for plane-parallel chambers were analyzed by Benmakhlouf and Andreo (2011)). Current developments on the mean excitation energies for the electronic stopping powers of water and graphite, that may affect substantially the dosimetry of all radiotherapy beam types, will be discussed under a framework of consistency in the basic data used throughout the entire dosimetry chain, and their impact on a possible future scenario for reference dosimetry presented.

2 Fundamentals of reference dosimetry. Background

For sake of clarity and subsequent use throughout this work, expressions generalized for all types of high-energy radiotherapy beams of quality Q , for the determination of absorbed dose to water under reference conditions, $D_{w,Q}(z_{\text{ref}})$, using an ionization chamber calibrated in terms of air-kerma and absorbed dose to water will be given in this background section.

Recall that the fundamental Bragg-Gray expression relating the absorbed dose in two media through their stopping-power ratio is modified using a chamber specific perturbation correction factor for the relevant beam quality, which accounts for changes in the particle fluence at the point of measurement caused by the presence of the chamber. The various types of perturbation correction factors are usually written as a product of independent corrections, so that stopping-power ratios calculated for homogeneous “unperturbed” media can be used, i.e.

$$D_{w,Q}(z_{\text{ref}}) = D_{\text{air-ch},Q} s_{w\text{-air},Q} \left(\prod_j p_{\text{ch}_j} \right)_Q = D_{\text{air-ch},Q} s_{w\text{-air},Q} p_{\text{ch},Q} \equiv D_{\text{air-ch},Q} F_{\text{ch},Q} \quad (1)$$

where $D_{\text{air-ch},Q}$ is the mean absorbed dose in the chamber air cavity and, for simplicity in the notation, a factor $F_{\text{ch},Q} = s_{w\text{-air},Q} p_{\text{ch},Q}$ has been introduced. Note that $F_{\text{ch},Q}$ is commonly determined in Monte Carlo dosimetry simulations directly as the ratio $D_{w,Q}/D_{\text{air-ch},Q}$, which yields a “perturbed” stopping-power ratio (Sempau *et al.* (2004)). The $F_{\text{ch},Q}$ is also used to determine Monte Carlo-derived chamber perturbation correction factors, $p_{\text{ch},Q}$, where the influence of the various components of a chamber is analyzed comparing the resulting absorbed dose in the air cavity, $D_{\text{air-ch},Q}$, following the addition or replacement of each chamber component, with the dose to a point in water in the absence of the chamber, $D_{w,Q}$ (approximated by a very small water volume), and assuming that $s_{w\text{-air},Q}$ is known, see e.g. Sempau *et al.* (2004) and Wulff *et al.* (2008a).

Equation (1) provides the basis for the reference dosimetry of any type of high-energy radiotherapy beam based on air-kerma calibration coefficients for ^{60}Co , $N_{K,\text{air},\text{Co60}}$ (see e.g. TG-21, Schulz *et al.* (1983) or TRS-277, Andreo *et al.* (1987)) through the well-known $N_{D,\text{air}}$ coefficient, which for any beam type of quality Q can be written as

$$N_{D,\text{air},Q} = N_{D,\text{air},\text{Co60}} \frac{W_{\text{air},Q}}{W_{\text{air},\text{Co60}}} = N_{K,\text{air},\text{Co60}} (1 - \bar{g}_{\text{air}})_{\text{Co60}} \left(\prod_i k_{\text{ch}_i} \right)_{\text{Co60}} \frac{W_{\text{air},Q}}{W_{\text{air},\text{Co60}}} \quad (2)$$

where $\bar{g}_{\text{air}}$ is the mean fraction of the initial kinetic energy of the secondary electrons generated by ^{60}Co γ -rays that is converted to bremsstrahlung in air, and $\prod k_{\text{ch}}$ is the product of correction factors taking into account the lack of air equivalence of the chamber wall and its build-up cap, k_{m} , attenuation and scattering in the chamber components, k_{att} , and, if relevant, a k_{cel} factor that corrects for the presence of a central electrode. Note that these are essentially equivalent

to the corrections used in ionometric primary standards, in which the mean absorbed dose to the air cavity is determined from a measurement of the charge produced in a known air volume (c.f. Büermann and Burns (2009)). The above yields

$$D_{w,Q}(z_{\text{ref}}) = M_{w,Q} N_{D,\text{air},\text{Co60}} \frac{W_{\text{air},Q}}{W_{\text{air},\text{Co60}}} F_{\text{ch},Q} \quad (3)$$

$M_{w,Q}$ being the charge collected by the user chamber at the reference depth in a water phantom, corrected for influence quantities. For megavoltage photon and electron beams, where $W_{\text{air},Q} \cong W_{\text{air},\text{Co60}}$, expression (3) coincides with that used in conventional air-kerma protocols, while in the case of proton and heavier ion beams the ratio of the mean energies required to produce an ion pair in dry air, W_{air} , must be taken into account.

In parallel with the above, for the more straight forward case of absorbed dose to water standards, the reference absorbed dose to water in any type of high-energy radiotherapy beam is given by (see e.g. TRS-398, Andreo *et al.* (2000))

$$D_{w,Q}(z_{\text{ref}}) = M_{w,Q} N_{D,w,\text{Co60}} k_{Q,Q_0} \quad (4)$$

where

$$k_{Q,Q_0} = \frac{N_{D,w,Q}}{N_{D,w,\text{Co60}}} \quad (5)$$

and $N_{D,w,Q}$ are the calibration coefficients at the respective quality “q”, specifically measured for the user chamber. When calibration coefficients measured at qualities different from ^{60}Co are not available, equation (5) is approximated by

$$k_{Q,\text{Co60}}^{\text{calc}} = \frac{F_{\text{ch},Q}}{F_{\text{ch},\text{Co60}}} \frac{W_{\text{air},Q}}{W_{\text{air},\text{Co60}}} \quad (6)$$

for which values were given in TRS-398 (and for megavoltage photons and electrons in other dosimetry protocols as well). Note that in this case, both $F_{\text{ch},Q}$ and $F_{\text{ch},\text{Co60}}$ are calculated quantities.

3 Current status of ^{60}Co γ -ray key data

In an ideal case, reference dosimetry based on expressions (3) and (4) should coincide for any beam quality. At the time TRS-398 was published in 2000 this was not the case, and for ^{60}Co γ -rays the two expressions differed by about 1% for various types of ionization chambers (see Figure 19 in TRS-398). The situation was explained in terms of the K_{air} and D_w standards for ^{60}Co then available at the BIPM and other national metrology laboratories.

Three important issues have occurred since. The first was an increase of 0.54% in the K_{air} standard of the BIPM in 2007, increasing by this amount the ionization chamber calibration coefficients $N_{K,\text{air},\text{Co60}}$ traceable to this standard; note that the BIPM ionometric D_w standard was not changed at that time because of the ongoing development of a calorimetric standard, and furthermore is unlikely to change because of the good agreement between the BIPM ionometric and calorimetric standards. The second was a series of Monte Carlo calculations by different authors on ionization chamber perturbation correction factors. The third was developments in basic dosimetry data possibly leading to new recommendations for the I -values for graphite and water; these will be discussed separately below.

For photon beams the lack of equivalence to water of the material of a chamber wall is taken into account using the p_{wall} perturbation correction factor. An empirical two-component expression was given by Almond and Svensson (1977) to correct for this effect which, in spite of its simplicity, was used in TRS-398 as the only source then available. Wall perturbation correction factors for cylindrical chambers (NE-2571) have subsequently been calculated using the *EGSnrc* Monte Carlo system (Kawrakow *et al.* (2011)) by Buckley and Rogers (2006) and Wulff *et al.* (2008a), and values between 0.6% and 0.2% higher than the values included in TRS-398, obtained for ^{60}Co and for high megavoltage photon energies respectively (see Figure 1). With regard to the displacement correction factor, p_{dis} , different data sets, either from experimental data of Johansson *et al.* (1978), or from the “first scatter” analytical calculations of Cunningham and Sontag (1980), have been used to correct for this effect in dosimetry protocols such as TRS-398 and AAPM TG-51 (Almond *et al.* (1999)). Monte Carlo calculations by different authors (e.g. Wang and Rogers (2008); Wulff *et al.* (2008a)) have shown differences with the TRS-398 data of up to 0.8% for ^{60}Co ; these led Swanpalmer and Johansson (2012) to refine the experimental determinations of Johansson *et al.* (1978) obtaining good agreement with the new calculations. The different values shown in Figure 2 illustrate the expected change for a NE-2571 chamber. Central electrode perturbation correction factors, p_{cel} , for NE-2571 Farmer-type cylindrical ionization chambers in high-energy photon beams have been calculated by Buckley *et al.* (2004) and Wulff *et al.* (2008a), and in this case the difference between the values in TRS-398 and those from the references quoted is within 0.2%.

The combined effect of the new Monte Carlo data on p_{wall} , p_{dis} and p_{cel} for a NE-2571 chamber, keeping unchanged $s_{\text{w-air,Co60}}$, is to increase $F_{\text{ch,Co60}}$ by 1.5% approximately. Consequently, if $F_{\text{ch,Q}}$ would remain unaltered for this chamber type, as a priori would be the case for electrons, protons and heavier charged particles, k_{Q} , and therefore $D_{\text{w}}(z_{\text{ref}})$, would decrease by the same amount according to equations (6) and (4) respectively. In the case of megavoltage photons, the decrease would be smaller but still close to 1% (see Figures 1 and 2 for the differences in p_{wall} and p_{dis} , respectively). This conundrum requires a solution providing a consistent reference dose determination in the entire range of radiotherapy beams.

It has been overlooked so far that for ^{60}Co γ -rays the ratio of ionization chamber calibration coefficients in terms of absorbed dose to water and air-kerma, $N_{D,\text{w,Co60}}$ and $N_{K,\text{air,Co60}}$, yields the value of $F_{\text{ch,Co60}}$ through the $N_{D,\text{air,Co60}}$ coefficient, as

$$N_{D,\text{w,Co60}}/N_{D,\text{air,Co60}} \equiv F_{\text{ch,Co60}} = (s_{\text{w-air}} p_{\text{ch}})_{\text{Co60}} \quad (7)$$

where $N_{D,\text{air,Co60}}$ was defined in equation (2). The factor $F_{\text{ch,Co60}}$ is henceforth referred to as an experimental value, noting that $N_{D,\text{air,Co60}}$ includes the product of the chamber corrections $k_{\text{m}}k_{\text{att}}k_{\text{cel}}$ and the value of $(1 - \bar{g}_{\text{air}})$ for ^{60}Co .

Based on current BIPM standards, calibration coefficients from the IAEA Dosimetry Laboratory for a sample of 91 NE-2571 chambers yield an average ratio $N_{D,\text{w,Co60}}/N_{K,\text{air,Co60}} = 1.0914$ with a standard deviation of the data of 0.14%, which results in $F_{\text{ch,Co60}} = 1.1036$. The calibration data are shown in Figure 3, where significant chamber-to-chamber differences can be seen; note that these include the combined influence of the build-up caps and waterproof sleeves used. This experimental value of $F_{\text{ch,Co60}}$ agrees within about 0.12% with the value given in TRS-398 (1.102, see the rightmost column of Table 37 in TRS-398). The current ratio between $D_{\text{w,Co60}}(N_{D,\text{w}})$ and $D_{\text{w,Co60}}(N_{K}-N_{D,\text{air}})$ has the same level of agreement, as

$$\frac{D_{\text{w,Co60}}(N_{D,\text{w}})}{D_{\text{w,Co60}}(N_{K}-N_{D,\text{air}})} = \frac{N_{D,\text{w,Co60}}}{N_{D,\text{air,Co60}}F_{\text{ch,Co60}}} \rightarrow \frac{(F_{\text{ch,Co60}})_{\text{exp}}}{(F_{\text{ch,Co60}})_{\text{TRS-398}}} \quad (8)$$

thus superseding the approximate 1% difference quoted in the TRS-398 Code of Practice, specif-

ically 0.7% for the NE-2571 chamber. Numerical details of the calculations involved, rounded to three decimals, are given in Table 1; note that all the Monte Carlo calculated values shown have a statistical standard uncertainty $u_A \simeq 0.1\%$. Compared with the experimental value of $F_{\text{ch,Co60}}$, the difference of about 1.5% raised by the published Monte Carlo data on chamber perturbation factors mentioned above is not consistent with the use of the current key data and BIPM K_{air} and D_w standards if consistency throughout the entire dosimetry chain is sought. A different scenario could however be foreseen for the future on the light of other changes in key dosimetry quantities, that will be discussed in detail below.

To provide a more specific and detailed comparison with Monte Carlo calculations, new simulations have been carried out where an improved geometry description of the NE-2571 ionization chamber has been coded using information provided in the Nuclear Enterprises Ltd Report 3 (NE (1984)). Note that most references above were based on a simplified geometry of this chamber, as described by Aird and Farmer (1972). User codes in the current *EGSnrc* Monte Carlo system (Kawrakow *et al.* (2011)) have been used to derive air-kerma related quantities $N_{K,\text{air,Co60}}$ and $k_m k_{\text{att}} k_{\text{cel}}$ (*cavity*, Kawrakow *et al.* (2009)), and absorbed dose to water related quantities $N_{D,w,\text{Co60}}$, $D_w/D_{\text{air}} = F_{\text{ch,Co60}}$ (*egs_chamber*, Wulff *et al.* (2008b); Wulff (2010)), all with the mentioned statistical standard uncertainty $u_A \simeq 0.1\%$. The chamber geometry was described using the *egspp* library (Kawrakow *et al.* (2009)). The cut-off energies for particle production and transport in the calculations were set to 1 keV for photons and electrons. Rayleigh scattering and electron impact ionization were taken into account, and the XCOM photon cross sections and NIST bremsstrahlung cross sections selected for the simulations. All other parameters were left to their defaults as defined in the current *EGSnrc* version (V4-r2-3-2). Material data sets were prepared with restricted electronic mass stopping powers for $I_{\text{water}} = 75$ eV and $I_{\text{graphite}} = 78$ eV and other I -values from ICRU Report 37 (ICRU (1984)). The resulting figures are also included in Table 1. Comparing TRS-398 values and the new Monte Carlo calculations with ^{60}Co experimental data, it can be seen that the current status is

- (a) $F_{\text{ch,Co60}}[\text{TRS-398}]$ differs by -0.1%,
- (b) $D_{w,\text{Co60}} (N_{D,w}/N_K) [\text{TRS-398}]$ differs by -0.1%,
- (c) $F_{\text{ch,Co60}}[\text{MC}]$ differs by +1.0%, and
- (d) $N_{D,w}/N_K[\text{MC}]$ differs by +0.6%.

It is emphasized that the present Monte Carlo calculations would decrease the difference in $p_{\text{ch,Co60}}$ with TR-398 from 1.5% (references above) to 1.1%.

4 Beam quality factors k_Q for megavoltage photon beams

In the case of megavoltage photons, calculated beam quality factors would be affected by the increase in the values of p_{ch} predicted by the Monte Carlo calculations cited above, notably those of ^{60}Co . Values of k_Q have been provided by Wulff *et al.* (2008a) and Muir and Rogers (2010) in the form of tables and/or polynomial fits. Both sets of results, which in Wulff's case have been expanded to include source-surface-distance (SSD) and source-chamber-distance (SCD) configurations, as well as those from new Monte Carlo calculations according to the description above, have been obtained using the *egs_chamber* user code (Wulff *et al.* (2008b); Wulff (2010)). They all agree remarkably well despite the improved geometry description of the NE-2571 chamber, a finding which is consistent with previous observations of Wulff *et al.* (2010). The results are shown in Figure 4(a) along with the TRS-398 data, where sigmoidal fits of the form $k_Q = a/(1 + e^{(b-TPR_{20,10})/c})$ have been included for visualization purposes. An increasing difference with beam quality between the Monte Carlo and TRS-398 data can be seen, which becomes about 0.8% at the highest beam qualities. This difference is mainly due to the

large increase of p_{ch} at ^{60}Co discussed in the preceding section, entering into the factor $F_{\text{ch},\text{Co60}}$ in the denominator of k_Q , as for high photon energies the different perturbation factors entering into $F_{\text{ch},Q}$ (numerator of k_Q) do not differ from those in TRS-398 by more than 0.2%-0.3% (see Figures 1 and 2). Although it is almost certain that the Monte Carlo k_Q values would not vary much if certain key dosimetry data are changed (to be discussed later), as they include ratios of calculated quantities, a change in TRS-398 would again not be consistent with current metrology standards.

In addition, it is of importance to emphasize that (a) the common standard uncertainties of about 0.1% usually obtained in Monte Carlo calculations are only of the statistical type (u_A), and (b) the uncertainty of W_{air} still is one of the largest sources of uncertainty in ionization chamber dosimetry. Using the same relative standard uncertainty estimate for W_{air} as in TRS-398, Muir and Rogers (2010) stated a “systematic relative uncertainty”¹ of 0.85% for their calculated k_Q photon values, which is quite similar to the combined standard uncertainty estimate given in TRS-398, so that the two sets of data overlap considerably (see Figure 4(b)). There have been attempts by Muir *et al.* (2011) to decrease the uncertainty of their Monte Carlo calculated k_Q values by assigning any possible difference between the *EGSnrc* calculated and their own experimental k_Q values to a new W_{air} and $u(W_{\text{air}})$ estimate, but their approach is not endorsed here due to reasons that become apparent when the arguments below on experimental values are considered.

A comparison with experimental data of the Monte Carlo calculated values and those in TRS-398 is of importance in the present context. Figure 5 shows a compilation by Andreo (2000) of results obtained at primary standards laboratories, some of which were updated by Aalbers *et al.* (2008), that has been extended to include calorimetry determinations by Krauss and Kapsch (2007) and McEwen (2010); these two sets have stated uncertainties considerably lower than previous data. As above, sigmoidal fits have been included that in the case of the experimental values is weighted with their stated uncertainties. It can be observed that the experimental curve is positioned practically between the two sets of calculated values, showing no preference for one set over the other; the McEwen calorimetry results practically lie over the TRS-398 curve, although this might be a coincidence. An additional conclusion from this figure is that the scatter of the experimental data, possibly influenced by differences in the standards but, more importantly, due to chamber-to-chamber differences that include the influence of their waterproof sleeves (as in Figure 3 for ^{60}Co), shows the appropriateness of using values specifically measured for the user chamber in order to maintain consistency through the entire dosimetry chain. The chamber-to-chamber experimental differences also show why relying on a single source of experimental values to derive W_{air} and $u(W_{\text{air}})$ is not endorsed in this work.

To complicate the picture above even further, Wulff *et al.* (2008a) have shown a dependence of k_Q for the NE-2571 chamber for megavoltage photons on the mean excitation energy of graphite, the I -value entering into the stopping power formula, which results in differences of about 0.5% in k_Q for I -values of 78 eV and 86.8 eV; the k_Q values are higher for the higher I_{graphite} . An analysis of the potential impact of specific changes in I -values on the electronic mass stopping powers of materials of interest in reference dosimetry, and on the relevant stopping-power ratios required for the complete dosimetry chain, is therefore relevant.

¹Note that, quoting resolution INC-1 (1981) of the International Committee for Weights and Measures (Giacomo (1981); Kaarls (1981)), the Guide to the Expression of Uncertainty in Measurement (GUM) states that ‘the term “systematic uncertainty” can be misleading and should be avoided’ (JCGM (2008)).

5 Status of key data for reference dosimetry

5.1 The I -value of water

Despite the fact that liquid water is the most widely used “standard medium” in radiation dosimetry, it is still a substance subject to considerable debate from the perspective of energy loss by all types of charged particles, basically described by the well-known Bethe’s stopping power formulae (c.f. ICRU Reports 37 and 49 (ICRU (1984, 1993))). Recall that the mass electronic stopping power formula includes the logarithm of the mean excitation energy, the I -value, closely related to the electronic structure of a substance through its optical oscillator-strength (OOS) spectrum, $df(W)/dW$ (see e.g. Fano (1963) or Inokuti (1971)),

$$\ln I = \frac{\int_0^\infty \ln W \frac{df(W)}{dW} dW}{\int_0^\infty \frac{df(W)}{dW} dW} \approx \frac{\sum_i \ln E_i f_i}{\sum_i f_i} \quad (9)$$

where the integrals extend over all possible ionization and excitation atomic energy levels and $df(W)/dW$ is the number of electrons having energy W (i.e., oscillators with the same harmonic frequency). In practice, the denominator is approximated by the atomic number Z of the stopping medium, i.e. one associates a single oscillator to each atomic shell, $f_i = Z_i$, with binding energy E_i . Classical electrodynamics for dielectric media, on the other hand, establishes a direct relationship between the OOS and the dielectric response function (DRF) of a material, the latter being deduced from optical models based on experimental data or on semi-empirical approaches; the OOS can thus be determined practically from experimental grounds and an I -value derived.

For heavy particles with charge z and relativistic velocity β , the mass electronic stopping power formula is often written as

$$\frac{1}{\rho} S_{el} = 4\pi r_e^2 m_e c^2 N_A \frac{Z}{A} \frac{z^2}{\beta^2} L(\beta) \quad (10)$$

where r_e and $m_e c^2$ are the electron classic radius and its rest mass, N_A the Avogadro constant, and Z and A the atomic number and mass of the absorbing medium. The factor $L(\beta)$, called the stopping number, is given by a power series of z having the form

$$L(\beta) = L_0(\beta) + z L_1(\beta) + z^2 L_2(\beta) \quad (11)$$

where the first term is given by

$$L_0(\beta) = \ln \left(\frac{2m_e c^2 \beta^2}{(1 - \beta^2)I} \right) - \beta^2 - \frac{C(\beta)}{Z} - \frac{\delta(\beta)}{2} \quad (12)$$

in which $C(\beta)$ and $\delta(\beta)$ are the shell and density effect corrections, respectively. The terms $z L_1(\beta)$ and $z^2 L_2(\beta)$ correspond to the Barkas and Bloch corrections, respectively, taking into account the stopping power dependence on the sign of the incident particle charge (Barkas) and the departure from the Born approximation (both corrections). The approximate contribution of the different terms to the stopping number as a function of the energy are shown in Figure 6 for protons in water, illustrating the small size of the Barkas and Bloch corrections which are significant at low energies only, but are always smaller than the shell correction.

At the time of the development of ICRU-37 it was considered that the uncertainty of I_{water} did not play a substantial role in the stopping power of electrons at energies of interest in dosimetry. This was a reasonable assumption considering the uncertainties in radiation dosimetry achievable at that time. Today, however, the ICRU-37 assumption can be considered a debatable issue in the light of the current level of estimated uncertainties in the field, where stopping-power ratios for radiotherapy dosimetry are assumed to have an estimated uncertainty of a few tenths of a per cent. In addition, in the case of protons and heavier charged particles it has been shown that the value of I_{water} is critical for the position of the Bragg peak (Andreo (2009)), and that its uncertainty and that of the I -value for human tissues jeopardizes the spatial accuracy of clinical dose delivery in radiotherapy with heavy charged particles (Andreo (2009), Besemer *et al.* (2013)).

Since the comprehensive analysis of I -values in ICRU-37 a substantial number of investigations have produced various estimates of I_{water} using either dielectric-response functions (DRF) based on photon experimental data at low energies or stopping-power and range measurements of protons and heavier charged particles at high energies, where the conditions for Bethe's theory are valid and the influence of the corrections in the stopping power expression small, as shown in Figure 6. The I_{water} values so obtained are influenced by the intrinsic approximations made in each optical model or experimental approach, yielding a range of values that differ considerably. Furthermore, most of the determinations lack uncertainty estimations, and when they exist they are usually not consistent with current recommendations for the statement of uncertainties (e.g. JCGM (2008)). This diversity of I_{water} values has triggered investigations on their effect on stopping-power ratios for dosimetry but, interestingly, research has mainly been focused on carbon ions (e.g. Geithner *et al.* (2006); Henkner *et al.* (2009)). No attempt has yet been made for a proposal towards a harmonized value of the mean excitation energy of liquid water taking into account the considerable amount of data available.

ICRU-37 recommended an I_{water} value of 75 eV with an estimated uncertainty “smaller than or equal to 5%”. As described by Berger and Paul (1995), this value was obtained from the analysis of only four sets of values, two from $DRFs$ by Ritchie *et al.* (1978) and Ashley (1982) and two from stopping-power and range measurements in protons and pions by Thompson (1952) and Nordin and Henkelman (1979) respectively. In a “post-concluded” report footnote ICRU-49 referred to a new experimental determination by Bichsel and Hiraoka (1992) in 70 MeV protons leading to a value of 79.7 ± 0.5 eV, “larger than the recommended 75 ± 3 eV but still lying within the limits of error quoted in ICRU-37”. This value was confirmed by Bichsel *et al.* (2000) in experiments with carbon ions, obtaining 80 ± 1.3 eV, although a number of approximations were made in the experimental determination.

In an analysis by Paul *et al.* (2007) a value implicitly recommended in ICRU Report 73 (ICRU (2005)) of 67.2 eV was questioned, and based on the DRF -based value calculated by Dingfelder *et al.* (1998) of 81.8 eV and that measured by Bichsel and Hiraoka, the authors suggested a value of 80.8 ± 2 eV, well outside the uncertainty limits of ICRU-37. Shortly after, Paul (2007) referred to a previously published indirect experimental determination by Sihver *et al.* (1998), obtained in the comparison of an analytical model with experimental depth-ionization curves of 195 MeV and 270 MeV carbon ions, concluding that “the value of 75 eV from ICRU-49 agrees best with Sihver's experimental value”. The same set of experimental data with carbon ions was used by Krämer *et al.* (2000) to benchmark the physical model used for the radiotherapy treatment planning at the GSI centre in Darmstadt, Germany, stating that a value of 77 eV was required in their case to reproduce measured Bragg peak positions. The implicit low value of 67.2 eV in the stopping power data of ICRU-73 was subsequently corrected by ICRU (2009) and a tentative value of 78 eV recommended, which was based solely on ion measurements by Schardt *et al.* (2008), described in a GSI scientific report.

From the perspective of electrodynamics of dielectric media, a recent study by Emfietzoglou *et al.* (2009) has suggested an I_{water} value of 77.8 eV based on a DRF deduced from the most recent x -ray spectroscopy data for liquid water (Hayashi *et al.* (2000)); from an analysis of the DRF properties, these authors also provided a semi-quantitative uncertainty margin of ± 1 eV. This significant study included a thorough compilation of previously published values, mostly derived using analogous numerically-based approaches, some of which relied on different experimental reflectance and spectroscopy data (the so-called REF and $IXSS$ data sets, see Table 2). These I_{water} values varied between the 72.5 eV of Tan *et al.* (2004) and the 82.4 eV of Emfietzoglou *et al.* (2005).

A compilation by Burns and Andreo (2012) of experimental data and DRF -based values, used for work commissioned for an ICRU task group, is given in Table 2; the values have been selected from a broad search and analysis of published data, already initiated in Vatnitskiy *et al.* (2011). The selection excludes certain I_{water} values where important corrections have not been taken into account, for instance multiple scattering corrections in low-energy electron measurements or corrections in the stopping powers of heavy charged particles at low energies (see Figure 6), or significant details for the derivation of I_{water} not given.

Whereas it is usual that experimental determinations include an uncertainty estimate, this is, however, not a straightforward task in DRF -based studies where a large number of steps and numerical procedures are involved. Burns and Andreo made an uncertainty estimate for the DRF -based data using the results of a set of publications by Emfietzoglou and collaborators (see Table 2) based on different physical models and optical data that can be considered representative of the entire set of DRF values. The different models introduced a standard uncertainty of 2.5 eV and the optical data 3.3 eV. In summary, this analysis resulted in the mean DRF -based value for I_{water} of 78.4 eV with a standard uncertainty of 4.2 eV (which is very close to the standard deviation of the DRF -based data set). For the experimental values, Burns and Andreo used a weighted statistical analysis, based on the Mandel-Paule method (Mandel and Paule (1970)) in which the stated experimental uncertainties were increased to estimates that result in a Birge-ratio equal to one (Birge (1932)); the required increase was 1.8 eV (added in quadrature). The result of this analysis is the mean experimental value 77.8 eV with standard uncertainty 2.0 eV. The experimental result is then combined with that of the theoretical data, yielding the final rounded value $I_{\text{water}} = 78$ eV with a standard uncertainty of 2 eV, see figure 7. This value happens to be in good agreement with the ICRU (2009) tentative value, which, as already mentioned, does not take into account DRF -based determined values.

5.2 The I -value for graphite

Ionometric primary standards based on graphite-walled cavity ionization chambers (c.f. Büermann and Burns (2009)) require the value for W_{air} and the stopping-power ratio $s_{\text{graphite-air}}$. These quantities are also of importance in different steps of reference radiotherapy dosimetry based on air-kerma and absorbed dose to water calibration coefficients, and consistency requires that the values be identical throughout the entire dosimetry process. The values in current use are based on $W_{\text{air}} = 33.97$ eV and $I_{\text{graphite}} = 78.0$ eV for the measured (bulk) graphite density (ICRU (1984)).

A recent analysis has been made by Burns (2012) of results obtained in over forty experiments that have determined either W_{air} , I_{graphite} , or the product $W_{\text{air}}s_{\text{graphite-air}}$ for ^{60}Co γ -rays. This work updates a previous analysis of Burns (2009) by including additional data and making robust and self-consistent estimates of the required key quantities. The results of this process were the values $W_{\text{air}} = 33.97 \pm 0.11$ eV, identical to that currently recommended but with a higher uncertainty, $s_{\text{graphite-air}} = 0.9926$ with relative standard uncertainty 0.32%, and the

product $W_{\text{air}} s_{\text{graphite-air}} = 33.72$ eV with standard uncertainty 0.08%. The resulting value for I_{graphite} depends on the treatment of the density effect in graphite, the best estimate being the value of 81.1 ± 2.0 eV obtained when using the grain density ($\rho = 2.265$ g cm⁻³) in the evaluation of the graphite stopping power.

6 Potential impact of new I -values on reference dosimetry

With regard to water, the most significant impact of the 4% increase in I_{water} would be a decrease in the water-to-air stopping-power ratio, which for all types of megavoltage radiotherapy beams is calculated to be between approximately 0.3% and 0.6%. Figure 8 shows the ratio of $s_{\text{w-air}}$ at the reference depth resulting from the newly proposed I_{water} value and from that of ICRU-37, 78 eV and 75 eV respectively, for photons and electron beams. It is observed that the decrease is practically constant for electron beams of different qualities (R_{50}), being about 0.3%, while it varies from 0.6% for ⁶⁰Co to 0.3% for the highest photon beam quality ($TPR_{20,10} = 0.8$). The calculations of $s_{\text{w-air}}$ were made with the *EGSnrc* user code *SPRRZnrc* (Rogers *et al.* (2011)) using 10 clinical electron beam spectra taken from Ding and Rogers (1995) and 14 photon spectra from the classic set of Mohan *et al.* (1985) and from Sheikh-Bagheri and Rogers (2002). For the restricted stopping power data used in the Monte Carlo calculations, density effect corrections consistent with this I_{water} were obtained using version 2 of the *STAR* package as distributed by the IAEA (Berger (1993)).

For protons and carbon ions, Figure 9 illustrates the depth variation of $s_{\text{w-air}}$ for the two I_{water} values in two mono-energetic beams, showing in both cases a practically constant difference of about 0.4% to 0.5% at the plateau and at the distal edge of the Bragg-peak, where the abrupt increase in $s_{\text{w-air}}$ occurs (Medin and Andreo (1997)). In this case, the Monte Carlo calculations were made with the *SHIELD-HIT* v10 code (N. Sobolevsky, priv comm.; see Gudowska *et al.* (2004) for a description of the code) in conjunction with stopping powers obtained with *STAR* v2 for protons, and a renormalization of the ICRU-73 values using the *BEST* computer code described by Berger and Paul (1995) for carbon ions.

The influence of the increased I_{water} on calculated ion chamber perturbation factors is, on the other hand, well below the differences above, becoming practically negligible. It is clear then that when reference dosimetry is based on ratios of $s_{\text{w-air}}$ values at two beam qualities, the changes mentioned have a minor effect (up to 0.3%) for most particle types, as is the case in determinations based on absorbed dose to water standards, through k_Q values; a more detailed global analysis is presented below. When reference dosimetry is based on air-kerma standards and $s_{\text{w-air}}$ does not appear in a ratio, the estimated decrease in stopping-power ratios apply fully, bringing us back to the ⁶⁰Co issue where the decrease in $s_{\text{w-air}}$ would be of 0.6%.

More significant implications can be inferred in the case of I_{graphite} , where the recent analysis of Burns (2012) raises its value from 78 eV to 81 eV. New graphite stopping powers would enter into $p_{\text{ch,Q}}$ calculations yielding changes of the order of a few tenths of a per cent. Of larger significance, however, is that a new I_{graphite} could affect all the air-kerma standards for ⁶⁰Co, including the BIPM standard, reducing it by an estimated 0.7% and therefore decreasing the calibration coefficients $N_{K,\text{air,Co60}}$ and $N_{D,\text{air,Co60}}$ by the same amount. As the BIPM standard for absorbed dose to water is not expected to be modified due to the reasons noted in Section 3, this decrease would approximately cancel the 0.54% increase of 2007 and return to a situation similar to that before 2007. Consequently, the $F_{\text{ch,Co60}}$ value given in TRS-398 would have to be modified, requiring an increase of the order of 0.7%-0.8% in order to agree with the experimental value. On the other hand, this would be the most favourable situation for the new Monte Carlo $F_{\text{ch,Q}}$ calculations, which using the new stopping powers would agree at the level of about 0.1% with the experimental value of $F_{\text{ch,Co60}}$.

The availability of the BIPM key comparison database (KCDB, see <http://kcdb.bipm.org/>) enables the present analysis to be referred to worldwide standards rather than restricting it to the BIPM standards. The KCDB provides the results of comparisons of national primary standards with the BIPM standards. By taking the mean value of these results, ratios of the “world-to-BIPM” K_{air} and D_{w} standards of 1.0014 and 0.9975, respectively, are obtained. These can be used to arrive at conclusions de-coupled from the BIPM and linked to world averages of $N_{K,\text{air},\text{Co60}}$ and $N_{D,\text{w},\text{Co60}}$, independent of a particular laboratory. This process yields an $F_{\text{ch},\text{Co60}}$ value differing from TRS-398 by about 0.4% and still agreeing with the new Monte Carlo value within 0.3%.

The estimated changes for a NE-2571 chamber are summarized in Table 3, where all the quantities have been updated according to electronic stopping powers using the new I -values, including the *EGSnrc* Monte Carlo calculations; electronic stopping power data were obtained as in the case of water described above. It is worth noting that the product of chamber corrections $k_{\text{m}}k_{\text{att}}k_{\text{cel}}$ remains practically unchanged in these new calculations, so that the difference in $N_{D,\text{air},\text{Co60}}$ is solely due to the change in $N_{K,\text{air},\text{Co60}}$. The estimates are given separately for calibrations traceable to the BIPM and to world averages. The current values in TRS-398 for $F_{\text{ch},\text{Co60}}$ etc are included for comparison. The rightmost column gives the predicted modifications in our Monte Carlo calculated values following a potential update of I -values in the form of the ratio future/current; note that the quantities shown become modified whenever they do not involve ratios of similar Monte Carlo quantity estimates, as is the case with $N_{D,\text{w}}$ and N_K . For the other quantities one can see that the controversial $p_{\text{ch},\text{Co60}}$ values discussed earlier are confirmed only because there is a balance with the change in $s_{\text{w-air},\text{Co60}}$, as $F_{\text{ch},\text{Co60}}$ must remain constant. It can be observed that the new Monte Carlo values change at most by about half a per cent with respect to the calculations based on the currently recommend I -values used in Table 1.

Comparing this future scenario for ^{60}Co experimental data with the current TRS-398 values and the new Monte Carlo calculations following the adoption of new mean excitation energies, the status would be

- (a) $F_{\text{ch},\text{Co60}}[\text{TRS-398}]$ would differ by -0.8% (BIPM) and -0.4% (world),
- (b) $D_{\text{w},\text{Co60}}(N_{D,\text{w}}/N_K)[\text{TRS-398}]$ would differ by -0.8% (BIPM) and -0.4% (world),
- (c) $F_{\text{ch},\text{Co60}}[\text{MC}]$ would differ by -0.1% (BIPM) and +0.3% (world), and
- (d) $N_{D,\text{w}}/N_K[\text{MC}]$ would differ by -0.1% (BIPM) and +0.3% (world).

that is, compared with Table 1, the differences for TRS-398 and for the Monte Carlo data with respect to the BIPM standards would become practically reversed. Compared with the world average of standards the two data sets would lie within an interval between -0.4% and +0.3%.

As already mentioned, beam quality factors for megavoltage beams are not expected to change due to the use of ratios of the quantities discussed above. This has been verified for the NE-2571 chamber and the photon beam qualities of Figure 8a, calculating by Monte Carlo simulation the factor $F_{\text{ch},\text{Q}}$ directly as the ratio $D_{\text{w},\text{Q}}/D_{\text{air-ch},\text{Q}}$, and determining k_{Q} according to equation (6). The decrease obtained for the various $F_{\text{ch},\text{Q}}$ varies between 0.2% and 0.5%, differences that include the potential changes both in $s_{\text{w-air}}$ and $p_{\text{ch},\text{Q}}$, but the differences in k_{Q} values are in all cases smaller than 0.2%, confirming the expected trend. It needs to be emphasized, however, that the constancy in the Monte Carlo calculated k_{Q} values does not solve the problematic situation discussed earlier in relation to their comparison with experimental values and the preference for beam quality factors specifically measured for the user chamber.

6.1 The special case of proton reference dosimetry

The analysis of proton reference dosimetry presents an additional challenge because, in addition to the $F_{\text{ch,Q}}$ and $F_{\text{ch,Co60}}$ factors already discussed, the mean energy required to produce an ion pair in dry air in proton beams, $W_{\text{air,Q}}$, needs to be taken into account. This quantity has, prior to the publication of IAEA TRS-398 and ICRU Reports 59 and 78 (ICRU (1998, 2007)), most often been determined by comparing ionization chamber dosimetry using the N_K - $N_{D,\text{air}}$ formalism with calorimetry measurements according to (see eq. (3)):

$$W_{\text{air,Q}} = \frac{D_{\text{w,Q}}^{\text{calor}}(z_{\text{ref}})}{M_{\text{w,Q}}(z_{\text{ref}})N_{D,\text{air,Co60}}} \frac{W_{\text{air,Co60}}}{F_{\text{ch,Q}}} \quad (13)$$

If the relative changes of the factors on the right hand side are small, the change in $W_{\text{air,Q}}$ can be expressed as:

$$\Delta(W_{\text{air,Q}}) \approx \Delta(W_{\text{air,Co60}}) - \Delta(N_{D,\text{air,Co60}}) - \Delta(F_{\text{ch,Q}}) \quad (14)$$

A change in $F_{\text{ch,Q}}$ would solely be based on that of $s_{\text{w-air}}$ for protons (-0.4%), given that Monte Carlo studies have indicated that the chamber perturbation correction factor for the NE-2571 in proton beams is close to unity (Palmans et al. 2001; Verhaegen and Palmans 2001; Palmans 2011). Thus, the value of $W_{\text{air,Q}}$ would solely be affected by the changes in $N_{D,\text{air,Co60}}$ (0.7%) and $F_{\text{ch,Q}}$, as $W_{\text{air,Co60}}$ remains constant (Burns (2012)). Note, however, that all the determinations of the $W_{\text{air,Q}}$ value for protons according to equation (13) had been made prior to the change of the BIPM air-kerma standard (and comparable changes to other primary air-kerma standards) in 2007, hence the net change from those determinations amounts to +0.2%. The estimated changes in the different components would then yield an overall increase in $W_{\text{air,Q}}$ of about 0.6%, i.e. from the current 34.23 J/C to 34.44 J/C. A small number of publications on the determination of $W_{\text{air,Q}}$ prior to the publication of IAEA TRS-398, as well as all the papers on this topic during the last seven years, were based on a comparison of ionization chamber dosimetry using the $N_{D,\text{w}}$ formalism and calorimetry. Note that because the arguments provided on the N_K - $N_{D,\text{air}}$ formalism are based on the ratio of experimental coefficients in ^{60}Co , the change in $W_{\text{air,Q}}$ determined via the $N_{D,\text{w,Co60}}$ route would be entirely consistent with this estimated increase, as

$$W_{\text{air,Q}} = \frac{D_{\text{w,Q}}^{\text{calor}}(z_{\text{ref}})}{M_{\text{w,Q}}(z_{\text{ref}})N_{D,\text{w,Co60}}} \frac{W_{\text{air,Co60}}F_{\text{ch,Co60}}}{F_{\text{ch,Q}}} \quad (15)$$

thus confirming the estimate of $W_{\text{air,Q}} = 34.44$ J/C. If the relative changes of the different factors on the right hand side are small, the change in $W_{\text{air,Q}}$ can be expressed as:

$$\Delta(W_{\text{air,Q}}) \approx \Delta(W_{\text{air,Co60}}) + \Delta(F_{\text{ch,Co60}}) - \Delta(F_{\text{ch,Q}}) \quad (16)$$

i.e., no change in the value of $N_{D,\text{w,Co60}}$ is accounted for since the absorbed dose to water standard of the BIPM has been unaltered.

The combination of changes mentioned in these possible scenarios would not affect current TRS-398 calculated k_Q values for the NE-2571 chamber in radiotherapy proton beams. Indeed, the calorimetric determinations of $W_{\text{air,Q}}$ are essentially measurements of k_Q and if consistency is maintained in the data used for deriving $W_{\text{air,Q}}$ and in the subsequent re-calculation of k_Q , the latter would remain unaffected; this is reflected in the cancellation of the various changes shown in Table 4. The cancellation confirms the need for maintaining consistency in an analysis that unavoidably must include the data in the complete dosimetry chain. These arguments and

estimates would also be applicable to calorimetrically determined $W_{\text{air,Q}}$ values for ions heavier than protons, unless specific new values of $W_{\text{air,Q}}$ for these particles, different from those in TRS-398, would become available. It is also worth noting that although the discussion above has been focused on the BIPM standards, the final estimates for $W_{\text{air,Q}}$ and k_Q would be identical using the world average of standards.

To conclude, it needs to be recalled that the current $W_{\text{air,Q}}$ value for protons originates from the re-evaluation by Medin *et al.* (2000) of a compilation in ICRU Report 59 (ICRU (1998)), in which several dosimetry inconsistencies were found. This set of data was updated and statistically analysed in TRS-398 (Andreo *et al.* (2000)), leading to the recommended current value (34.23 J/C). As reviewed in Palmans (2012), a subsequent update and analysis by Jones (2006) suggested using only calorimetric data, obtaining for this specific data set a $W_{\text{air,Q}}$ value consistent with that in TRS-398, which is now endorsed by the ICRU (ICRU (2007)). Although our predicted increase over the currently recommended value of $W_{\text{air,Q}}$ for protons would be independent of the ionometric standard and formalism used, N_K - $N_{D,\text{air}}$ or $N_{D,\text{w,Co60}}$, our work suggests that there could be a need for revising the current recommendation. An examination of the various compilations and analysis deriving a $W_{\text{air,Q}}$ value shows that the issue of data consistency has not been fully addressed. For example in the most recent analysis, by Jones (2006), the data had mostly been corrected for the difference in stopping-power ratios water-to-air (those by Medin and Andreo (1997) versus Janni (1982) or ICRU (1993)) but differences in other basic data included in the dosimetry protocols used, especially AAPM Report 16 (Lyman *et al.* (1986)), the first ECHED (Vynckier *et al.* (1991)) or more recent protocols, had been ignored. Also, the values of $F_{\text{ch,Co60}}$ used in the derivation of $W_{\text{air,Q}}$ from a comparison of ionization chamber dosimetry using the $N_{D,\text{w}}$ formalism and calorimetry, may not be consistent with experimental values across all chamber types (at least ten different chamber types have been involved in the evaluations leading to the data compiled by Jones). Thus, even if Allisy-Roberts *et al.* (2009) have shown that standards worldwide are in excellent agreement (see also the BIPM key comparison database (KCDB); the standard deviation of the results for K_{air} worldwide is 0.2%) and it is most likely that the projected change in the BIPM K_{air} standard will also be implemented in other national standards, the lack of data consistency in various steps of the dosimetry chain used to derive $W_{\text{air,Q}}$ advises a future revision as suggested above.

7 Summary and conclusions

Triggered by the substantial changes in ionization chamber perturbation correction factors for ^{60}Co γ -rays suggested by recent Monte Carlo calculations, which would cause a decrease of about 1.5% in the reference dosimetry of all types of charged particles (electrons, protons and heavier ions) based on calculated k_Q values, a detailed analysis of the data used throughout the complete dosimetry chain has been conducted.

Taking into account that the ratio of ionization chamber calibration coefficients in ^{60}Co in terms of absorbed dose to water and air-kerma, $N_{D,\text{w,Co60}}$ and $N_{K,\text{air,Co60}}$, yields an experimental value of $F_{\text{ch,Co60}} = (s_{\text{w-air}} p_{\text{ch}})_{\text{Co60}}$ through the $N_{D,\text{air,Co60}}$ coefficient, data provided by the IAEA Dosimetry Section for a large set of NE-2571 chambers have been used as experimental reference. These calibrations are traceable to current BIPM K_{air} and D_{w} standards in use since 2007. The average experimental $F_{\text{ch,Co60}}$ value has been compared with that deriving using the Monte Carlo calculations mentioned above, using new simulations carried out for the present work, and with the value included in IAEA TRS-398. It has been shown that TRS-398 data agrees at the level of 0.12% with the experimental reference value, superseding the approximate 1% difference quoted in the protocol, specifically 0.7% for the NE-2571 chamber. The use of new $p_{\text{ch,Co60}}$ resulting

from recent Monte Carlo calculations, yielding a 1.5% difference in reference dosimetry, cannot be justified in conjunction with current fundamental data and BIPM standards if consistency in the entire dosimetry chain is sought. New Monte Carlo calculations carried out for this work decrease the difference in $p_{\text{ch,Co60}}$ with TRS-398 from 1.5% to 1.1%, but still the difference with the experimentally determined $F_{\text{ch,Co60}}$ is 1%.

For megavoltage photons, Monte Carlo calculated beam quality factors k_Q for the NE-2571 chamber have been compared to those in TRS-398. When the same uncertainty is considered in both cases for the mean energy required to produce an ion pair in dry air, $W_{\text{air,Q}}$, the two sets of data overlap considerably. They have been compared with k_Q measurements at standards laboratories, whose results lie practically between the two sets of calculated values, showing no preference for one set over the other. The observed chamber-to-chamber differences (also seen for ^{60}Co), shows the appropriateness of using k_Q values specifically measured for the user chamber.

Current developments on the mean excitation energies for the mass electronic stopping powers of water and graphite have been presented, proposing a weighted average value of $I_{\text{water}}=78 \pm 2.0$ eV, which is based on published experimental values and values determined using dielectric response functions (*DRF*). Adopting this increase in I_{water} over the current recommended value (75 eV) would decrease the water-to-air stopping-power ratio for all types of megavoltage radiotherapy beams between 0.3% and 0.6% approximately. The implications of a recently suggested new value for I_{graphite} , raising it from 78 eV to 81 eV, have also been analyzed, and as a result of the corresponding potential change in the ^{60}Co BIPM standard for K_{air} of 0.7%, the $N_{K,\text{air,Co60}}$ and $N_{D,\text{air,Co60}}$ of users chambers would decrease by the same amount.

The impact of adopting these new mean excitation energies would be to raise the experimental $F_{\text{ch,Co60}}$, which for the NE-2571 chamber and referring to BIPM standards would require an increase of about 0.8% with respect to the current TRS-398 value. Monte Carlo $F_{\text{ch,Q}}$ calculations using the new stopping powers would, on the other hand, agree at a level of 0.1% with the ^{60}Co experimental value of $F_{\text{ch,Co60}}$, confirming the need for consistency in the dosimetry chain data. Should world average standards be used as reference, the figures would become +0.4% for TRS-398 and -0.3% for the Monte Carlo calculation. Megavoltage photons k_Q values have been calculated with this $F_{\text{ch,Co60}}$ and the new stopping power data used to determine $F_{\text{ch,Q}}$ at other beam qualities. Although the latter decrease by amounts of between 0.2% and 0.5%, when they enter as a ratios in k_Q the differences with previous k_Q calculated values are in all cases smaller than 0.2%. This constancy in the Monte Carlo calculated k_Q values does not resolve, however, the observed differences between calculated and measured k_Q values and the preference remains for beam quality factors specifically measured for user chambers.

In the case of proton beams the largest consequence of the changes mentioned would be the need for increasing $W_{\text{air,Q}}$ by about 0.6%, as this quantity is derived from the combination of calorimetric and ionometric measurements. The combination of the changes mentioned in this possible scenario would result in no change for the current TRS-398 calculated k_Q (NE-2571) for radiotherapy proton beams. The same conclusion applies for ions heavier than protons. Also in these advanced radiotherapy modalities, the need for maintaining consistency in an analysis that unavoidably must include the complete dosimetry chain is demonstrated.

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10 Tables and Figures

Table 1: Comparison of dosimetry quantities at the reference quality of ^{60}Co γ -rays for NE-2571 ionization chambers. The experimental reference is for a set of calibration coefficients from the IAEA Dosimetry Laboratory for 91 chambers, see Figure 3, traceable to current BIPM K_{air} and D_{w} standards (as of 2007).

	Past (< 2007)	Present (≥ 2007)	TRS-398 ^a	Monte Carlo present ^b
$N_{D,\text{w},\text{Co60}}$ (IAEA)	45.28	45.28		
$N_{K,\text{air},\text{Co60}}$ (IAEA)	41.26	41.48		
$N_{D,\text{w}}/N_K$	1.097		1.091	1.098
$k_{\text{m}}k_{\text{att}}k_{\text{cel}}^{\text{c}}$	0.992			0.988
$1 - \bar{g}_{\text{air}}$	0.997			
$N_{D,\text{air}}$	40.81	41.03		
$N_{D,\text{w}}/N_{D,\text{air}} = F_{\text{ch},\text{Co60}}$	1.110	1.104		
$F_{\text{ch},\text{Co60}} = s_{\text{w-air}}p_{\text{ch}}$	1.110	1.104	1.102	1.114
$s_{\text{w-air}}(\Delta = 10 \text{ keV})$	1.133	1.133	1.133	1.134
p_{ch} (from above)	0.979	0.974	0.972	0.983
$D_{\text{w}}(N_{D,\text{w}}/N_K)$ [TRS-398]	1.007	1.001		

^a From Table 37 in IAEA TRS-398, Andreo *et al.* (2000).

^b This work, based on improved geometry description.

^c $k_{\text{m}}k_{\text{att}}=0.985$ (TRS-277); $k_{\text{cel}}=1.007$ ($1/p_{\text{cel}}$ in TRS-398 Table 37.)

Table 2: Compilation of experimental (measured energy-range distributions) and dielectric response function (DRF)-based published values of the mean excitation energy of liquid water used in the present analysis.

Reference	I_{water} (eV)	stated		Method	Comments
		std unc (eV)	adopted ^a std unc (eV)		
Thompson (1952)	75.4	1.0 ^b	2.0	Experimental	340 and 200 MeV protons, based on $I_{\text{Cu}}=322$ eV
Nordin and Henkelman (1979)	74.6	1.4 ^b	2.3	Experimental	60 MeV pions
Bichsel and Hiraoka (1992)	79.7	0.3	1.8	Experimental	70 MeV protons, based on $I_{\text{Al}}=166$ eV
Krämer <i>et al.</i> (2000) - Sihver <i>et al.</i> (1998)	77.0	2.0 ^c	2.7	Experimental	195 MeV and 270 MeV carbon ions
Bichsel <i>et al.</i> (2000)	80.0	0.7	1.9	Experimental	290 MeV carbon ions
Kumazaki <i>et al.</i> (2007)	78.4	0.8	2.0	Experimental	150 MeV, 190 MeV and 230 MeV protons
Scharadt <i>et al.</i> (2008)	78.0	1.0	2.1	Experimental	Ions (^1H , ^3He , ^7Li , ^{12}C , ^{16}O) up to 400 MeV
Ritchie <i>et al.</i> (1978)	75.0		4.2	DRF	REF optical data ^d
Ashley (1982)	75.4		.	DRF	Semi-empirical model
LaVerne and Mozumder (1986)	74.9		.	DRF	Semi-empirical model
Dingfelder <i>et al.</i> (1998)	81.8		.	DRF	Semi-empirical model
Akkerman and Akkerman (1999)	74.0		.	DRF	Semi-empirical model
Tan <i>et al.</i> (2004)	72.5		.	DRF	Semi-empirical model
Emfietzoglou (2003)	80.9		.	DRF	REF optical data ^d
Emfietzoglou and Nikjoo (2005)	85.4		.	DRF	REF optical data ^d
Emfietzoglou and Nikjoo (2005)	80.7		.	DRF	IXSS optical data ^e
Emfietzoglou <i>et al.</i> (2005)	82.4		.	DRF	IXSS optical data ^e
Emfietzoglou <i>et al.</i> (2009)	77.8	1.0	.	DRF	IXSS optical data ^e
Garcia-Molina <i>et al.</i> (2009)	79.4		4.2	DRF	IXSS optical data ^e

^a The adopted standard uncertainties for the experimental values are chosen to give a Birge ratio of unity for this data set. The standard uncertainty of 4.2 eV for the mean of the DRF values is derived as described in the text.

^b Uncertainties quoted by Berger and Paul (1995) as used in ICRU-37 (1984).

^c This value is taken as the standard deviation of the experimental data set and is consistent with the authors' statement of a Bragg-peak shift of 5 mm for a 2 eV change in I_{water} .

^d Reflectance measurements by Heller *et al.* (1974).

^e Inelastic x -ray scattering spectroscopy by Hayashi *et al.* (2000).

Table 3: Potential changes in dosimetric quantities at the reference quality of ^{60}Co γ -rays for NE-2571 ionization chambers due to the adoption of new mean excitation energies, I_{water} and I_{graphite} . The experimental references $N_{D,w}/N_{D,\text{air}} = F_{\text{ch,Co60}}$ are the estimated updates of the current calibration coefficients from the IAEA Dosimetry Laboratory in Table 1, traceable to the BIPM and to the world average of standards. The scenario for the future includes new stopping powers and assumes a 0.7% decrease in the K_{air} standards.

	Future (rel to BIPM)	Future (rel to world)	TRS-398 ^a	Monte Carlo future ^b	Monte Carlo future/present
$N_{D,w,\text{Co60}}$ (IAEA)	45.28	45.16			
$N_{K,\text{air,Co60}}$ (IAEA)	41.20	41.25			
$N_{D,w}/N_K$	1.099	1.095		1.098	1.000
$k_{\text{m}}k_{\text{att}}k_{\text{cel}}$ ^b	0.992			0.992	1.004
$1 - \bar{g}_{\text{air}}$	0.997				
$N_{D,\text{air}}$	40.75	40.81			
$N_{D,w}/N_{D,\text{air}} = F_{\text{ch,Co60}}$	1.111	1.107			
$F_{\text{ch,Co60}} = s_{w,\text{air}}p_{\text{ch}}$	1.111	1.107	1.102	1.110	0.996
$s_{w,\text{air}}(\Delta = 10 \text{ keV})$	1.127		1.133	1.127	0.994
p_{ch} (from above)	0.986	0.982	0.972	0.984	1.002
$D_w(N_{D,w}/N_K)$ [TRS-398]	1.008	1.004			

^a From Table 37 in IAEA TRS-398, Andreo *et al.* (2000)

^b This work, based on new electronic stopping powers

Table 4: Potential changes in $W_{\text{air},Q}$ and in the calculated values of k_Q for radiotherapy proton and heavier ion beams due to the adoption of new mean excitation energies, I_{water} and I_{graphite} as well as other changes in air-kerma standards. The changes are determined from those estimated for the quantities F_{ch} and W_{air} for the qualities ^{60}Co and Q .

Quantity	Estimated change (%)	Comment
$W_{\text{air},\text{Co60}}$	0	see Burns (2012)
$N_{D,\text{air},\text{Co60}}$	-0.2	due to change in $N_{K,\text{air},\text{Co60}}$ from pre-2007 value
$N_{D,\text{w},\text{Co60}}$	0	
$F_{\text{ch},\text{Co60}}$	+0.2	experimental ratio $(N_{D,\text{w}}/N_{D,\text{air}})_{\text{Co60}}$
$F_{\text{ch},Q}$	-0.4	due to change in $s_{\text{w-air},Q}$, assumes no change in $p_{\text{ch},Q}$
$W_{\text{air},Q}$	+0.6	eqs.(13) and (15) yielding 34.44 J/C
$k_{Q,\text{Co60}}^{\text{calc}}$	0	eq. (6)

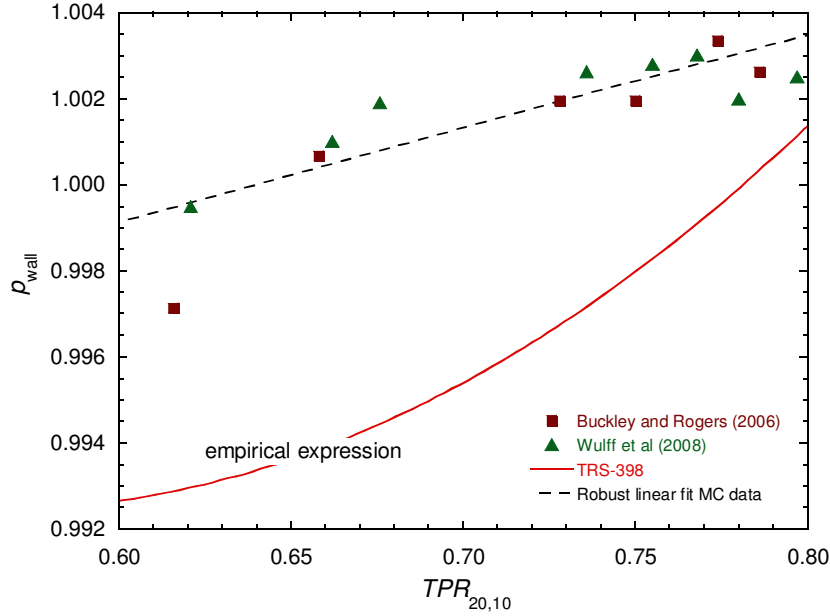


Figure 1: Chamber wall perturbation correction factors for a Farmer NE-2571 as a function of photon beam quality. The solid line corresponds to the empirical expression by Almond and Svensson (1977) used in IAEA TRS-398 and the dashed line is a robust linear fit to Monte Carlo calculated values by different authors (symbols). Adapted from Benmakhlouf and Andreo (2011).

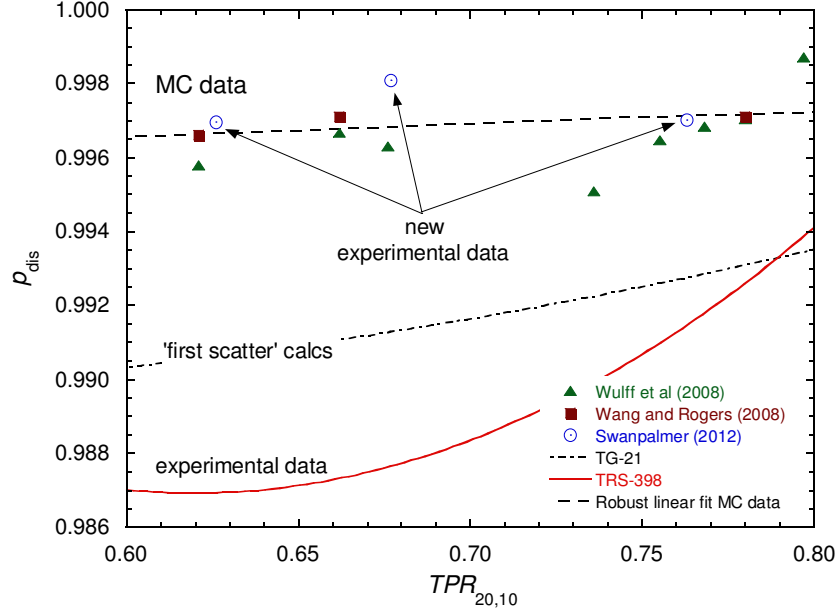


Figure 2: Displacement perturbation correction factors for a Farmer NE-2571 as a function of photon beam quality. The solid line corresponds to the experimental data of Johansson *et al.* (1978) used in IAEA TRS-398, and the dashed-dotted line to the calculations of Cunningham and Sontag (1980) used in AAPM TG-51. The dashed line is a robust linear fit to Monte Carlo calculated values by different authors (symbols). The arrows indicate new experimental data (open dotted circles) by Swanpalmer and Johansson (2012).

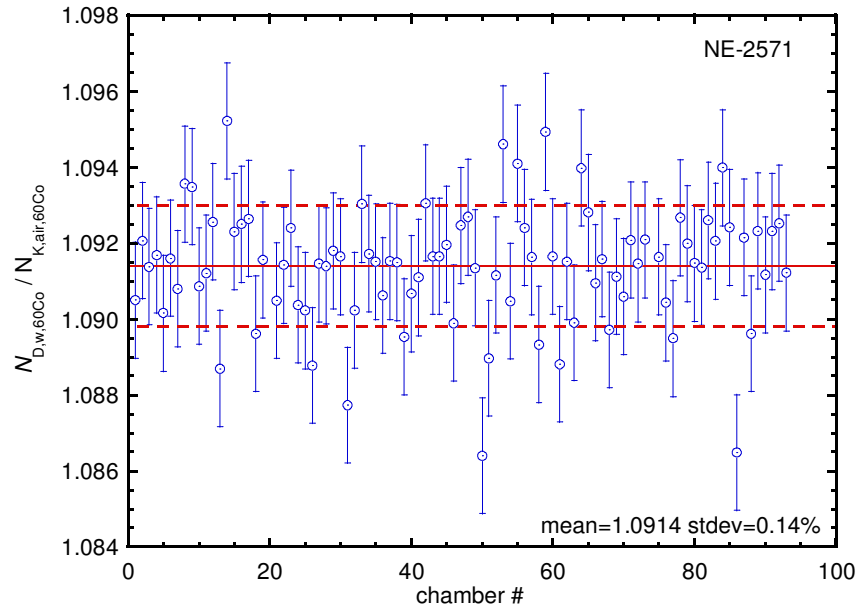


Figure 3: Ratio of calibration coefficients $N_{D,w,Co60}/N_{K,air,Co60}$ traceable to current BIPM K_{air} and D_w standards for a sample of 91 NE-2571 chambers. The chamber-to-chamber differences include the combined influence of build-up caps and waterproof sleeves. The mean value (solid horizontal line) and $\pm$ standard deviation of the data (dashed lines) are indicated. Data courtesy of the IAEA Dosimetry Section.

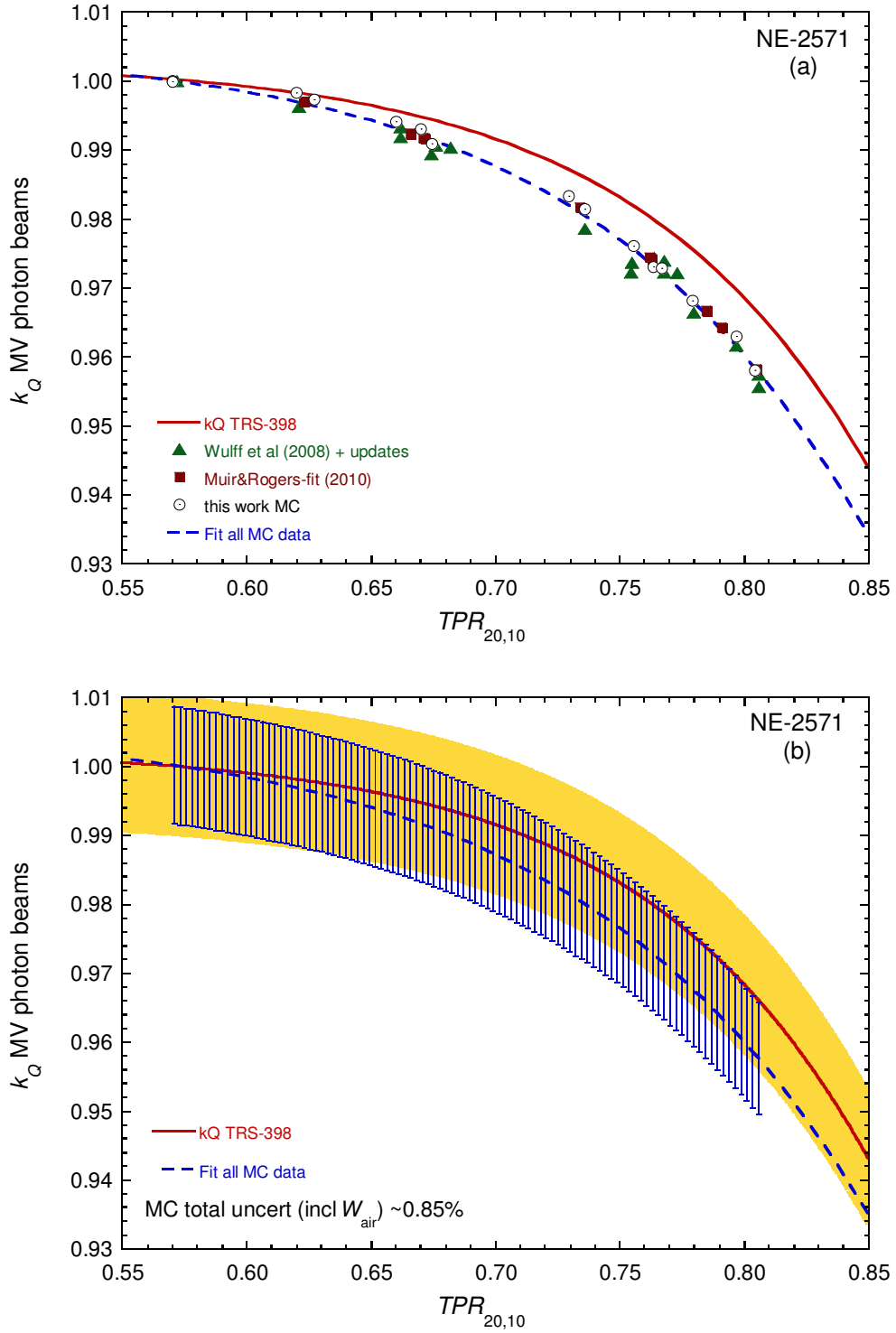


Figure 4: Comparison of calculated beam quality correction factors, k_Q , for a NE-2571 Farmer-type chamber in megavoltage photon beams. (a) The solid line corresponds to the data in IAEA TRS-398. The symbols correspond to the Monte Carlo calculations described in the text; the dashed line is a sigmoidal fit to the MC data. (b) Same as (a) but showing the standard uncertainty of the k_Q values given in IAEA TRS-398 and in Muir and Rogers (2010); for clarity the data points are omitted. The data sets agree within the overall uncertainty of each, which includes the uncertainty of W_{air} .

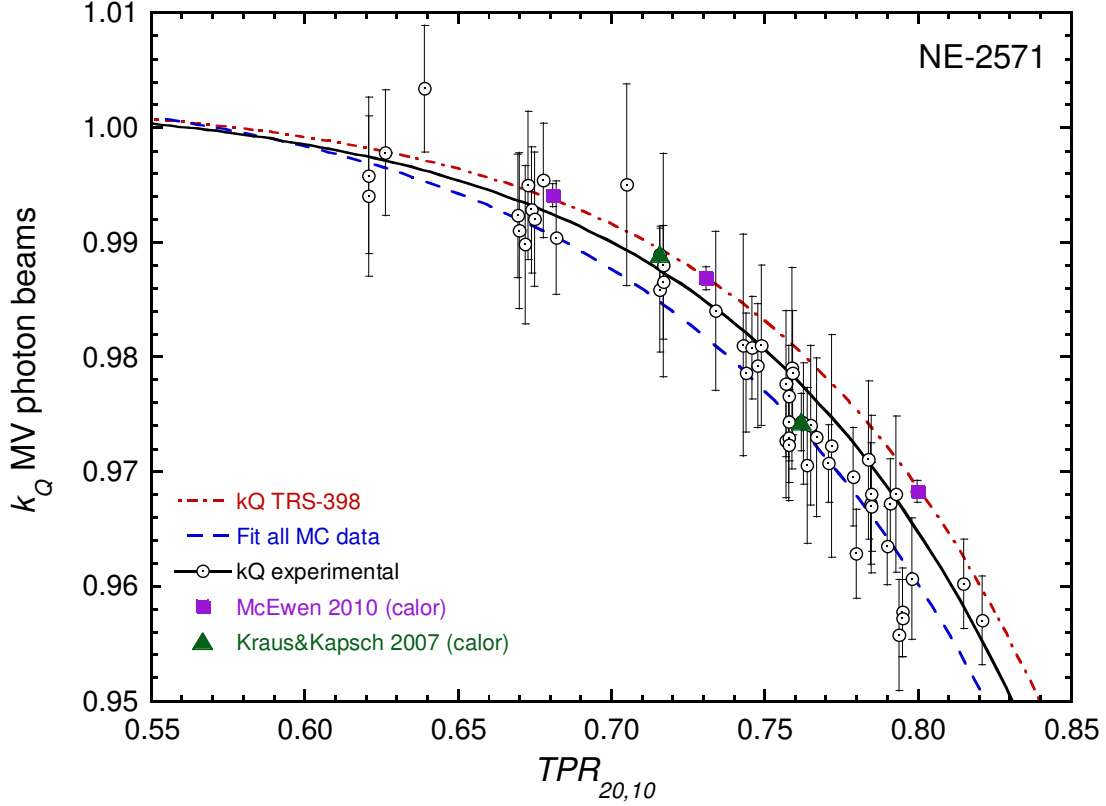


Figure 5: Comparison of experimental and calculated beam quality correction factors, k_Q , for a NE-2571 Farmer-type chamber in megavoltage photon beams. The symbols correspond to measurements in standard laboratories world-wide, where the most recent values (filled symbols) are based on water calorimetry; the solid line is a sigmoidal fit to the data weighted by the standard uncertainties stated by the laboratories. The upper dashed-dotted line corresponds to the data in IAEA TRS-398 and the lower dashed line to the Monte Carlo calculations described in the text.

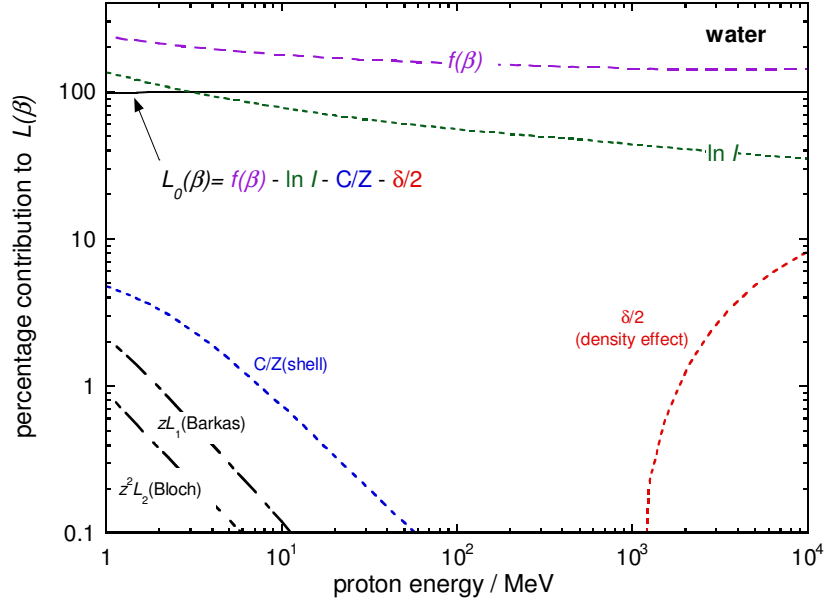


Figure 6: Contribution of the various corrections to the stopping number of protons in water, shown as a percentage of $L(\beta)$, see equations (8-10). The contribution ordinate exceeds 100% because some of the terms are negative. Data calculated with the *BEST* computer code (acronym for *BE*the *ST*opping, Berger and Paul (1995)).

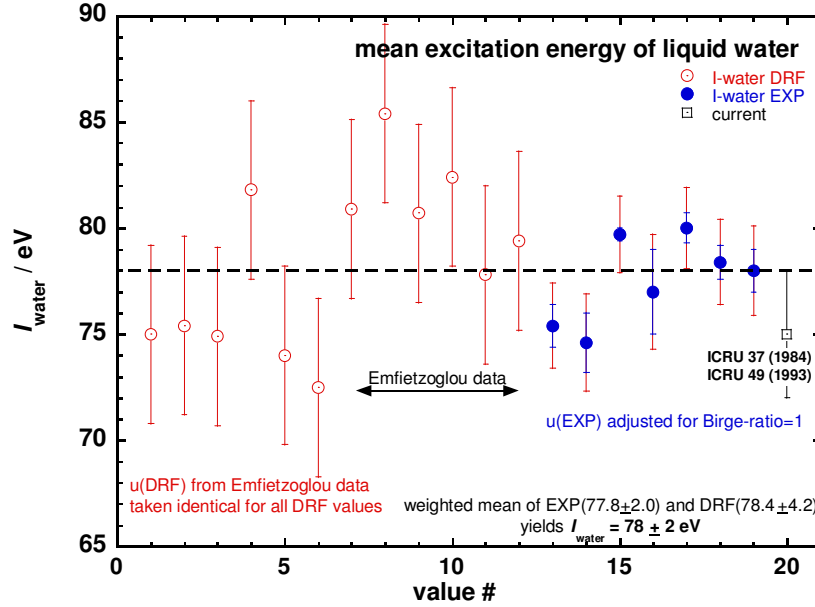


Figure 7: Weighted average value of the mean excitation energy of liquid water, I_{water} , dashed line, derived from the experimental (filled circles) and *DRF*-based (open circles) published values given in Table 2. The stated experimental uncertainties (short uncertainty bars) have been adjusted to yield a Birge-ratio of one (larger bars). Identical uncertainties are assumed for all the *DRF*-based values, obtained from the analysis of data sets by Emfietzoglou and collaborators based on different optical models and data.

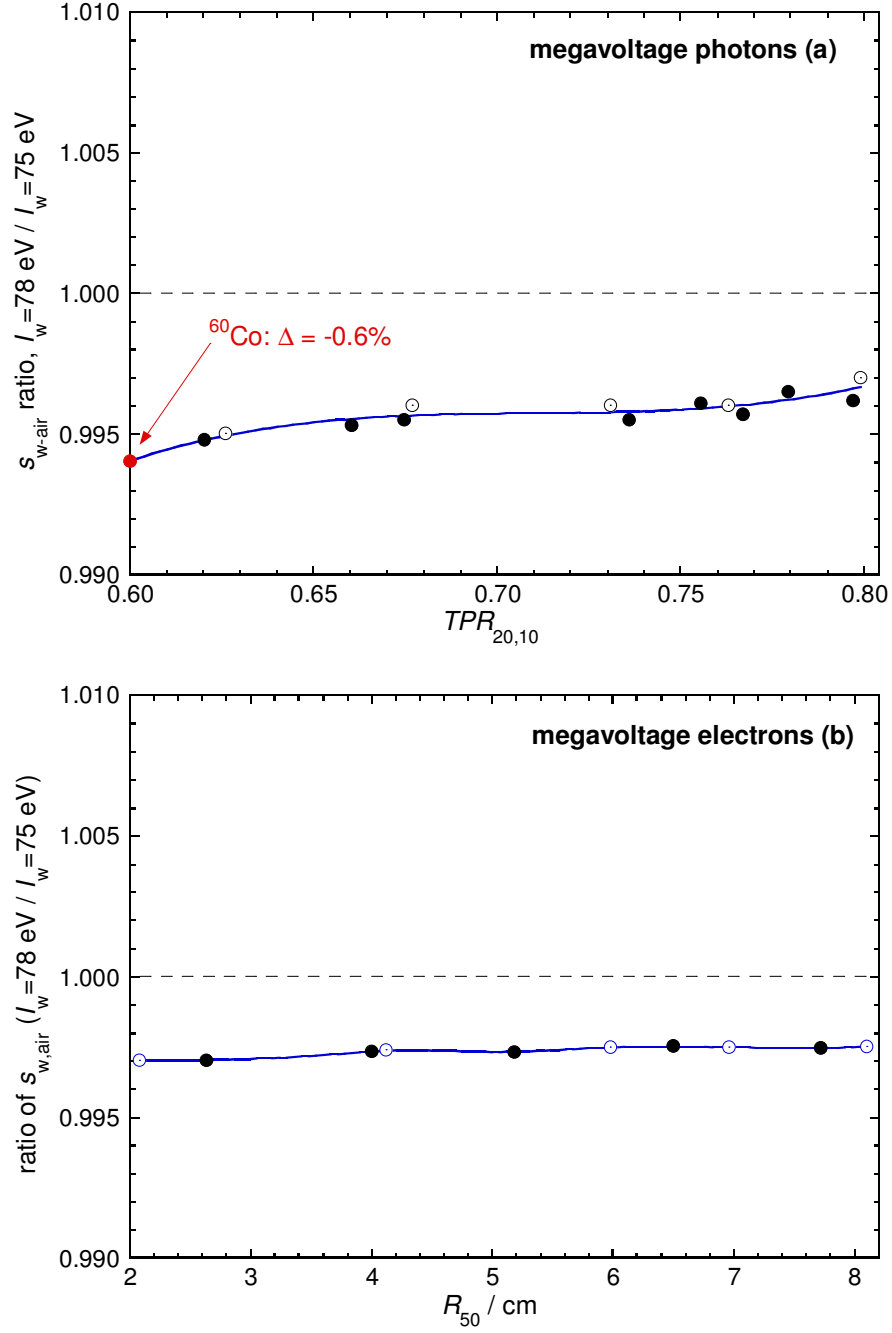


Figure 8: Influence of an increase in the I_{water} value on the water-to-air stopping-power ratio for megavoltage photons (a) and electrons (b). The difference between using $I_{\text{water}}=75 \text{ eV}$ (ICRU-37 and ICRU-49) and $I_{\text{water}}=78 \text{ eV}$ (this work) varies between -0.6% for ^{60}Co and -0.3 to -0.4% for high energy photons and electrons. Data computed using the *EGSnrc* code *SPRRZnrc* (Rogers *et al* 2011).

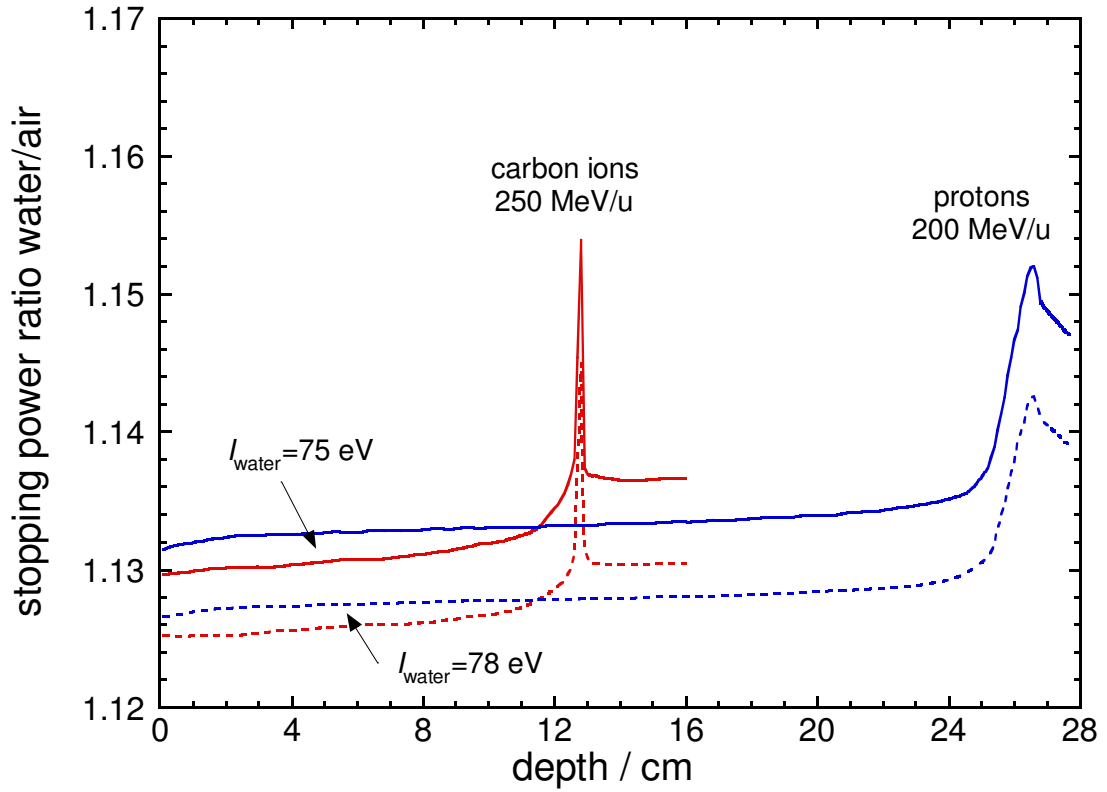


Figure 9: Influence of an increase in the I_{water} value on the water-to-air stopping-power ratios for protons (200 MeV/u) and carbon ions (250 MeV/u). The difference between using $I_{\text{water}}=75 \text{ eV}$ (ICRU-37 and ICRU-49, solid lines), and $I_{\text{water}}=78 \text{ eV}$ (this work, dashed lines) is approximately 0.4%. Data computed using the *SHIELD-HIT* Monte Carlo code, v10 (N. Sobolevsky, priv. comm.).