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Use of Monte Carlo simulations for uncertainty evaluation: A proposed approach for a challenging issue in the dosimetry of high dose per pulse electron beams using plane-parallel chambers

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Summary. — This paper describes a Monte Carlo (MC) approach to assess the ion recombination correction, k_s and its associated uncertainty, $u(k_s)$, in plane-parallel chambers used in high dose-per-pulse electron beam dosimetry. The proposed method was applied to assess k_s and $u(k_s)$ as a function of the ratio Q_1/Q_2, *i.e.*, the charge collected at polarizing voltages V_1 and V_2, in a plane-parallel chamber with electrode spacing $\ell = 2\,\text{mm}$. Data were fitted to a general quadratic function with the aim to derive an analytical equation for easy and direct computation of k_s and $u(k_s)$ in clinical dosimetry.

1. – Introduction

The assessment of the ion recombination factor, k_s, represents a major issue in the dosimetry of electron beams with dose-per-pulse >10 mGy if it is determined using an ionization chamber [1]. In this scenario k_s is largely overestimated if it is assessed using the traditional two-voltage method recommended by currently available international protocols [2]. To overcome this issue, three alternative models have been proposed in the literature allowing for the presence of a free-electron component, p [3]:

$$\begin{aligned} f' &= \frac{1}{u}\ln\left(1+\frac{e^{pu}-1}{p}\right), \quad f'' = p+\frac{1}{u}\ln\left[1+(1-p)\,u\right], \\ f''' &= \lambda+\frac{1}{u}\ln\left(1+\frac{e^{\lambda(1-\lambda)u}-1}{\lambda}\right), \end{aligned} \tag{1}$$

where $\lambda = 1-\sqrt{1-p}$ and $u = \mu\ell^2 r/V$ with μ being a constant depending on the gas in the chamber cavity, ℓ the electrode spacing, r the charge density per radiation pulse and V the polarizing voltage. Ultimately, k_s is given by the inverse of the charge collection efficiency f. An expression for the free electron fraction, p, was derived by Boag *et al.* [4] as

$$p = \frac{w\tau}{\ell}\left(1-e^{-\frac{\ell}{w\tau}}\right), \tag{2}$$

where w and τ are the lifetime and the drift velocity of the free electrons in the gas filling the cavity, respectively.

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2. – Propagation of distributions using a Monte Carlo approach

Because the quantity u is obtained by numerical methods, partial derivatives of eqs. (1) cannot be directly derived and the law of propagation of uncertainty described in the *Guide to the Expression of Uncertainty in Measurement* (GUM) [5] cannot be applied.

To overcome this issue, in the present study we propose a Monte Carlo approach to assess k_s and its standard uncertainty, $u(k_s)$. In particular, M random values can be generated for each input variable in eqs. (1), each with an assigned probability density function. Then, for each iteration the possible values of the input random variables will be sampled according to their distributions and the output variable $(k_s)_r$ $(r = 1, ..., M)$ can be calculated accordingly. Finally, the standard uncertainty, $u(k_s)$, is given by

$$u(k_s) = \frac{1}{M}\sqrt{M\sum_{r=1}^{M}(k_s)_r^2 - \left(\sum_{r=1}^{M}(k_s)_r\right)^2}. \tag{3}$$

2˙1. *Monte Carlo assessment of the free electron component, p.* – The free electron component, p, can be assessed through a MC approach generating random input values for all quantities appearing in eq. (2). Building on the study of Laitano *et al.* [6], the electron drift velocity (w, expressed in cm s^{-1}) and the electron lifetime in the air cavity (τ, expressed in s) can be approximated by the following equations:

$$\begin{aligned} w &= a + b\left[\left(1 - e^{-cE}\right) - \frac{d}{n}\left(1 + \frac{ce^{-nE} - ne^{-cE}}{n - c}\right)\right], \\ \tau &= a\left(1 - e^{-bE}\right) + c\left(1 - e^{-dE}\right), \end{aligned} \tag{4}$$

where E is the electric field strength (V cm^{-1}), determined as $E = V/\ell$, with V the chamber voltage and ℓ the electrode spacing, and the parameters a, b, c, d, e and n are determined from the fit, with $n = d + e$ (cm V^{-1}). The assessment of w and τ can be performed through a MC approach by generating random input values for the variables $\{V, \ell, a, b, c, d, e, n\}$ and $\{V, \ell, a, b, c, d\}$, respectively. Adopting a conservative approach, in the present study a continuous uniform distribution was assigned to all quantities in eqs. (4), *i.e.*, each quantity was treated as if it was equally probable for its value to lie anywhere within the lower (α_-) and upper limit (α_+) of a rectangular distribution (with $\alpha = (\alpha_+ - \alpha_-)/2$, being the half-width of the interval) [7]. Both V and ℓ were randomly sampled assigning a rectangular distribution to experimental values. For the chamber voltage, V, a 1% half-width of the interval of the uniform distribution was considered. Based on manufacturers' specification, for the electrode spacing, ℓ, a 10% half-width of the interval of the uniform distribution was considered instead (up to a maximum half-width of ± 0.1 mm). The parameters $\{a, b, c, d, e, n\}$ and $\{a, b, c, d\}$, along with their uncertainties, were previously determined fitting literature data of w and τ [6] against E with eqs. (4). Table I reports the values of the fitting parameters and the associated half-width of the interval of the uniform distribution, derived from the fit uncertainty.

2˙2. *Determination of the variable u.* – The determination of the charge collection efficiency requires the knowledge of the variable u. The modified two-voltage analysis [6]

TABLE I. – *Fitting parameters for w and τ.*

Fitting parameters for w (electron drift velocity)		α (half-width of the uniform distribution)
a	$7.033 \cdot 10^4$ (cm s^{-1})	1.4%
b	$3.481 \cdot 10^7$ (cm s^{-1})	1.0%
c	$1.014 \cdot 10^{-4}$ (cm V^{-1})	1.3%
d	$3.441 \cdot 10^{-3}$ (cm V^{-1})	0.3%
e	$8.401 \cdot 10^{-4}$ (cm V^{-1})	0.5%
Fitting parameters for τ (electron lifetime)		α (half-width of the uniform distribution)
a	$6.629 \cdot 10^{-8}$ (cm s^{-1})	7.1%
b	$1.776 \cdot 10^{-4}$ (cm s^{-1})	2.0%
c	$6.360 \cdot 10^{-8}$ (cm V^{-1})	7.5%
d	$1.803 \cdot 10^{-4}$ (cm V^{-1})	4.8%

can be applied to experimental data to calculate the charge collection efficiency described by eqs. (1)

$$\frac{Q_1}{Q_2} = \frac{V_1}{V_2} \frac{\ln\left[1 + \frac{e^{(p_1 u_1)} - 1}{p_1}\right]}{\ln\left[1 + \frac{e^{\left(\frac{V_1}{V_2} p_2 u_1\right)} - 1}{p_2}\right]}, \tag{5}$$

$$\frac{Q_1}{Q_2} = \frac{p_1 u_1 + \ln\left[1 + (1 - p_1)\, u_1\right]}{p_2 u_1 + \left(\frac{V_2}{V_1}\right) \ln\left[1 + \left(\frac{V_1}{V_2}\right)(1 - p_2)\, u_1\right]}, \tag{6}$$

$$\frac{Q_1}{Q_2} = \frac{\lambda_1 u_1 + \ln\left\{1 + \left(\frac{1}{\lambda_1}\right)\left[e^{\lambda_1(1-\lambda_1)u_1} - 1\right]\right\}}{\lambda_2 u_1 + \left(\frac{V_2}{V_1}\right) \ln\left\{1 + \left(\frac{1}{\lambda_2}\right)\left[e^{\lambda_2(1-\lambda_2)\frac{V_1}{V_2}u_1} - 1\right]\right\}}. \tag{7}$$

Equations (5), (6) and (7) can be numerically solved for u_1 implementing the iterative Levenberg-Marquardt algorithm. For a given ionization chamber, the pair of charge values Q_1 and Q_2 can be derived from experimental measurements at the corresponding pair of chamber voltages V_1 and V_2 (with $V_1 > V_2$). Ultimately, MC sampling can be performed using experimentally determined mean values of Q_1 and Q_2 and considering a Gaussian probability density function with variance determined as the square of the typical experimental standard deviation (about 0.5%).

3. – Results and conclusions

The proposed MC approach was applied to assess the uncertainty associated with the ion recombination correction, k_s as a function of the ratio Q_1/Q_2, *i.e.*, the charge collected at polarizing voltages V_1 and V_2 (with $V_1 = (400 \pm 4)V$, $V_2 = (100 \pm 1)V$) in a typical plane-parallel ionization chamber used in the dosimetry of high dose per pulse IORT electron beams, with electrode spacing $\ell = (2.0 \pm 0.1)$ mm (*e.g.*, Roos, PPC40).

The results are reported in fig. 1. The charge collection process described by the model f_s''' in eq. (1) results in k_s values halfway between those obtained from models f_s' and f_s'' (fig. 1 (a)), confirming previous findings [1]. Interestingly, fig. 1(b) shows that there are no significant differences in the relative standard uncertainties obtained for the three models, in the considered Q_1/Q_2 range (1.05–1.70). Previous research demonstrated that the model f_s''' in eqs. (1) (corresponding to the correction factor here referred to as k_s''') is the most accurate in determining the ion recombination factor [6,8].

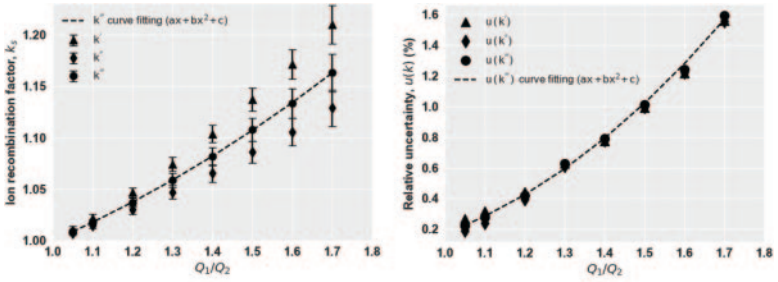

Fig. 1. – (a) k_s values determined according to eqs. (1) as a function of the ratio Q_1/Q_2. Relative standard uncertainties were determined using the proposed MC approach (eq. (3)) (b) Relative standard uncertainties as a function of the ratio Q_1/Q_2.

With this in mind, in this study we fitted simulated data of k_s''' and $u(k_s''')$ to a general quadratic function of the form $y = ax + bx^2 + c$ (with $x = Q_1/Q_2$) with the aim to derive an analytical equation for use in clinical dosimetry. The best fitting quadratic models for k_s''' and $u(k_s''')$ are reported below

$$k_s''' = -0.01734\left(\frac{Q_1}{Q_2}\right) + 0.09252\left(\frac{Q_1}{Q_2}\right)^2 + 0.92482, \tag{8}$$

$$u(k_s''') = -1.99168\left(\frac{Q_1}{Q_2}\right) + 1.474456\left(\frac{Q_1}{Q_2}\right)^2 + 0.69010. \tag{9}$$

Equations (8) and (9) can be used for typical Q_1/Q_2 values in the range 1.05–1.70, *i.e.*, dose per pulse in the range 0.1–70 mGy, approximately (with $V_1 \approx 4V_2$). It is worth noticing that there is a controversy in the literature on the best method to assess the ion recombination correction. A recent research published by our group indicated that an additional uncertainty component (type-B uncertainty) can be introduced to account for the differences between models f_s', f_s'' and f_s''' in eqs. (1). According to the proposed approach, the combined relative uncertainty would be given by the sum in quadrature of the MC uncertainty (type A, $u(k_s)^A$, as determined by eq. (9)) and the above-mentioned additional (type B, $u(k_s)^B$) component, *i.e.*, $u(k_s)_{tot} = \sqrt{(u(k_s)^A)^2 + (u(k_s)^B)^2}$. Our investigations into this area are still ongoing and further research is needed to assess if fitting models, such as eqs. (8) and (9) can be established for plane parallel ionization chambers with different electrode spacing and for different V_1/V_2 ratios.

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