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A parametrization of the CT number of a substance and its use for stoichiometric calibration

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Abstract A method to carry out stoichiometric calibrations of CT scanners employed in radiotherapy treatment planning is proposed. The method is based on a simple parametrization of the CT number of a substance, which involves only two variables to describe the substance (electron density and one effective atomic number) and one parameter to describe the beam. The method was tested experimentally on a group of beams. A set of no tissue-like substances of known densities and elemental compositions were employed as calibrators. CT number-to-density curves (RED curves) were calculated with the proposed parametrization and compared to those measured with a commercial density phantom. Differences between the electron densities assigned by the calculated RED curves and the measured ones were in the range 0.009–0.019 (RMS). The proposed method may be employed to carry out accurate stoichiometric calibrations by using only one suitable substance as calibrator, not necessarily tissue-like.

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Introduction

Radiotherapy treatment planning systems calculate doses to inhomogeneities by employing some corrections based on the knowledge of the electron densities of human tissues. Nowadays, this information is commonly obtained from CT images. The electron density of a tissue can be

obtained from its CT number by using a functional relation between both variables called Relative Electron Density (RED) curve. This relation depends on the spectral characteristics of the CT beam and must be established in each case. The calculation of this curve is referred to as the “calibration” of the CT unit. Traditionally, two methods have been described to carry out this calibration.

The first method is the calibration with substitutes [1,2], which employs a set of commercially available tissue equivalent materials. Their CT numbers are experimentally measured and plotted against their electron

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densities. The main advantage of this method is its simplicity. However, the accuracy of the calibration depends on the quality of the substitutes, which must be selected with caution.

The second method is the stoichiometric calibration, which is considered to be more precise than the calibration with substitutes [3–6]. It is based on the use of an expression to calculate the CT numbers of selected body tissues from their tabulated elemental compositions and electron densities. Most of the authors who have followed this approach have used the Schneider's parametrization [3], an expression for the CT number involving three variables to describe the substance (electron density and two effective atomic numbers) and three parameters to describe the beam. These parameters must be calculated by measuring the CT number values of certain materials with known compositions and densities, called calibrators. However, tissue substitutes have normally been employed as calibrators [3,4,6], which may lead to think that a commercial phantom with tissue substitutes is always needed to carry out a stoichiometric calibration and that both calibration methods are not independent.

The purpose of this paper is to provide a simple parametrization for the CT number of a substance which may be employed to carry out reliable stoichiometric calibrations by using calibrators which are not necessarily tissue-like. The parametrization involves only two variables to describe the material and one parameter to describe the beam. This parametrization was published and used by the authors in previous works [7,8]. The current paper is a revised and improved version of the theoretical basis of this model, which is put in context and deducted as a last consequence of the works by Rutherford and Henson. The experimental set up for testing and applying the parametrization has also been improved in this paper with the use of a new phantom designed by the authors for data acquisition. Experimental data of six beams from two CT units dedicated to radiotherapy treatment planning simulation have been included. Moreover, comparisons of the proposed parametrization with the Schneider's one and with calibrations carried out with a commercial density phantom have also been added to this revision.

Theoretical background

The mass attenuation coefficient of a compound can be calculated with the expression:

$$\mu_m = \sum_i w_i \mu_{m,i} \quad (1)$$

where w_i is the mass fraction of the i -th element in the compound and $\mu_{m,i}$ its corresponding mass attenuation coefficient. Although this expression, known as the "mixture rule", has some limitations because it ignores the effects related to the molecular structure of the compound, errors from this approximation are less than a few percent above 10 keV [9]. For a given energy E in the range of diagnostic X-rays, the mass attenuation coefficient of the i -th element can be written as:

$$\mu_{m,i} = N_A \frac{Z_i}{A_i} \cdot g(Z_i; E) \quad (2)$$

where N_A is the Avogadro's number and Z_i and A_i are the atomic and mass numbers of the element, respectively. The function g describes the atomic cross section of the element, and it is the sum of the Klein–Nishina cross section (σ_{KN} , incoherent scattering), the photoelectric effect contribution (σ_{PH}) and a correction term (δ) to account for deviations due to coherent scattering and binding energy effects (these binding effects may be neglected because of the high energy of the X-ray photons compared to the binding energies). Expressions of the form $A \cdot E^{-m} \cdot Z_i^n$ were used by Rutherford *et al.* [10] to parametrize the photoelectric and coherent contributions.

According to equation (2), the ratio of the mass attenuation coefficients of the i -th element for two given energies E_1 , E_2 , can be written as:

$$\frac{\mu_{m,i}(E_1)}{\mu_{m,i}(E_2)} = \frac{g(Z_i; E_1)}{g(Z_i; E_2)} = f(Z_i; E_1, E_2) \quad (3)$$

Rutherford *et al.* [10] proposed the use of this function f to define the effective atomic number Z_{ef} of a compound from the ratio of its mass attenuation coefficients for two given energies, as follows:

$$\frac{\mu_m(E_1)}{\mu_m(E_2)} = f(Z_{ef}, E_1, E_2) \quad (4)$$

and showed that this effective atomic number could be accurately measured by scanning the material with two CT beams of different energies. Frija *et al.* [11] used this effective atomic number measured with a CT scanner to calculate the compositions of different body tissues.

In a theoretical analysis of equation (3), Henson [12–14] showed that, for a given pair of energies in the range [50 keV...100 keV] and $Z_i \leq 20$, the value of Z_{ef} defined by equation (4) was unique and, although it depended slightly on E_1 and E_2 , it was almost constant over that range of energy. Although this means that the effective atomic number defined by equation (4) could be calculated in the considered ranges as a function of the elemental composition of the material, Henson did not propose any expressions to calculate it in this way.

Material and methods

Parametrization of the photon attenuation coefficient

To obtain an expression for Z_{ef} as a function of the elemental composition of the compound, let us try the following parametrization for $g(Z_i; E)$ in the range [50 keV...100 keV] and $Z_i \leq 20$:

$$g(Z_i; E) = \lambda(E) + \nu(E) \cdot Z_i^n \quad (5)$$

The function $\lambda(E)$ is intended to represent the contribution of the incoherent scattering, whereas the term $\nu(E) \cdot Z_i^n$ is intended to take into account the contribution from the photoelectric effect, σ_{PH} , and the correction term, δ , simultaneously. Using equations (5), (2) and (1) the linear attenuation coefficient μ (in cm^{-1}) of a compound with mass density ρ_m (in g/cm^3) results:

Table 1 Values of α for $n = 3.21$ ($k = 2$). R^2 is the coefficient of determination for each of the fits.

E (keV)	α	R^2
50	0.8238 ± 0.0003	1.0000
60	0.8874 ± 0.0001	1.0000
80	0.9463 ± 0.0002	1.0000
100	0.9702 ± 0.0002	1.0000

$$\frac{\mu(E)}{\rho} = \lambda(E) + \nu(E) \cdot Z_{\text{ef}}^n \quad (6)$$

where ρ is the electron density (in electrons/cm³):

$$\rho = N_A \cdot \rho_m \cdot \sum w_i \frac{Z_i}{A_i} \quad (7)$$

and Z_{ef} is the effective atomic number, calculated as:

$$Z_{\text{ef}} = \left(\frac{\sum w_i \cdot \frac{Z_i}{A_i} \cdot Z_i^n}{\sum w_i \cdot \frac{Z_i}{A_i}} \right)^{1/n} \quad (8)$$

Using the symbol $*$ to denote values relative to water, equation (6) becomes:

$$\frac{\mu^*(E)}{\rho^*} = \alpha(E) \cdot (1 - Z_{\text{ef}}^{*n}) + Z_{\text{ef}}^{*n} \quad (9)$$

where α is defined as:

$$\alpha(E) = \frac{1}{1 + \frac{\nu(E)}{\lambda(E)} \cdot Z_{\text{ef},w}^n} \quad (10)$$

$Z_{\text{ef},w}$ is the effective atomic number of water.

Calculation of n and α

The value of n and the function $\alpha(E)$ for the energy and atomic number ranges considered by Henson [13,14], i.e. [50 keV...100 keV] and $Z_i \leq 20$, were obtained by fitting the tabulated linear attenuation coefficients available in the NIST X-ray attenuation databases [15] to equation (9). As most biological materials contain varying proportions of the elements H, C, N, O, F, Na, Mg, P, S, Cl, K and Ca, only these elements were considered.

The best value for n was taken as the one that minimized the sum of the residuals resulting from the linear fits of $\mu_i^*(E_j)/\rho_i^* - Z_i^{*n}$ vs. $1 - Z_i^{*n}$ (see equation (9)) for the energies $E_j = 50$ keV...100 keV. The minimization was done numerically. Five values of n : 2.75, 3.00, 3.25, 3.50 and 3.75 were selected, and their corresponding sums of

the residuals were calculated. The minimum of this function was then calculated by fitting these data to a quadratic function. Once known the best value of n , the values of $\alpha(E_j)$ were obtained as the corresponding slopes in the linear fit of $\mu_i^*(E_j)/\rho_i^* - Z_i^{*n}$ vs. $1 - Z_i^{*n}$.

Parametrization of the CT number

The CT number in Hounsfield units of a substance can be expressed as [5]:

$$N_{\text{CT}} = (\mu_{\varepsilon}^* - 1) \cdot (N_{\text{CT},w} - N_{\text{CT},\text{air}}) + N_{\text{CT},w} \quad (11)$$

where $N_{\text{CT},w}$ and $N_{\text{CT},\text{air}}$ are the CT numbers for water and air, respectively (in a well calibrated scanner, the values $N_{\text{CT},w} = 0$ and $N_{\text{CT},\text{air}} = -1000$ can be assumed; the explicit use of these two values in equation (11) allows to incorporate some possible differences in the calibration of the scanners). $\mu_{\varepsilon}^* = \mu^*(\varepsilon)$ is the relative to water measured effective linear attenuation coefficient of the substance, corresponding to an effective energy of the beam ε , according to the definition by McCullough [9]. By introducing equation (9) into equation (11), we obtain:

$$\frac{h}{\rho^*} = \alpha_{\varepsilon} (1 - Z_{\text{ef}}^{*n}) + Z_{\text{ef}}^{*n} \quad (12)$$

where:

$$h = \frac{N_{\text{CT}} - N_{\text{CT},w}}{N_{\text{CT},w} - N_{\text{CT},\text{air}}} + 1 \quad (13)$$

and $\alpha_{\varepsilon} = \alpha(\varepsilon)$ denotes the value of α for the energy ε .

Stoichiometric calibration

Equation (13) was employed for the stoichiometric calibration of two CT units dedicated to radiotherapy treatment planning simulation: a Picker AQSYM and a SIEMENS Tomoscan 64. The following materials were used as calibrators: sodium chloride, calcium carbonate, calcium chloride, sulphur, lactose and magnesium oxide. All of them were commercially available in the form of powder. The purity of their chemical compositions satisfied the Spanish pharmaceutical regulations and was better than 95% in all cases, according to the manufacturer. The samples were prepared in cylindrical recipients of 3 cm diameter and 4 cm height (around 30 cm [3]). Volumes were evaluated with two different methods: the measurement of the internal dimensions of the cylinders and by weighing them on a scale once filled with water. The volume uncertainty was estimated by comparing both results. The recipients were filled with the substances, sealed and weighed on a scale and their mass densities calculated. The electron

Table 2 Differences (in percent) between calculated (equation (9)) and tabulated linear attenuation coefficients. Calculated values correspond to $n = 3.21$ and the values of α listed in Table 1.

E (keV)	H	C	N	O	F	Na	Mg	P	S	Cl	K	Ca
50	-0.5	-0.5	-0.2	0.1	0.1	0.1	0.0	0.0	-0.4	-0.1	0.0	0.2
60	0.0	-0.3	-0.2	-0.1	-0.2	-0.1	-0.1	0.1	-0.2	-0.1	0.0	0.1
80	0.2	-0.3	-0.3	-0.3	-0.5	-0.4	-0.4	0.0	-0.3	0.0	0.1	0.1
100	0.5	0.0	0.0	-0.1	-0.3	-0.4	-0.4	0.0	-0.3	0.0	0.1	0.2

Figure 1 Linear fit of the attenuation coefficients of the elements H, C, N, O, F, Na, Mg, P, S, Cl, K and Ca to equation (14) ($n = 3.21$) for the energies 6 keV and 100 keV. Slopes (α) and coefficients of determination (R^2) are shown in the figure. See Table 1 for the rest of values in the energy range [50 keV...100 keV].

densities and effective atomic numbers were then evaluated by using equations (7) and (8), respectively. The electron density uncertainties were evaluated from the volume uncertainties. The effective atomic number uncertainties were estimated taking into account some of the impurities referred by the manufacturer and were considered negligible ($\leq 0.4\%$).

A cylindrical PMMA phantom of 32 cm diameter and 5 cm height, with a hole of 3 cm diameter in its center, was built by the authors to simulate a standard abdomen. The samples were placed in the center of the phantom and scanned. Standard abdomen protocols with three different values of kVp were chosen: 100 kVp, 130 kVp and 140 kVp for the Picker AQSYM and 100 kVp, 120 kVp and 140 kVp for the SIEMENS Tomoscan 64. The CT number of each of the materials was taken as the average value in a circular ROI of 1 cm diameter in the center of the image. Its uncertainty was evaluated from the standard deviation in the ROI and the number of pixels.

The value of α_e for each beam was obtained by fitting the measured CT numbers to equation (12) ($h/\rho^* - Z_{ef}^{*n}$ vs. $1 - Z_{ef}^{*n}$). With these values of α_e , RED curves were

Figure 2 α as a function of the energy. The solid line corresponds to the values calculated by equation (16) with $A = 12,179$ and $p = 2.8$. Uncertainties of α are too small to be seen (smaller than the size of the symbol; see Table 1).

generated by calculating with equation (13) the CT numbers of a selection of human tissues: lung, adipose, breast, muscle, liver, bone-spongiosa, bone-sacrum, bone-vertebral column (D6, L3), bone-humerus, bone-skull, bone-mandible and bone-cortical. The elemental compositions and mass densities defined by ICRP Publication 23 [16] were used in equations (7) and (8) for the calculation of their electron densities and effective atomic numbers.

The uncertainties of α_e and the CT number of tissues were calculated by a numerical simulation of the uncertainties of the dependent variable $h/\rho^* - Z_{ef}^{*n}$. Random values of this variable for each material were generated assuming Gaussian distributions for h and ρ^* (with known means and standard deviations) and the corresponding values of α_e and the CT numbers of tissues were found. This method allowed calculating the probability distributions for α_e and the CT numbers. Their uncertainties were directly found from the standard deviations of these distributions (with $k = 2$).

RED curves for the selected beams were also calculated by using the Schneider's stoichiometric calibration method. The Schneider's parametrization of the CT number is [3]:

Table 3 Calibrators used to determine the effective energies of beams. Z_{ef} corresponds to $n = 3.21$ (equation (8)). $Z_{ef} = 7.463$ for water.

Material	Composition	ρ_m (g/cm ³)	ρ^*	Z_{ef}^*	Z_{ef}	Z_{coh}	Z_{ph}
Magnesium oxide	MgO	0.23	0.21 ± 0.01	1.444	10.780	10.558	10.840
Lactose	$C_{12}H_{22}O_{11} \cdot H_2O$	0.96	0.92 ± 0.03	0.937	6.993	6.717	7.050
Sulphur	S	0.76	0.69 ± 0.03	2.144	16.000	16.000	16.000
Sodium chloride	NaCl	1.45	1.25 ± 0.05	2.042	15.243	14.896	15.336
Calcium chloride	$CaCl_2$	0.93	0.81 ± 0.03	2.444	18.240	18.160	18.264
Calcium carbonate	$CaCO_3$	1.38	1.25 ± 0.05	2.058	15.358	13.786	15.733

Table 4 Description of the body tissues used for the stoichiometric calibrations (data from ICRP Publication 23). Z_{ef} corresponds to $n = 3.21$ (equation (8)). $Z_{\text{ef}} = 7.463$ for water.

Tissue	ρ_m (g/cm ³)	ρ^*	Z_{ef}^*	Z_{ef}	Z_{coh}	Z_{ph}
Lung (inhale)	0.260	0.258	1.014	7.571	7.096	7.693
Adipose	0.950	0.951	0.857	6.399	5.982	6.497
Breast	1.020	1.014	0.937	6.996	6.569	7.094
Muscle	1.050	1.040	1.010	7.534	7.037	7.669
Liver	1.060	1.050	1.012	7.552	7.057	7.685
Bone-spongiosa	1.180	1.150	1.355	10.112	8.355	10.636
Bone-Sacrum	1.290	1.244	1.454	10.855	9.065	11.368
Bone-Vertebral column (D6. L3)	1.330	1.278	1.500	11.193	9.372	11.705
Bone-Humerus	1.460	1.389	1.613	12.039	10.144	12.539
Bone-Skull	1.610	1.517	1.689	12.603	10.798	13.073
Bone-Mandible	1.680	1.577	1.718	12.825	11.038	13.286
Bone-Cortical	1.920	1.780	1.813	13.533	11.833	13.961

Table 5 Tissue substitutes in CIRS Model 062 electron density phantom.

Material	ρ_m (g/cm ³)	ρ^*
Lung (inhale)	0.195	0.190
Adipose	0.967	0.952
Breast (50/50)	0.991	0.976
Muscle	1.062	1.043
Liver	1.071	1.052
Trabecular bone	1.161	1.117
Dense bone 800 mg/ml HA	1.609	1.512

$$\frac{h}{\rho^*} = K_{\text{KN}} + K_{\text{coh}} Z_{\text{coh}}^{1.86} + K_{\text{ph}} Z_{\text{ph}}^{3.62} \quad (14)$$

where Z_{coh} and Z_{ph} are the coherent and photoelectric atomic numbers, respectively, calculated as follows:

$$Z_{\text{coh}} = \left(\frac{\sum w_i \cdot \frac{Z_i}{A_i} \cdot Z_i^{1.86}}{\sum w_i \cdot \frac{Z_i}{A_i}} \right)^{1/1.86} \quad Z_{\text{ph}} = \left(\frac{\sum w_i \cdot \frac{Z_i}{A_i} \cdot Z_i^{3.62}}{\sum w_i \cdot \frac{Z_i}{A_i}} \right)^{1/3.62} \quad (15)$$

and K_{KN} , K_{coh} and K_{ph} are three beam dependent parameters. These three constants were calculated by fitting the CT number values of the calibrators to equation (14). A multilinear regression fit was employed. The resulting RED curves were compared to those generated by equation (12).

The uncertainties of the parameters and the CT number of tissues were again obtained from simulation of the uncertainties of the variable h/ρ^* . This method allowed finding the probability distributions of the free parameters together with their correlation.

A calibration phantom CIRS Model 062 was employed to measure a reference RED curve for each of the six beams analyzed. According to Pemler *et al.* [17], although the materials available in this phantom are only approximately tissue equivalent, the calculated RED curves can be considered correct. The tissue substitutes available in this phantom were: lung (inhale), adipose, breast (50/50), muscle, liver, trabecular bone and dense bone 800 mg/ml HA (hydroxyapatite). The samples were placed in the center of the cylindrical PMMA phantom and scanned in the same conditions as the calibrators. The RED curves generated in this way, which will be referred to as the measured ones, were compared to the calculated ones.

Results

The best value of n was 3.21. Table 1 lists the corresponding values of α , together with their uncertainties ($k = 2$), and the value of the coefficient of determination for each of the fits. Table 2 shows the differences (in percent) between the attenuation coefficients calculated with equation (6) and the tabulated ones [15] for the selected elements. The values of $\mu_i^*/\rho^* - Z_i^{*3.21}$ against $1 - Z_i^{*3.21}$ for the energies 60 keV and 100 keV, as an example, are

Table 6 CT number values (and standard deviations) for the calibrators (Table 3) in Picker ACQSYM and SIEMENS Tomoscan 64 CT scanners.

Material	Picker AQSYM			SIEMENS Tomoscan 64		
	100 kVp	130 kVp	140 kVp	100 kVp	120 kVp	140 kVp
Air	−890 (14)	−905 (12)	−909 (12)	−944 (20)	−944 (21)	−939 (17)
Water	0 (14)	2 (13)	3 (15)	−17 (22)	−23 (15)	−25 (17)
Magnesium oxide	−632 (15)	−660 (14)	−664 (13)	−677 (22)	−686 (15)	−702 (18)
Lactose	−84 (16)	−79 (16)	−77 (15)	−96 (24)	−92 (21)	−88 (21)
Sulphur	322 (59)	161 (54)	123 (52)	305 (60)	158 (53)	85 (48)
Sodium chloride	935 (23)	757 (19)	713 (19)	955 (37)	796 (36)	688 (32)
Calcium chloride	757 (25)	522 (25)	461 (21)	744 (46)	532 (39)	403 (36)
Calcium carbonate	986 (27)	805 (23)	758 (24)	1052 (51)	856 (45)	720 (37)

Table 7 Values of α_e (equation (12), $k = 2$) and the corresponding effective energies ε (equation (16), $k = 2$) for Picker ACQSYM and SIEMENS Tomoscan 64 CT scanners.

kVp	α_e	ε (keV)
Picker ACQSYM/100 kVp	0.919 ± 0.005	68 ± 1.6
Picker ACQSYM/130 kVp	0.941 ± 0.004	77 ± 2.0
Picker ACQSYM/140 kVp	0.947 ± 0.005	81 ± 2.9
SIEMENS Tomoscan 64/100 kVp	0.921 ± 0.004	69 ± 1.4
SIEMENS Tomoscan 64/120 kVp	0.938 ± 0.005	76 ± 2.3
SIEMENS Tomoscan 64/140 kVp	0.948 ± 0.003	81 ± 1.8

plotted in Fig. 1. The coefficients of determination are also included in the figure. Fig. 2 plots α as a function of the energy. The solid line corresponds to the fit to the expression:

$$\alpha = \frac{1}{1 + A \cdot E^{-p}} \quad (16)$$

with values $A = 12,179$ and $p = 2.8$ (E in keV). The use of this expression is suggested by the definition of α (equation (10)). The agreement with the tabulated values of α is better than 0.08%.

Table 3 shows the compositions, mass densities, relative electron densities (equation (7)) with their uncertainties ($k = 2$) and relative effective atomic numbers (equation (8) with $n = 3.21$, $Z_{ef} = 7.463$ for water) of the calibrators used. Their coherent and photoelectric atomic numbers (equation (15)) are also listed.

Figure 3 Fit of the measured CT numbers (Table 6) for the PICKER ACQSYM/130 kVp beam to equation (12). The slope corresponds to the value of α_e (see Table 7). Uncertainties of the dependent variable are too small to be seen (smaller than the size of the symbol). For the uncertainty of the slope see Table 7.

Table 4 shows the mass densities, relative electron densities and relative effective atomic numbers (equations (7) and (8)) of the human tissues used for the calculation of the RED curves [16]. Coherent and photoelectric atomic numbers are also shown (equation (15)).

Table 5 lists the mass and electron densities relative to water, according to the manufacturer, of the tissue substitutes provided with the CIRS Model 062 phantom.

The measured CT numbers (and standard deviations) of the calibrators for the six beams analysed are shown in Table 6. The values of α_e (equation (12)) and the corresponding effective energies (equation (16)) for each of the beams, together with their uncertainties ($k = 2$), are listed in Table 7. The linear fits for two of the beams are shown in Figs. 3 and 4. The values of K_{KN} , K_{coh} and K_{ph} of the Schneider parametrization (equation (14)) and their uncertainties ($k = 2$) are shown in Table 8.

The CT numbers of the selected body tissues calculated with equations (12) and (14) are listed in Tables 9 and 10. The measured CT numbers of the phantom tissue substitutes are shown in Table 11.

Table 12 shows the differences in the electron densities predicted by the calculated and the measured RED curves for a given CT number. Figs. 5 and 6 compare the three RED curves obtained for two of the beams, as an example.

Discussion

The parametrization of the CT number proposed in this paper is a consequence of the simple parametrization introduced for the relative linear attenuation coefficient (equation (6)). Although the use of a term for every single attenuation process (coherent scattering, incoherent

Figure 4 Fit of the measured CT numbers (Table 6) for the SIEMENS Tomoscan 64/120 kVp beam to equation (12). The slope corresponds to the value of α_e (see Table 7). Uncertainties of the dependent variable are too small to be seen (smaller than the size of the symbol). For the uncertainty of the slope see Table 7.

Table 8 Values of the Schneider's parameters (equation (14), $k = 2$) for PICKER ACQSYM and SIEMENS Tomoscan 64 CT scanners.

kVp	K_{coh}	K_{ph}	K_{KN}
Picker ACQSYM/100 kVp	$(5.5 \times 10^{-3}) \pm (3.0 \times 10^{-3})$	$(6.8 \times 10^{-6}) \pm (1.7 \times 10^{-5})$	$(8.1 \times 10^{-1}) \pm (1.0 \times 10^{-1})$
Picker ACQSYM/130 kVp	$(4.3 \times 10^{-3}) \pm (3.1 \times 10^{-3})$	$(3.5 \times 10^{-6}) \pm (1.7 \times 10^{-5})$	$(8.5 \times 10^{-1}) \pm (1.1 \times 10^{-1})$
Picker ACQSYM/140 kVp	$(4.7 \times 10^{-3}) \pm (2.5 \times 10^{-3})$	$(-1.8 \times 10^{-6}) \pm (1.5 \times 10^{-5})$	$(8.5 \times 10^{-1}) \pm (8.0 \times 10^{-2})$
SIEMENS Tomoscan 64/ 100 kVp	$(4.8 \times 10^{-3}) \pm (3.0 \times 10^{-3})$	$(1.1 \times 10^{-5}) \pm (1.5 \times 10^{-5})$	$(8.4 \times 10^{-1}) \pm (1.0 \times 10^{-1})$
SIEMENS Tomoscan 64/ 120 kVp	$(4.4 \times 10^{-3}) \pm (3.3 \times 10^{-3})$	$(4.1 \times 10^{-6}) \pm (1.8 \times 10^{-5})$	$(8.6 \times 10^{-1}) \pm (1.0 \times 10^{-1})$
SIEMENS Tomoscan 64/ 140 kVp	$(4.1 \times 10^{-3}) \pm (1.8 \times 10^{-3})$	$(1.9 \times 10^{-6}) \pm (1.1 \times 10^{-5})$	$(8.6 \times 10^{-1}) \pm (5.8 \times 10^{-2})$

Table 9 Calculated CT numbers ($k = 2$) of the body tissues for the PICKER ACQSYM CT scanner.

Tissue	This paper's method (equation (12))			Schneider's method (equation (14))		
	100 kVp	130 kVp	140 kVp	100 kVp	130 kVp	140 kVp
Lung	-659 ± 0.1	-671 ± 0	-673 ± 0.1	-652 ± 9	-665 ± 12	-668 ± 8
Adipose	-70 ± 2	-62 ± 1	-59 ± 2	-67 ± 34	-61 ± 49	-62 ± 37
Breast	-1 ± 1	5 ± 0.7	7 ± 1	16 ± 36	17 ± 50	16 ± 36
Muscle	38 ± 0.2	40 ± 0.1	41 ± 0.2	65 ± 36	61 ± 49	60 ± 34
Liver	47 ± 0.3	50 ± 0.2	51 ± 0.3	75 ± 37	71 ± 49	70 ± 35
Bone-spongiosa	269 ± 12	238 ± 7	231 ± 12	270 ± 32	240 ± 57	225 ± 36
Bone-sacrum	424 ± 18	376 ± 11	365 ± 18	427 ± 32	381 ± 61	360 ± 35
Bone-vertebral column (D6, L3)	491 ± 21	433 ± 13	421 ± 21	493 ± 31	439 ± 63	415 ± 35
Bone-humerus	706 ± 31	620 ± 19	601 ± 32	699 ± 28	620 ± 73	585 ± 39
Bone-skull	933 ± 41	819 ± 25	794 ± 42	927 ± 27	823 ± 78	779 ± 43
Bone-mandible	1040 ± 46	913 ± 27	884 ± 46	1032 ± 26	916 ± 82	868 ± 46
Bone-cortical	1425 ± 64	1248 ± 38	1208 ± 64	1410 ± 38	1249 ± 96	1182 ± 57

scattering and photoelectric effect) may be considered more complete from a formal point of view, the agreement of equation (6) with the tabulated attenuation coefficients in the energy and atomic number ranges considered is better than 0.5%, the same than the agreement achieved by using the Rutherford's parametrization [10], on which the Schneider's method is based. Hence, increasing the number of parameters does not seem to have any practical effects

in the ranges considered, and the use of a single effective atomic number calculated with an effective exponent seems to be a very good approach.

The expression proposed in this paper for the CT number (equation (12)) means a considerable simplification compared to the Schneider's parametrization (equation (14)). The multilinear regression fit carried out to calculate the three beam dependent parameters of the Schneider's

Table 10 Calculated CT numbers ($k = 2$) of the body tissues for the SIEMENS Tomoscan 64 CT scanner.

Tissue	This paper's method (equation (12))			Schneider's method (equation (14))		
	100 kVp	120 kVp	140 kVp	100 kVp	120 kVp	140 kVp
Lung	-704 ± 0.1	-706 ± 0.1	-703 ± 0	-695 ± 4	-698 ± 6	-698 ± 6
Adipose	-90 ± 2	-89 ± 2	-87 ± 1	-78 ± 26	-78 ± 24	-87 ± 27
Breast	-18 ± 1	-21 ± 1	-21 ± 1	7 ± 20	2 ± 24	-10 ± 27
Muscle	23 ± 0.1	16 ± 0.2	14 ± 0.1	56 ± 17	47 ± 26	33 ± 26
Liver	32 ± 0.2	25 ± 0.2	23 ± 0.1	67 ± 17	57 ± 26	43 ± 26
Bone-spongiosa	261 ± 9	223 ± 9	200 ± 5	276 ± 31	233 ± 27	203 ± 29
Bone-sacrum	422 ± 13	366 ± 14	333 ± 8	440 ± 32	378 ± 29	339 ± 30
Bone-vertebral column (D6, L3)	492 ± 16	427 ± 16	388 ± 10	510 ± 33	438 ± 31	395 ± 31
Bone-humerus	715 ± 23	623 ± 24	566 ± 14	728 ± 42	626 ± 36	568 ± 38
Bone-skull	950 ± 30	830 ± 32	756 ± 19	967 ± 43	836 ± 40	763 ± 44
Bone-mandible	1060 ± 34	928 ± 35	846 ± 21	1077 ± 46	932 ± 43	853 ± 47
Bone-cortical	1460 ± 47	1279 ± 49	1165 ± 29	1475 ± 55	1276 ± 52	1172 ± 60

Table 11 Measured CT numbers (and standard deviations) of the tissue substitutes (Table 5) for PICKER ACQSYM and SIEMENS Tomoscan 64 CT scanners.

Material	Picker ACQSYM			SIEMENS Tomoscan 64		
	100 kVp	100 kVp	130 kVp	100 kVp	120 kVp	140 kVp
Lung (inhale)	−720 (16)	−720 (16)	−733 (15)	−784 (22)	−775 (18)	−783 (20)
Adipose	−64 (17)	−64 (17)	−53 (14)	−94 (23)	−82 (21)	−73 (19)
Breast (50/50)	−31 (15)	−31 (15)	−22 (14)	−60 (23)	−50 (21)	−51 (19)
Muscle	43 (16)	43 (16)	44 (15)	12 (24)	15 (21)	19 (21)
Liver	53 (17)	53 (17)	54 (14)	17 (26)	23 (23)	28 (21)
Trabecular bone	252 (15)	252 (15)	217 (16)	224 (26)	189 (21)	175 (18)
Dense bone 800 mg/ml HA	919 (34)	919 (34)	798 (30)	953 (48)	839 (37)	786 (31)

Table 12 Differences in relative electron densities predicted by the Schneider's method, this paper's method and the calibrated values (Tables 5 and 11).

Beam	This paper's method vs. Schneider's method		This paper's method vs. CIRS Model 062		Schneider's method vs. CIRS Model 062	
	RMS	MAX	RMS	MAX	RMS	MAX
Pickier ACQSYM/ 100 kVp	0.007	0.013	0.014	0.026	0.013	0.024
Pickier ACQSYM/ 130 kVp	0.004	0.009	0.011	0.020	0.009	0.016
Pickier ACQSYM/ 140 kVp	0.008	0.016	0.011	0.019	0.011	0.020
Siemens Tomoscan 64/100 kVp	0.010	0.017	0.011	0.020	0.015	0.030
Siemens Tomoscan 64/120 kVp	0.009	0.017	0.010	0.016	0.011	0.017
Siemens Tomoscan 64/ 140 kVp	0.005	0.010	0.020	0.027	0.018	0.023

Figure 5 Measured and calculated RED curves for the PICKER ACQSYM – 130 kVp beam. The uncertainties of N_{CT} (see Table 10) have not been represented to avoid confusion among data. **Figure 6** Measured and calculated RED curves for the SIEMENS Tomoscan 64 – 120 kVp beam. The uncertainties of N_{CT} (see Table 10) have not been represented to avoid confusion among data.

method, K_{KN} , K_{coh} and K_{ph} seems to be very unstable, as the uncertainties obtained for these parameters show (see Table 8). These uncertainties, however, do not produce CT number uncertainties as large as we would expect (see Tables 9 and 10), because of the correlation among these parameters. It is interesting to observe the different behaviour of the CT number uncertainties produced by both methods. Whereas Schneider's method produces an increasing CT number uncertainty in the whole range of h , equation (12) produces negligible uncertainties over the range $0 \leq h \leq 1$.

In spite of the simplification, the CT number values of the body tissues calculated by both methods (see Tables 9 and 10) are very similar, the differences being almost negligible and smaller than the uncertainties. The biggest differences appear in the central region, for the breast, muscle and liver tissues. As the electron densities of the muscle and liver substitutes which have been employed are the same than the electron densities considered for these tissues (the differences are smaller than 0.3%), their measured and calculated CT number values can be directly compared (this is not the case for the breast substitute, because the difference of electron densities is 3.8%). This comparison permits us to conclude that our method gives better results than equation (14) in this region. This may be a consequence of the fact that equation (12) does incorporate the constraint $h = 1$ for $Z_{ef}^* = \rho^* = 1$, whereas equation (14) does not. Unless we have enough calibrators placed around this central region, this constraint is not guaranteed after the fit, and the CT numbers calculated with equation (14) can be slightly shifted. However, in spite of these small differences in the central region, the RED curves generated by both methods are almost identical. The calculated relative electron densities for a given CT number value show average differences (RMS) smaller than 0.01 (see Table 12).

The stoichiometric calibration method has been used by other authors as a sort of correction or fine adjustment to the substitutes calibration method, using commercial tissue substitutes as calibrators [3–6]. This seems to suggest that both methods are not independent. However, it has to be noted that the RED curves obtained in this paper were calculated by using no tissue equivalent substances as calibrators, with very good results, as the comparison with the measured RED curves show. When using equation (12), any substances can be employed to calculate α , as long as their electron densities and chemical composition are well known and within range ($Z \leq 20$). As a consequence of involving only one beam dependent parameter, equation (12) allows using a single calibrator to carry out the stoichiometric calibration. The parameter α_e can be calculated as:

$$\alpha_e = \frac{h/\rho^* - Z_{ef}^{*n}}{1 - Z_{ef}^{*n}} \quad (17)$$

However, if only one calibrator is going to be used, attention must be paid to its uncertainty. Taking for granted the chemical purity of the calibrator, the uncertainty of α_e is proportional to $1/(1 - Z_{ef}^{*n})$. The closer Z_{ef}^* is to 1, the greater the uncertainty is. As an example, the values of α_e and their uncertainties for one of the beams

Table 13 Values of α for each calibrator. SIEMENS Tomoscan 64 CT scanner.

Material	100 kVp	120 kVp	120 kVp
Magnesium oxide	0.832 ± 0.137	0.850 ± 0.133	0.894 ± 0.123
Lactose	0.980 ± 0.219	1.045 ± 0.221	1.074 ± 0.223
Sulphur	0.909 ± 0.011	0.930 ± 0.009	0.940 ± 0.009
Sodium chloride	0.928 ± 0.006	0.943 ± 0.005	0.953 ± 0.005
Calcium chloride	0.926 ± 0.006	0.942 ± 0.006	0.952 ± 0.005
Calcium carbonate	0.920 ± 0.006	0.938 ± 0.005	0.950 ± 0.005

have been calculated with equation (17) for each of the calibrators used. The results are listed in Table 13. As we see, the best values of α_e , those with smaller uncertainties and closer to the values obtained with the least squares method (see Tables 8 and 9), correspond to the materials with higher effective atomic numbers: calcium chloride and calcium carbonate. Substances with relative effective atomic numbers close to 1, "light" substances, should not be used alone when calculating the effective energy of a beam.

Apart from the reduction in the number of free parameters, the feasibility of calculating the effective energy of a beam directly from the value of α also represents a difference compared to the Schneider's approach. In the Schneider's parametrization, the explicit energy dependence of the parameters is not considered. The determination of α and the effective energy by fitting measured CT number values to equation (12), directly follows the definition of the effective energy by Millner *et al.* [18]: the resulting energy from the maximum correlation coefficient between the CT numbers and the linear attenuation coefficients of different substances placed in a water filled phantom. Judy and Adler [19] demonstrated that the Millner's method was equivalent to the McCullough's definition [9]. The approach proposed in this paper is especially suitable, because no tabulated attenuation coefficients have to be used in the process and calculation of effective energy takes place straightforward.

It is clear that the use of an effective energy for polychromatic beams must be taken as an approximation, because of the beam hardening effect. This effect can be eliminated nowadays to a high degree by simulating a monoenergetic behaviour of the beam with corrections carried out by algorithms involved in the reconstruction process. The attenuation values of the different materials are averaged over energy according to a location independent spectral function [20,21], making the CT number of a substance almost independent from its position on the image. Although this dependence is small, it should be taken into account when analysing the total uncertainty in the conversion of CT numbers into electron density for clinical applications. However, this effect has not been considered in this paper when comparing the RED curves to each other, because all the CT number values were measured at the same position, the center of the phantom.

Conclusions

The parametrization of the CT number of a substance proposed in this paper reduces the number of variables involved in the calculation of stoichiometric calibrations compared to other often used parametrizations: only one effective atomic number instead of two and only one beam dependent parameter instead of three. With this method, accurate stoichiometric calibrations for radiotherapy treatment planning can be easily established by using a single material not necessarily tissue-like.

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