On the equivalence of image-based dual-energy CT methods for the
determination of electron density and effective atomic number in
radiotherapy

Christian Möhler\textsuperscript{a,b}, Patrick Wohlfahrt\textsuperscript{c,d}, Christian Richter\textsuperscript{c,d,e,f}, Steffen Greilich\textsuperscript{a,b,}\textsuperscript{⁎}

\textsuperscript{a} German Cancer Research Center (DKFZ), 69120 Heidelberg, Germany
\textsuperscript{b} National Center for Radiation Research in Oncology (NCRO), Heidelberg Institute for Radiation Oncology (HIRO), 69120 Heidelberg, Germany
\textsuperscript{c} OncoRay – National Center for Radiation Research in Oncology, Faculty of Medicine and University Hospital Carl Gustav Carus, Technische Universität Dresden, Helmholtz-Zentrum Dresden – Rossendorf, 01307 Dresden, Germany
\textsuperscript{d} Institute of Radiooncology, Faculty of Medicine and University Hospital Carl Gustav Carus, Technische Universität Dresden, 01307 Dresden, Germany
\textsuperscript{e} German Cancer Research Center (DKFZ), 69120 Heidelberg, Germany
\textsuperscript{f} German Cancer Consortium (DKTK), 01307 Dresden, Germany

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ABSTRACT

Dual-energy computed tomography enables the determination of relative electron density and effective atomic number. As this can increase accuracy in radiotherapy treatment planning, a substantial number of algorithms for the determination of the two quantities has been suggested – most of them based on reconstructed CT images. We show that many of these methods share a common theoretical framework. Equations can be transformed from one method to the other by re-definition of the calibration parameters. We suggest that further work should be spent on practical calibration and the reliability of CT numbers rather than on the theoretical framework.

1. Introduction

It was already recognized in the early days of computed tomography (CT) that the use of two different X-ray energies enables additional characterization of the imaged object [1]. More specifically, it allows to determine radiological tissue parameters such as electron density relative to water, \( \tilde{n} \), and effective atomic number, \( Z_{eff} \) [2]. The determination of these tissue parameters is of particular interest for the improvement of dose calculation in particle therapy treatment planning: they can be used either directly (e.g., electron density) or as proxy for other quantities (e.g., the effective atomic number as a proxy for the mean excitation energy) to calculate stopping-power ratios via the Bethe formula [3,4]. Since the introduction of dedicated clinical dual-energy CT (DECT) scanners [5], an increasing number of algorithms for DECT-based \( \tilde{n}/Z_{eff} \) determination is found in literature [6–16].

Many of these methods are performed on reconstructed images, although a calculation on projection data is also conceivable [13,17–20]. In principle, the latter can implicitly account for beam hardening, but requires congruent projections during DECT acquisition, which excludes for example application in a dual-source scanner. In contrast, image-based approaches rely on ideal CT numbers, which can be reasonably achieved using effective beam hardening correction methods employed during image reconstruction. In addition, image-based algorithms do not interfere with the specific reconstruction algorithm used and are therefore more seamlessly implemented.

Most of the image-based algorithms share a common theoretical framework that was elaborated in the 1970s. They use, however, different notation, different definition of parameters and different forms of final equations or their derivation. In this note, we show that most of the above cited algorithms are mathematically equivalent.

To this end, we first review the development of the methods for \( \tilde{n}/Z_{eff} \) determination and the derivation of the respective equations (Section 2). Secondly, we demonstrate the mathematical equivalence of several methods by listing the necessary parameter transformations and discuss potential differences in the calibration procedure (Section 3).

2. Materials and methods

Before showing in Section 3 the mathematical equivalence of the image-based algorithms published in Refs. [7,9–11,16,21], we derive the corresponding equations for \( \tilde{n} \) and \( Z_{eff} \) in a general framework to establish a convenient notation and to highlight specific features.

The basis of the framework is the parameterization of the single-element photon absorption cross section in terms of photon energy, \( E \),...
and atomic number of the target material, \( Z \), in the general form [22]
\[
\sigma(E, Z) = A(E) + B(E)C(Z)
\]
(1)
which is a necessary condition for the coherent definition of \( Z_{\text{eff}} \).

The attenuation coefficients relative to water, \( \beta_{\text{eff}} \equiv \mu_{\text{eff}}/\rho_{w} \), for the lower \((s = 1)\) and higher \((s = h)\) energy X-ray spectra are obtained from Eq. (1) as (appendix of Ref. [23]):
\[
\beta_{\text{eff}} = \frac{\mu_{\text{eff}}}{\rho_{w}} = \left[ \tilde{\mu}_{A} + \frac{C(Z_{\text{eff}})}{B_{\text{eff}}} \right] \quad \text{(2)}
\]

The step from Eq. (1) to Eq. (2) is rather non-trivial. It requires to
(i) correctly superpose the elemental cross sections (i.e., a sum over all elements present in the compound) in conjunction with a consistent definition of \( Z_{\text{eff}} \) (see Eq. (6) below);
(ii) apply proper spectral weighting (i.e., an integration over \( E \) and %
(iii) relate the photon absorption of the material to that of water.

Eq. (2) can then be expressed as a system of two linear equations in the unknowns \( \tilde{\mu} \) and \( \beta_{\text{eff}}(C(Z_{\text{eff}})) \), with a matrix of initially four coefficients, which later constitute the calibration parameters:
\[
\begin{pmatrix}
\tilde{\mu}_{b} & \tilde{\mu}_{i}
\end{pmatrix} = 
\begin{pmatrix}
\tilde{\mu}_{A} & \tilde{\mu}_{B}
\end{pmatrix} \left[ \tilde{\mu}_{A} + \frac{C(Z_{\text{eff}})}{B_{\text{eff}}} \right]
\]
(3)

This equation is similar to Eq. (7) in Heismann et al. [7]. Notice, however, that in contrast to Ref. [7], which uses the mass density, the relative electron density appears in our Eq. (3) and the \( E \) and \( Z \) dependence is not specified at this point. Inverting Eq. (3) yields
\[
\begin{pmatrix}
\tilde{\mu}_{b} \\
\tilde{\mu}_{i}
\end{pmatrix} = 
\begin{pmatrix}
B_{1} & B_{0} \\
-A_{1} & A_{0}
\end{pmatrix}^{-1} \begin{pmatrix}
\tilde{\mu}_{A} \\
\tilde{\mu}_{B}
\end{pmatrix}
\]
(4)
where the coefficients were redefined according to \( X = \tilde{X}/(\tilde{\mu}_{A}B_{\text{eff}} - \tilde{\mu}_{B}) \) with \( X \in [A_{0}A_{1}, B_{0}, B_{1}] \) and corresponding \( \tilde{X} \). We believe this form of the equations illustrates important aspects of the approach very clearly:

(i) It is easily seen that in this framework the relative electron density can be determined independently of the effective atomic number – but not vice versa. In particular, the derived relative electron density is independent of the specific form of \( C(Z) \).

(ii) The first entry of the vector in Eq. (4) yields
\[
\tilde{\mu}_{b} = B_{1}\tilde{\mu}_{A} - B_{0}\tilde{\mu}_{i} \quad \text{(5)}
\]
This equation allows for a physical interpretation: only the relative magnitude of the coefficients associated to the photoelectric effect (\( B_{i} \)) influences the result for the relative electron density of different materials (i.e., with different \( \mu_{i} \)), while the coefficients associated to Compton scattering (\( A_{i} \)) contribute only to an overall normalization via the definition of the coefficients \( X \) above. Eq. (5) can thus indeed be regarded as a subtraction of the photoelectric effect (c.f., the method of ‘dual-energy subtraction’ by Saito [9]).

(iii) To determine the effective atomic number (e.g., via the second entry in Eq. (4)), the dependency \( C(Z) \) has to be specified, which is often done by introducing an exponent \( m \) [2], yielding
\[
C(Z_{\text{eff}}) = \frac{\tilde{\mu}_{A}\tilde{\mu}_{B}}{B_{\text{eff}}^{m}} + 1
\]
(6)

### 3. Results

In table 1, the six investigated image-based approaches for DECT-based calculation of \( \tilde{\mu}/\rho_{w} \) are listed.\(^1\) The corresponding equations for \( \tilde{\mu} \) and \( Z_{\text{eff}} \) determination in each of these approaches are mathematically equivalent to Eqs. (5) and (6) in the framework established in the last section. This equivalence is manifest by straight-forward arithmetic transformation after applying the according re-definitions of the involved parameters (last column in Table 1). Due to the equivalence of each of the listed approaches to the framework established in Section 2, the approaches are also mutually equivalent.

Eqs. (5) and (6) initially contain a total of five parameters (the four coefficients plus the exponent parameter), to be either fixed or determined by calibration. This parameter space can be further reduced by choosing to fix the water calibration point (for water: \( \tilde{\mu}_{b} = \tilde{\mu}_{i} = 1, \quad Z_{\text{eff}} = Z_{\text{eff},w} \)), yielding the parameter relations \( B_{0} = B_{1} = 1 \) and \( A_{0} = Z_{\text{eff},w}^{m} + A_{1} \). This eliminates one parameter in each of the Eqs. (5) and (6), leaving only one free calibration parameter for \( \tilde{\mu} \) determination (e.g., \( B_{1} \)) and two more for \( Z_{\text{eff}} \) determination (e.g., \( A_{1}, m \)). The minimum set of two calibration parameters (e.g., \( B_{1}, A_{1} \)) is obtained by further fixing the exponent \( m \) to some known value, typically between 3.0 and 3.5 (Table 1).

\(^1\) Some of the DECT approaches mentioned in the introduction are not calibration-based [6,8] or working with parameterizations that are more complex than Eq. (1) [14]. Consequently, these methods are not compatible with the presented framework and are not included in the study.

| ID  | Reference                  | \( \tilde{\mu} \) eq. | \( Z_{\text{eff}} \) eq. | Fix water calibration | \( m \) | Parameter transformations |
|-----|----------------------------|------------------------|---------------------------|-----------------------|--------|-----------------------------|
| BRO | Brooks (1977) [21]          | (4), (6), (10)         | (4), (6), (10)             | Yes                   | 3.1    | \( Q_{1} = Z_{\text{eff},w}^{m}B_{0}/A_{0}, \) \( Q_{2} = Z_{\text{eff},w}^{m}B_{1}/A_{1} \) |
| HEI | Heismann et al. (2003) [7]  | (16)\(^a\)             | (17)                       | No                    | 3.0    | \( \beta = \tilde{\mu}_{A} = \tilde{\mu}_{B}, \) \( \tilde{g}_{1} = \tilde{g}_{1}, \) \( \tilde{g}_{2} = \tilde{g}_{2} \) |
| SA1 | Saito (2012) [9]            | (1), (2)               | –                          | Yes                   | –      | \( \alpha = B_{n} \) |
| LAN | Landry et al. (2013) [10]   | –                      | (9)                        | No                    | 3.3    | \( \alpha = B_{n}, \) \( \tilde{c}_{n} = -B_{A}, \) \( \tilde{d}_{n} = B_{A} \) |
| HUE | Hünemohr et al. (2014) [11] | (14)                   | (19)                       | Yes                   | 3.1    | \( \gamma_{L} = \frac{\tilde{q}}{B_{n}^{m} - B_{n}^{m}} + 1 \) |
| SA2 | Saito and Sagara (2017) [16] | (1), (2)               | (8)                        | Yes                   | 3.3    | \( \alpha = B_{n}, \) \( \tilde{c}_{n} = -B_{A}, \) \( \tilde{d}_{n} = B_{A} \) |

\(^a\) Mass density replaced by relative electron density.

\(^b\) The equality \( \tilde{\mu}_{A} = \tilde{\mu}_{B} \) is an additional assumption in HEI (see Section 4).
4. Discussion

We proved the mathematical equivalence of several image-based approaches for DECT-based \( \tilde{\rho}/Z_{eff} \) determination (Table 1). Certain statements about novelty have thus to be treated with care in this context: apparent differences in the final formulation of the employed equations are of mostly cosmetic nature, with no impact on the applicability or accuracy of the method.

There remains, however, a certain freedom concerning calibration choices, e.g., whether to fix the water calibration point or the exponent parameter \( m \). Both SA12 and HUE work with a minimal set of calibration parameters (\( \alpha, \beta \) and \( c, d \) respectively). Besides different values for \( m \), these methods are therefore fully equivalent. In contrast, the water calibration point was not fixed in LAN. Therefore, this approach involves four calibration parameters, of which one can be eliminated by taking the ratio of \( \tilde{\rho}_L \) and \( \tilde{\rho}_W \) in Eq. (2). In HEI, the energy dependence of the Compton effect was neglected (\( \tilde{\rho}_H = \tilde{\rho}_W \)), leading to a slightly different formulation. This assumption seems unnecessarily strict, as it does not further reduce the parameter space, nor offers any obvious practical advantage over the other methods. Besides the calibration parameters from the theoretical framework, as described up to now, additional parameters have been introduced by some authors to account for certain imperfections in the CT system. In SA11, for example, the solution for relative electron density (Eq. (5)) was wrapped in an additional linear-regression model (with two parameters a, b) to account for potential bias in CT-scanner calibration.

In general, the above described differences in the number of parameters do not seem to have a major influence on the accuracy of the determined quantities, as was also observed by SA12 in their comparison to LAN (cf., Figs. 7 and 8 in SA12). On the other hand, the specific practical procedure for the calibration of the parameters (e.g., calibration setup) can have a substantial impact on the accuracy of the method [23]. We therefore suggest that further work should be spent on the improvement of calibration rather than the theoretical framework. In addition, the importance of image acquisition and reconstruction should be stressed, as the reliability of CT numbers is essential for the practical advantage over the other methods. Besides the calibration parameters the Compton term was neglected (\( \tilde{\rho}_H = \tilde{\rho}_W \)), leading to a slightly different formulation. This assumption seems unnecessarily strict, as it does not further reduce the parameter space, nor offers any obvious practical advantage over the other methods. Besides the calibration parameters from the theoretical framework, as described up to now, additional parameters have been introduced by some authors to account for certain imperfections in the CT system. In SA11, for example, the solution for relative electron density (Eq. (5)) was wrapped in an additional linear-regression model (with two parameters a, b) to account for potential bias in CT-scanner calibration.

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Conflict of interest

None declared.

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