Physical Density Estimations of Single- and Dual-energy CT Using Material-based Forward Projection Algorithm

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Research

Keywords: CT calibration, Dual-energy CT, Biological tissue, ICRP110 human phantom, HU-to-density curve

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Abstract

Purpose: This study aims to evaluate the accuracy of physical density prediction in single-energy CT (SECT) and dual-energy CT (DECT) by adapting a fully simulation-based method using a material-based forward projection algorithm (MBFPA).

Methods: We used biological tissues referenced in ICRU Report 44 and tissue substitutes to prepare three different types of phantoms for calibrating the HU-to-density curves. Sinograms were first virtually generated by the MBFPA with four representative energy spectra (i.e. 80 kV, 100 kV, 120 kV, and 6 MV) and then reconstructed to form realistic CT images by adding statistical noise. The HU-to-density curves in each spectrum and their pairwise combinations were derived from the CT images. The accuracy of these curves was validated using the ICRP110 human phantoms.

Results: The relative mean square errors (RMSEs) of the physical density by the HU-to-density curves calibrated with kV SECT nearly presented no phantom size dependence. The kV-kV DECT calibrated curves were also comparable with those from the kV SECT. The phantom size effect became notable when the MV X-ray beams were employed for both SECT and DECT due to beam hardening effects. The RMSEs were decreased using the biological tissue phantom.

Conclusions: Simulation-based density prediction can be useful in the theoretical analysis of SECT and DECT calibrations. The results of this study indicated that the accuracy of SECT calibration is comparable with that of DECT using biological tissues. The size and shape of the calibration phantom could affect the accuracy, especially for MV CT calibrations.

Keywords: CT calibration, Dual-energy CT, Biological tissue, ICRP110 human phantom, HU-to-density curve

Introduction

To establish the relationship between the computed tomography (CT) number (in Hounsfield units, HU) of a given voxel and the physical (or electron) density relative to water is one of the crucial processes that control the variance of patient dose calculations in radiotherapy treatment planning\(^1\sim^3\). The HU-to-density conversion is typically determined by calibration curves, which are experimentally
obtained from tissue-substitutes with known densities in a calibration phantom. Several studies have investigated the sensitivity of dose calculation for photon and particle beams relative to the accuracy of this conversion. A major concern of this approach is that the elemental composition of these substitutes may differ from that of biological tissues, and consequently, the adopted calibration curves may not be sufficiently accurate. One way to overcome this problem is the state-of-the-art stoichiometric calibration method introduced by Schneider et al., in which the specific parameters of a CT scanner are determined by the measurement of a few tissue-substitutes with known materials. Recently, this method has been re-examined in the context of single-energy CT (SECT) calibration for proton therapy treatment planning, and its accuracy was found to depend on the tissue-substitutes used for calibration. This dependency implies that the improvement of dual energy CT (DECT) over SECT should also be re-assessed, which may depend on the use of tissue substitutes as determined in a number of experiments for predicting relative stopping powers in proton therapy.

In this study, the accuracy of physical density prediction using SECT and DECT was evaluated, which is the first step in treatment planning. To reduce the uncertainty of the calibration, the HU-to-density conversion using biological tissues from ICRU Publication 44 was proposed. The approach in this study differs from the stoichiometric calibration by assuming that the X-ray spectra are known for the evaluation of the attenuation coefficients. In this case, CT values were reconstructed from the sinograms generated by the material-based forward projection algorithm (MBFPA), which has been utilised in model-based material decomposition, when the material composition of the object was determined. These CT values were then used to perform the calibration to obtain the HU-to-density look-up-table (LUT). Using this LUT, arbitrary CT images can be converted to density images. Namely, this approach is a full simulation of the clinical process because it is based on the modelling of the entire CT system, including the incident X-ray energy spectrum.

The aim of this study was threefold. First, the feasibility of the proposed approach using MBFPA for physical density prediction was presented, which is significantly relevant to estimate proton stopping powers for treatment planning. To achieve this, the HU-to-density curves were simulated using three types of phantoms, where phantom (size/shape and composition) dependence in the calibration was also analysed. Second, the advantage of DECT over SECT for calibrations based on the proposed approach
was quantitatively evaluated. Furthermore, the issue of whether a large energy gap in DECT, such as in the kilovoltage-megavoltage (kV-MV) range, could improve the accuracy of estimating the physical density was reassessed.

**Materials and Methods**

The schematic workflow is shown in Fig. 1. The method starts with the preparation of three types of two-dimensional material-based digital calibration phantoms. Next, virtual projections (or sinograms) were produced using MBFPA, and CT images were sequentially reconstructed with the sinograms. Using the reconstructed images, the HU-to-density LUTs were calculated for each phantom. Finally, these LUTs were validated by predicting the physical density distributions of the ICRP110 human phantom. Four different X-ray energy sources (i.e. 80 kV, 100 kV, 120 kV, 6 MV) were employed. Thus, four SECTs and their six pairwise combinations for DECTs were considered.

![Fig. 1. Workflow of the current study for total density evaluation. BT(A), TS, and BT(B) phantoms were used for the calibration, and the ICRU human phantoms were used for the validation (for more details, see the main text).](image-url)
Digital phantoms

Three types of phantoms were employed for the calibrations in this study, including the biological tissue (BT) phantoms in two different sizes and shapes, as well as the Gammex phantom (Gammex Inc., Middleton, WI). The former two are referred to as the BT(A) and BT(B) phantoms, respectively. The latter is known to have better tissue substitutes (TS) than the other tissue-mimicking phantoms\(^9\), and is hereon referred to as the TS phantom. The shape of BT(A) is similar to the Shepp-Logan phantom, whereas those of TS and BT(B) mimicked that of the Gammex phantom. The composed materials of BT(A) were taken from the ICRU publication 44\(^{13-15}\). Details of the elemental compositions and mass fractions are listed in Table I of Ref. 11 or Table I of Ref. 12. Following Hünemohr et al.’s study\(^{12}\), the mass fractions of six major elements (H, C, N, O, P, Ca) were normalised to provide a sum of 100%. Three of the materials were randomly selected to construct one BT(A) phantom; a total of 54 phantoms were generated. Meanwhile, the TS phantom was composed of one base material (solid water) and 12 insertions (LN-300, LN-450, AP6, BR12, water, SR2, LV1, IB3, B200, CB2-30%CaCO\(_3\), CB2-50%CaCO\(_3\), and SB3), which were generated with weight fractions and mass densities of 8 elements (H, C, N, O, Mg, Si, P, and Ca) provided in Ref.\(^9\). The BT(B) phantoms have the same shape as the TS phantom but consist of 12 standard human biological tissues\(^{13-15}\) and water instead of tissue-substitutes. By using different biological tissues, 6 phantoms were created. The width (major axis) and height (minor axis) of each BT(A) phantom were 260 mm and 197 mm, respectively, with a pixel scale of 1 mm, while the TS and BT(B) phantoms had a radius of 115 mm. Each of the insertions in the latter two had a radius of 13 mm. All the phantoms were placed in the air to obtain “complete” phantoms (images), for which the sizes were 300 \(\times\) 300 mm\(^2\) for the BT(A) and 512 \(\times\) 512 mm\(^2\) for the TS and BT(B). These three types of phantoms were considered for the following reasons: 1) to analyse the size and shape dependence by comparing the calibration results from the BT(A) and BT(B) phantoms, and 2) to analyse the material dependence by comparing the TS and BT(B) phantoms. Finally, 30 images were prepared from the ICRP110 human phantoms for validation, which consisted of five head, lung, and pelvis phantom slices for both, females and males, which were all 512 \(\times\) 512 mm\(^2\) in size with a 1-mm scale; six elements (H, C, N, O, P, and Ca) were considered. The specifics of all the phantoms used in this study are summarised in Table 1. The phantoms in the calibration are shown in Fig. 2, and the selected
ICRP110 human phantoms are shown in Figs. 3 and 4.

Fig. 2. Shape, size, and composition of the BT(A), TS, and BT(B) phantoms in the calibration.

- **BT(A)** 1-3: biological tissues
- **BT(B)** 5: Water, **Others**: biological tissues

Fig. 3. Ground truth of the selected ICRP110 human phantoms for female. The images in the first, second, and third row indicate head, lung, and pelvis, respectively.
Table 1. Specifics of all the phantoms used in this study.

<table>
<thead>
<tr>
<th>Name</th>
<th>Calibration</th>
<th>Validation</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>BT (A)</td>
<td>TS</td>
</tr>
<tr>
<td>Materials</td>
<td>Biological tissues</td>
<td>Tissue substitutes</td>
</tr>
<tr>
<td>Shape</td>
<td>Shepp-Logan</td>
<td>Gammex</td>
</tr>
<tr>
<td>Width (mm)</td>
<td>260</td>
<td>330</td>
</tr>
<tr>
<td>Height (mm)</td>
<td>197</td>
<td>330</td>
</tr>
<tr>
<td>Image (mm²)</td>
<td>300²</td>
<td>512²</td>
</tr>
<tr>
<td>Slice(s)†</td>
<td>54</td>
<td>1</td>
</tr>
</tbody>
</table>

†: number of phantoms (slices) used in calibration and validation.

**Virtual projection and reconstruction**

In this study, four different X-ray energies (80 kV, 100 kV, 120 kV, and 6 MV) were used for SECTs, and their six pairwise combinations for DECTs. This makes it simple to compare the results from SECT, kV-kV DECT, and kV-MV DECT. For diagnostic CT, an X-ray within the MV range is not applicable, whereas for image-guided radiation systems, equipment to produce clinical or non-clinical projection images with MV X-rays exists. In this study, a 6 MV X-ray, which is a typical X-ray energy used in...
radiation treatment, was selected. The spectra of the X-ray sources were obtained by Monte-Carlo (MC) simulations using the GEANT4 toolkit (version 10.4) for a linear accelerator with kV imaging capability (Synergy, Elekta, UK). For kV X-rays, low-energy photons generated from an anode were decimated by filters composed of aluminium and copper, and the beam shape was formed by lead-cone and cassette collimators. For the MV X-rays, the photons generated from the target were decimated by a flattening filter, and the beam shape was formed by primary, jaw, and multi-leaf collimators. In both cases, the energy spectrum was formed by the photons collected on the plane located 70 cm from the sources. Fig. 5 presents the X-ray spectra produced for the kV and MV beams. Using the spectra and the digital calibration phantoms indicated above, virtual projections using MBFPA were then simulated; further details can be found in the Appendix. The geometry of the simulated CTs with relevant factors is shown in Fig. 6. The source and detectors were rotated 360 degrees in 0.45-degree increments (in total 800 projections). There were 609 detectors, which were aligned in equal intervals (0.15 cm). Furthermore, random noise is inevitable in CT imaging, which is also a main source of artefacts. A Gaussian distributed random noise was added to the sinograms (detectors) for the simulations in this study, for which the strength was determined to produce a signal-to-noise ratio of ~20 in the reconstructed images of a homogeneous water phantom, which is consistent with that in clinical practice.

Fig. 5. Simulated X-ray spectra of 80 kV, 100 kV, 120 kV, and 6 MV. The mean energies were 48.70 keV, 53.24 keV, 59.28 keV, and 1.30 MeV, respectively.
For the calibrations, the average CT number (HU) of each material from the reconstructed images along with the corresponding physical density (known for the calibration phantoms) were used to form the LUTs. A fourth order polynomial was applied to relate the physical density $\rho$ with HU in Hounsfield units as follows:

$$\rho(HU) = c_0 + c_1 HU + c_2 HU^2 + c_3 HU^3 + c_4 HU^4, \quad (1)$$

where $c_i \ (i = 0, \cdots, 4)$ are the parameters; note, $c_0$ can be expressed with $c_i \ (i = 1, \cdots, 4)$ because $\rho(-1000) = 0$. Therefore, the last four can be determined from a least-squares fit to the LUT of the SECT scans. The values of the parameters may differ depending on the X-ray energies and calibration phantoms and should be treated accordingly.

**HU-to-density relation for DECT calibrations**

The $\Delta HU - \rho_e$ conversion method$^{22,23}$ was applied for the DECT calibration, however, the electron density $\rho_e$ was replaced with the physical density $\rho$. This is appropriate because $\rho$ is proportional to

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**Fig. 6.** Schematic of geometry applied in sinogram production. IDD and SDD indicate the isocenter-to-detector distance and the source-to-detector distance, respectively. A total of 609 detectors were used, and the size of each one was 0.15 cm.
The dual energy subtracted quantity $\Delta HU$ was defined as follows:

$$\Delta HU \equiv (1 + \alpha) HU_H - \alpha HU_L , \quad (2)$$

where $HU_H$ and $HU_L$ denote the high-energy and low-energy CT numbers in Hounsfield units, respectively. Further, $\alpha$ is a weighting factor for the subtraction, which is regarded as material-independent. Similar to a previous study,$^{22}$ the relation between $\Delta HU$ and $\rho$ was assumed to be linear for materials with low effective atomic numbers as follows:

$$\rho(\Delta HU) = \frac{a \Delta HU}{1000} + b , \quad (3)$$

where $a$, $b$, and $\alpha$ can be determined by a least squares fit to $(HU_H, HU_L) - \rho$ data obtained from DECT scans of materials with a known density $\rho$ in calibration phantoms, which is similar to the SECT calibration.

### Validation

The minimum $\chi^2$ value of the fitting curves for the physical density were evaluated for all three calibration phantoms. A total of 30 virtual images based on the ICRP110 human phantoms (shown in Table I and Figs. 3 and 4) were independently prepared via virtual projections and image reconstructions. The physical density distribution converted by the LUTs of each energy spectrum and calibration phantom were compared with the ground truth. Statistical analysis was performed to determine the differences in the RMSE among the chosen energies (for SECT), their combinations (for DECT), or the chosen calibration phantoms. In particular, the following differences were assessed: 1) between SECT and DECT, 2) between TS and BT(B), and 3) among the energies with BT(A) and BT(B). For the statistical analysis, a Student's t-test was employed for the first two cases, while Tukey's range test was employed for the last.

### Results

#### Generated sinograms and reconstructed images

Fig. 7 presents the representative sinograms generated from the MBFPA of the TS phantom with four energies, and Fig. 8 presents the corresponding reconstructed images.
SECT calibration results

A dataset of CT values and physical densities in the calibration phantoms can be derived from the above reconstructed images. The data points and fitted curves for all three phantoms and four energies are shown in Fig. 9. The three calibration phantoms present similar behaviours, which is reasonable because similar or same materials were used. However, the BT(A) phantoms present a relatively different behaviour compared to the TS and BT(B) phantoms in the case of 6 MV because the size of the former is smaller.
DECT calibration results

The data of $\Delta HU$ and $\rho$, as well as the fitted results, are shown in Fig. 10. It was found that the TS and BT(B) phantoms have similar behaviours in all six DECT calibrations, which are different from the BT(A) phantoms. However, in the case of kV SECTs, all three curves present similar behaviours, as shown in Fig. 9. This is because a fourth order polynomial was applied for the SECT fitting, while a linear relationship was assumed for the DECT calibration. Therefore, the difference in the data points is suppressed by the higher order terms in the SECT situation. However, for the DECT calibration, such differences become notable. In addition, the fact that the size/shape of BT(A) and BT(B) phantoms are different also implies that the physical density estimation in the $\Delta HU$ approach depends on (the size/shape of) the calibration phantoms as well. In particular, this dependence appears stronger in kV-MV DECT calibrations.

Fig. 9. HU-to-density relations of three calibration phantoms with 80 kV, 100 kV, 120 kV, and 6 MV in SECT. The CT values are referred to as “Effective HU” because this approach is based on simulations.
Validation using the ICRP110 human phantom

The validation results using the ICRP110 human phantom are shown in Table II, where the average RMSEs are listed for all the anatomies. No significant difference in the RMSEs was found between SECT and DECT ($p$-values: 0.26, 0.16, and 0.68 for BT(A), TS, and BT(B), respectively). Conversely, the predicted results from the calibrations using BT(B) phantom significantly improved compared to that using TS phantom in density calibration ($p$-values: < 0.01), although the mean RSME difference was less than 0.0093. For the energy dependence of the physical density estimation, the RMSEs of the
6 MV SECT were observed to be significantly larger than those of the others for BT(B), whereas no significant difference was observed in the use of BT(A), mainly caused by the lung area having the large size. In addition, the RMSEs of the 6 MV SECT from BT(A) phantoms are relatively better than those from BT(B) phantoms. More specifically, the smaller the calibration phantom, the more accurate the validation predictions are. However, such behaviours are not apparent in the kV SECT results.

Table 2. Predicted average RMSEs of ICRP110 phantom slices from BT(A), TS, and BT(B) phantoms with SECT and DECT.

<table>
<thead>
<tr>
<th>Calibration</th>
<th>Anatomy</th>
<th>SECT predictions</th>
<th>DECT predictions</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>80 kV</td>
<td>100 kV</td>
</tr>
<tr>
<td>BT(A)</td>
<td>Head</td>
<td>0.1230</td>
<td>0.1236</td>
</tr>
<tr>
<td></td>
<td>Lung</td>
<td>0.1507</td>
<td>0.1429</td>
</tr>
<tr>
<td></td>
<td>Pelvis</td>
<td>0.0793</td>
<td>0.0756</td>
</tr>
<tr>
<td>TS</td>
<td>Head</td>
<td>0.1362</td>
<td>0.1424</td>
</tr>
<tr>
<td></td>
<td>Lung</td>
<td>0.1589</td>
<td>0.1522</td>
</tr>
<tr>
<td></td>
<td>Pelvis</td>
<td>0.0759</td>
<td>0.0762</td>
</tr>
<tr>
<td>BT(B)</td>
<td>Head</td>
<td>0.1294</td>
<td>0.1375</td>
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<tr>
<td></td>
<td>Lung</td>
<td>0.1484</td>
<td>0.1456</td>
</tr>
<tr>
<td></td>
<td>Pelvis</td>
<td>0.0727</td>
<td>0.0745</td>
</tr>
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</table>

Discussions

This study presented the evaluation of both SECT and DECT calibrations based on the MBFPA and demonstrated that the accuracy of SECT calibration is comparable with that of DECT. In addition, the use of the biological tissue phantom in the calibration was found to improve the physical density prediction compared with that of the Gammex phantom composed of tissue substitutes.

Similar results have already been implicitly obtained by Goma et al. who performed SECT calibration using the stoichiometric method, which consists of characterising the CT scanner directly through CT scans of tissue substitutes, and subsequently predicting the CT numbers of biological tissues using this characterisation. The main difference between the stoichiometric calibration and the present MBFPA approach is that the former requires real CT images acquired from CT scanners, whereas the latter does
not. In this study, the CT scanners were modelled, characterised by X-ray energy spectra directly, by which various simulations, with not only the kV-range X-rays but also MV-range X-rays, could be performed. Furthermore, the density results cannot be validated for real patients in the stoichiometric calibration framework. However, using the proposed MBFPA-based calibration approach, the validation is now possible by preparing, for example, the reconstructed CT datasets using the ICRP110 human phantom, which could be considered as real patients to a certain extent. This study not only supported the results of Goma et al. but also newly presented that the tissue substitutes differ from the biological tissues in physical density calibration.

The results of this study indicated that kV-MV DECT is not as outperformed as it was expected to be. This is due to the large beam hardening effect in MV CT, compared to that in kV CT. This can be inferred from the fact that different sizes of the calibration phantoms provided different calibration curves with MV X-rays. For a more apparent indication, a simulation using monochromatic energy X-rays with 3 MeV was also performed, which does not suffer from beam hardening. In this case, no phantom size dependence in the calibration curves was observed. The magnitude of beam hardening in MV CT could also be observed in the homogeneous water phantom (of the same size as the TS phantom) by extracting the reconstructed CT values in the centre and peripheral regions. Their relative difference was ~17% for MV CT due to the cupping artefacts; however, this value is only ~10% for kV CT. Such ambiguity in the MV CT with a practical spectrum significantly affected the accuracy of the calibration. Hence, DECT with MV X-rays does not improve the accuracy of the physical density estimation as well as the SECT of MV X-rays. Furthermore, the use of MV X-rays passing through a titanium filter could, to a certain extent, reduce the beam-hardening effect.

Note that Yang et al. assessed the superiority of kV-MV DECT in determining proton stopping power by generating 1 MV beams from MC calculations. According to the authors, when CT number uncertainties and artefacts such as imaging noise and beam hardening effects were considered, the kV-MV DECT improved the perfectly of SPR estimation substantially over kV-kV or MV-MV DECT methods. The SPR estimation is directly influenced by the electron density (or physical density), and therefore, Yang et al.’s study implied a substantial decrease in the physical density uncertainties in kV-MV DECT. However, this study apparently supports the contrary. This might indicate that the beam hardening...
effects were underestimated in MV CT in Yang et al.’s study because the authors assumed the “average spectra” accurately modelled the CT scanner. Thus, the beam hardening effect should be carefully treated in MV CT.

The proposed method can be considered an improvement over previous stoichiometric approaches in which the parameters, depending on the X-ray spectrum, which characterise the CT scanner are determined by fitting to the effective linear attenuation coefficients of a given material, whereas the proposed method explicitly deals with the X-ray spectrum. Although the explicit handling of the X-ray spectrum is advantageous in CT calibration, the requirement of the X-ray spectrum imposes limitations for practical applications. That is, the exact energy spectrum of medical CT scanners is unknown, and its direct measurement is difficult because of the high photon flux. Nevertheless, novel methods to estimate X-ray spectra in practical CT scanners have been proposed in recent years\textsuperscript{25-27}. Therefore, it is reasonable to assume that X-ray spectra are currently available.

**Conclusions**

The proposed method using the MBFPA is useful in the theoretical analysis of physical density calibrations. The accuracy of SECT calibration is comparable with that of DECT calibration and is improved with the use of biological tissues. The size and shape of the calibration phantom could affect the accuracy, especially for MV CT, mainly because of the beam hardening effects. The present method based on the MBFPA can also be applied to various other studies, such as effective atomic number estimations and material decompositions.
Declarations

Ethics approval and consent to participate
Not applicable.

Consent for publication
Not applicable.

Availability of data and materials
The datasets used and/or analysed during the current study are available from the corresponding author upon reasonable request.

Competing interests
The authors declare that they have no competing interests.

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Authors’ contributions
KL and DF conceived the idea. The method was discussed for KL, DF, and AH. Based on the discussion, KL and AH developed the software, and KL and DF analysed the generated data. KL, AH, HL, and LG presented the obtained results. KL and AH drafted the manuscript. All authors read, modified, and approved the manuscript.

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Appendix: Material-based forward projection algorithm (MBFPA)

The material-based forward projection algorithm applied in the X-ray virtual projections is briefly introduced here. According to Lambert-Beer’s law, the photon number \( n_i \) in the \( i \)-th detector after penetrating the object with attenuation coefficient \( \mu_j \) in voxel \( j \) is as follows:

\[
n_i(E) = n_0(E)e^{\sum_j -a_{ij}\mu_j(E)}, \quad (A1)
\]

where \( E \) is the photon energy, \( n_0 \) is the photon number in the X-ray source, and \( a_{ij} \) is the photon pass length in voxel \( j \), representing an element of the “system matrix”. If the spectrum of the X-ray is considered (as bins), the total photon number in the \( i \)-th detector becomes the following:

\[
n^\text{total}_i = \sum_E \alpha(E)n_i(E) = \sum_E \alpha(E)n_0(E)e^{\sum_j -a_{ij}\mu_j(E)}, \quad (A2)
\]

where \( \alpha(E) \) is the fraction of the corresponding photon energy bin. \( \mu_j(E) \) is dependent on the atomic number \( Z \) and the density \( \rho \) of the materials in a voxel \( j \), which is expressed as a sum of the attenuation coefficients for each element \( m \) as follows:

\[
\mu_j(E, Z, \rho) = \sum_m w_m \mu_{m,j}(E, Z, \rho), \quad (A3)
\]

where \( w_m \) denotes the weight (fraction) of the \( m \)-th element. For the energy range considered in this study, the attenuation coefficient \( \mu_{m,j}(E, Z, \rho) \) can be written as the sum of the processes of the photoelectric effect, Compton scattering, and pair production as follows:

\[
\mu_{m,j}(E, Z, \rho) = \rho Z \frac{N_A}{A} [\sigma_{pe}(E, Z) + \sigma_{comp}(E) + \sigma_{pp}(E, Z)], \quad (A4)
\]

where \( N_A \) and \( A \) denote the Avogadro constant and atomic weight, respectively. \( \sigma \) is the cross section of the photon – matter interactions. The cross section of the photoelectric effect can be approximated by\(^{28}\) as follows:

\[
\sigma_{pe}(E, Z) = 3.45 \times 10^{-6} r_e^2 (1 + 0.008 Z) \frac{Z^3}{E^3} (1 - \frac{E_k}{4E} - \frac{E_k^2}{1.21E}), \quad (A5)
\]

where \( r_e = 2.81794 \) fm is the classical electron radius and \( E_k \) is the \( K \)-shell binding energy. The latter is ignored in this study. The Compton scattering cross section is theoretically expressed by the Klein–Nishina formula as follows:
\[ \sigma_{\text{comp}}(E) = 2\pi r_e^2 \left\{ \frac{1 + E}{E^2} \left[ \frac{2(1 + E)}{1 + 2E} - \frac{\ln(1 + 2E)}{E} \right] + \frac{\ln(1 + 2E)}{2E} - \frac{1 + 3E}{(1 + 2E)^2} \right\} \quad (A6) \]

The cross section of the pair production is approximated as follows:

\[ \sigma_{\text{pp}}(E, Z) = 0.2545r_e^2(E - 2.332) \frac{Z}{137} \quad (A7) \]

As a result, the virtual projections were simulated by a ray-tracing method to generate sinograms. The sinograms were simulated by considering the energy spectrum with a bin width of 1 keV in this study.
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Figure 1

Workflow of the current study for total density evaluation. BT(A), TS, and BT(B) phantoms were used for the calibration, and the ICRU human phantoms were used for the validation (for more details, see the main text).
Figure 2

Shape, size, and composition of the BT(A), TS, and BT(B) phantoms in the calibration.

- **BT(A)** 1-3: biological tissues
- **BT(B)** 5: Water, **Others**: biological tissues

Figure 3

Ground truth of the selected ICRP110 human phantoms for female. The images in the first, second, and third row indicate head, lung, and pelvis, respectively.
Figure 4

Ground truth of the selected ICRP110 human phantoms for male. The images in the first, second, and third row indicate head, lung, and pelvis, respectively.

Figure 5

Simulated X-ray spectra of 80 kV, 100 kV, 120 kV, and 6 MV. The mean energies were 48.70 keV, 53.24 keV, 59.28 keV, and 1.30 MeV, respectively.
Figure 6

Schematic of geometry applied in sinogram production. IDD and SDD indicate the isocenter-to-detector distance and the source-to-detector distance, respectively. A total of 609 detectors were used, and the size of each one was 0.15 cm.

Figure 7

Sinograms of the TS phantom with 80 kV, 100 kV, 120 kV, and 6 MV. The display value ranges are 0–0.01 for kV CT and 0.1–0.3 for MV CT.
Figure 8

Reconstructed images of the TS phantom with 80 kV, 100 kV, 120 kV, and 6 MV. The display value ranges of the attenuation coefficients (in units of cm⁻¹) are 0–0.4 for kV CT and 0–0.1 for MV CT.

Figure 9

HU-to-density relations of three calibration phantoms with 80 kV, 100 kV, 120 kV, and 6 MV in SECT. The CT values are referred to as “Effective HU” because this approach is based on simulations.
Figure 10

Effective ΔHU to density relations of the three calibration phantoms with 80 kV, 100 kV, 120 kV, and 6 MV in DECT.