X-ray dual energy spectral parameter optimization for bone Calcium/Phosphorus mass ratio estimation

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Abstract. Calcium (Ca) and Phosphorus (P) bone mass ratio has been identified as an important, yet underutilized, risk factor in osteoporosis diagnosis. The purpose of this simulation study is to investigate the use of effective or mean mass attenuation coefficient in Ca/P mass ratio estimation with the use of a dual-energy method. The investigation was based on the minimization of the accuracy of Ca/P ratio, with respect to the Coefficient of Variation of the ratio. Different set-ups were examined, based on the K-edge filtering technique and single X-ray exposure. The modified X-ray output was attenuated by various Ca/P mass ratios resulting in nine calibration points, while keeping constant the total bone thickness. The simulated data were obtained considering a photon counting energy discriminating detector. The standard deviation of the residuals was used to compare and evaluate the accuracy between the different dual energy set-ups. The optimum mass attenuation coefficient for the Ca/P mass ratio estimation was the effective coefficient in all the examined set-ups. The variation of the residuals between the different set-ups was not significant.

1. Introduction

Osteoporosis has been recognized as a worldwide disease that affects more than 75 million people in the United States, Europe and Japan [1,2]. Several methods [2,3] are available for measuring an individual's bone mineral status. Bone mineral density (BMD) is the gold standard measurement, determining the bone health, which primarily measures the quantity of bone in the skeleton. However, about one-half of fractures occur in women with a T-Score above the World Health Organization (WHO) diagnosis threshold of osteoporosis [1,4], suggesting that other factors, besides bone quantity, are involved in the appearance of fractures. The major and essential component of human bones is hydroxyapatite ($Ca_{10}(PO_4)_6(OH)_2$), a mineral form of calcium (Ca) and phosphorus (P) that gives bones their rigidity. Researchers [2,5,6] have determined alterations in skeletal Ca/P molar ratio. There are indications [5-10] that the alterations on Ca/P ratio have a negative effect on bone health.

In this study, an optimization in the Ca/P bone mass ratio estimation was held based on the dual energy method, previously described by in previous works of our group [7,8,11]. Simulated data were obtained using the K-edge filtering technique and single X-ray exposure. The modified X-ray output was attenuated by nine calibration points produced by various Ca/P mass ratios. The analysis presented here, investigates the use of effective or mean mass attenuation coefficient in Ca/P mass ratio estimation. The optimization was based on the minimization of the accuracy of Ca/P ratio, with respect to the coefficient of variation of the Ca/P ratio ($CV_{Ca/P}$). The standard deviation of the residuals was used to compare and evaluate the accuracy between the different dual energy set-ups.

2. Materials and Methods

2.1 Simulation input functions and parameters

The theory for the *in vivo* determination of Ca/P ratio, in the radius, was described previously [8,11]. The Ca/P mass ratio is obtained assuming that there is a three-component system: Ca, PO_4 and water (w). The photon beam is transmitted through an object of total thickness t, $t = t_{Ca} + t_{PO_4} + t_w$ where t_{Ca} is the thickness of calcium, t_{PO4} is the thickness of phosphate and t_w is the thickness of water. The total thickness was equal to 5cm, corresponding to a human forearm. Assuming that both surfaces of Ca and PO_4 were exposed to the same radiation beam and considering that the molecular weight ratio PO_4/P is 3.0679, the Ca/P mass ratio [7,11] is given by:

$$\frac{Ca}{P} = \frac{t_{Ca}}{t_{PO_4}} \cdot 3.0679 \qquad (1)$$

In a previous study [11], a wide range of filter materials and thicknesses, combined with different maximum tube voltages (kVps), were simulated producing the different set-ups. The set-ups were used for the dual energy spectra optimization, in the Ca/P mass ratio estimation. The simulation considers a photon counting energy dispersive detector that allows energy peak discrimination and counting.

2.2 Mass attenuation coefficients

In Table 1 the step thicknesses for Ca and PO_4 are shown, used to generate the detector data. The three pairs of Ca and PO_4 thicknesses correspond to molar ratios of 1.40, 1.58, and 1.67, respectively. The combined thicknesses results in 9 calibration points, where the total thickness of Ca, PO_4 and water is maintained constant.

Table 1. Ca and PO_4 calibration step thicknesses (in cm) used to generate simulated detector calibration data.

Material	Thickness (cm)		
Ca	0.0533	0.0671	0.0704
PO_4	0.1168	0.1017	0.0996

In the accuracy (~) determination [11] of the Ca/P mass ratio (Eq. 1), instead of the effective mass attenuation coefficient «/°$_{eff}$ that was used in the previous study [11,12], the mass attenuation coefficient, corresponding to the mean energy of the incident spectrum (mean mass attenuation coefficient, «/°$_{ME}$), can be used to estimate the Ca/P mass ratio. The accuracy of the estimated Ca/P mass ratio values was calculated for both «/°$_{eff}$ and «/°$_{ME}$ values.

For every calibration point, the residuals (¢) were calculated as the difference between the true (tr) and the estimated values (est) according to following equation:

$$¢ = Ca/P_{tr} - Ca/P_{est} \tag{2}$$

The standard deviation of the residuals (¢$_{rms}$) was used to compare and evaluate the accuracy between the different dual energy set-ups. ¢$_{rms}$ values close to zero indicates that the set-up has a smaller random error component. Different set-ups were examined, based on the K-edge filtering technique and single X-ray exposure [13]. This study used three set-ups with optimum $CV_{Ca/P}$ described in a previous study [11]. These are La (0.15cm, 100 kVp) (set-up S1), Ce (0.13cm, 100 kVp) (set-up S2) and Sm (0.13cm, 100 kVp) (set-up S3).

3. Results and Discussion

The accuracy values were calculated using both the effective («/°$_{eff}$) and mean («/°$_{ME}$) mass attenuation coefficients. For the set-ups S1, S2 and S3, the accuracy ranged from 2.31 to 5.18%, using «/°$_{eff}$ for the calculations, and from 8.33 to 18.98% using «/°$_{ME}$, respectively. Set-up S3 appeared to have the lower accuracy value (2.31%), as well as the optimum ¢$_{rms}$ (0.014) value. The results for set-ups S1, S2, S3 are shown in Table 2. The ¢$_{rms}$ values in three set-ups close to zero (Table 1) suggest that the errors from the Ca/P estimation will be sufficiently small in the calibration region. ¢$_{rms}$ values between the different set-ups were comparable. This implies that the accuracy values of each set-up are the main indicator for the optimum set-up and spectra optimization.

Table 2. ¢$_{rms}$ and accuracy range for the examined set-ups calculated with «/°$_{eff}$ and «/°$_{ME}$.

	«/°$_{eff}$		«/°$_{ME}$	
	¢$_{rms}$	α% (range)	¢$_{rms}$	α% (range)
set-up S1	0.033	3.60-4.22	0.067	15.47-18.98
set-up S2	0.019	4.25-5.18	0.066	15.49-18.61
set-up S3	0.014	2.31-2.97	0.077	8.33-12.31

The use of «/°$_{eff}$ instead of «/°$_{ME}$ provides results with lower accuracy values. The accuracy values can be up to 6 times higher if calculated with «/°$_{ME}$. In Table 3 the values of «/°$_{eff}$ and «/°$_{ME}$ are given for set-up S1. The «/°$_{ME}$ values are lower from the «/°$_{eff}$ values in all cases. These differences, in «/°$_{eff}$ and «/°$_{ME}$, justify the accuracy differences in Ca/P estimation.

Table 3. Mass attenuation coefficients of Ca, PO_4, w for set-up S1.

	«/°$_{eff}$	«/°$_{ME}$
$Ca_{(Ehigh)}$	0.7589	0.6866
$Ca_{(Elow)}$	2.2670	2.2570
$PO_{4\,(Ehigh)}$	0.2574	0.2458
$PO_{4\,(Elow)}$	0.5082	0.5069
$w_{(Ehigh)}$	0.2105	0.2072
$w_{(Elow)}$	0.2897	0.2897

The data from radius are included in this study solely as a proof-of-concept demonstration. The accuracy and the precision of measurements from bone phantoms and specimens is the subject of ongoing work in our lab.

4. Conclusions

Analysis of the bone composition increases sensitivity and specificity in metabolic bone diseases diagnosis and their monitoring. In this study an optimization in the Ca/P bone mass ratio estimation was investigated using the either the effective or mean mass attenuation coefficients. The use of the $«/°_{eff}$ instead of $«/°_{ME}$ provides results with lower accuracy values.

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