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# An Iterative Method for Computed Tomography Machine Calibration: Attenuation and Dual-Energy Computed Tomography Inversion from the Hounsfield Numbers

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ARTICLE INFO	A B S T R A C T
Article type: Original Paper	<b>Introduction:</b> Photoelectric effect and X-ray scattering determine the attenuation coefficient of materials in diagnostic radiology. This manuscript presents an iterative gradient search method to separate the reliable to the second determine the second determ
Article history: Received: Sep 13, 2019 Accepted: Feb 03, 2020	— contributions to attenuation from these two independent sources. This issue assumes importance due to two reasons, including 1) Electron density determination of scanned materials and 2) correct dose calculation in diagnostic radiology. Material and Matheda, A special water filled phantem which was custom built for simultaneous scanning.
Keywords: Compton Effect Photoelectric Effect	$\sim$ of 12 samples was used in the current study. Attenuation coefficient equations were iteratively solved to calculate the contributions from x-ray scattering and photoelectric effects. <b>Results:</b> Data converged after five iterations (within 1%). Error in the attenuation coefficient was measured at $\pm 3\%$ .
Computed Tomography	<b>Conclusion:</b> As evidenced by the obtained results, this method can be used to determine the Compton and photoelectric contributions with sufficient accuracy. Moreover, the inversion of Dual- Energy computed tomography (DECT) data for finding electron density and effective atomic number of materials also presents satisfactory results.

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# Introduction

Computed tomography (CT) is one of the most versatile and common non-invasive diagnostic tools in imaging the armamentarium. It is considered as having an excellent spatial and temporal resolution for the detection and characterization of various structures and organs in the human body [1, 2]. Image formation in CT systems utilizes the x-ray attenuation coefficient (depicted as  $\mu(E)$ ) of the material which is dependent on (a) the electron density, (b) effective atomic number of the material in the path of the x-ray beam, and (c) the effective energy of the source spectrum. Basic data from the CT are the Hounsfield unit (HU) values which relate the average attenuation coefficients of the materials ( $\hat{\mu}$  (V)) in the path of the x-ray beam to that of water ( $\hat{\mu}_w(V)$ ), where V is the excitation voltage of the x-ray source and the averages are calculated over the entire source spectrum and detector sensitivity

Due to the abovementioned applications, it is essential to accurately know the contributions of x-ray scattering and photoelectric effect to the total attenuation coefficient of the substance. X-ray scattering includes coherent+incoherent (i.e., Rayleigh scattering + Compton scattering) [3].

CT machines are standardized by the identification of the attenuations that are contributed to X-ray scattering and the photoelectric effect. Moreover, this

<sup>[3].</sup> Quantitative studies using CT system help the physicians to characterize normal and abnormal tissues and differentiate between them [4]. In addition, CT data are widely employed for (i) the assessment of mineral content in bones [5], (ii) tissue characterization by Dual-Energy CT (DECT) [6-8], and (iii) dose distribution calculations for radiation treatment planning in radiotherapy [9]. These references establish the first principles and the latest issues related to this field.

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identification in terms of constants a(V) and b(V) introduced in this paper yields satisfactory results for the inversion of electron density and effective atomic number of unknown substances i.e., they are the coefficients which are used for DECT inversion.

The method adopted in the current study was the CT machine calibration for the contributions of scattering and photoelectric effect using the HU values of substances with known electron density ( $\rho_e$ ) and effective atomic number ( $Z_{eff}$ ). When the coefficients for photoelectric effect and X-ray scattering are determined by calibration, they can be used to find ( $\rho_e$ ,  $Z_{eff}$ ) for unknown substances or DECT inversion.

# **Materials and Methods**

The HU values of the samples were recorded using a special phantom capable of determining the HU values of 12 samples by a single scan. It was performed to ensure that calibration data were obtained under identical conditions to the extent feasible. For data analysis, an iterative method was employed for the determination of x-ray scattering and photoelectric effect contributions.

## Experiment

For the experimental study, we employed a special phantom which was "custom-built" for the purpose of research. The basic design and the construction of this phantom are discussed in detail in our recent publication [10, 11]. The basic structure of the phantom can be surmised from the schematic diagram in Figure 1, while the actual arrangement of the body and test tubes are depicted in Figure 10f Reference [10]. The phantom is designed in a way to allow the beam hardening effect to be observed at different depths of the water phantom, and the added advantage is that 12 samples can be tested simultaneously.

The electron density  $(\rho_e)$  and effective atomic number  $(Z_{eff})$  of the samples were calculated from the known compositions of the mixtures that were employed in sample preparation. These calculations were performed using equtations1 and 2 as indicated below [12]:

$$\rho_e = \frac{\rho}{m_p} \times \frac{\sum_j \sum_i c(j) n(j,i) Z_i}{\sum_j \sum_i c(j) n(j,i) A_i}$$
(1)

$$Z_{eff}^{p} = \frac{\sum_{j} \sum_{i} c(j) n(j,i) Z_{i}^{p+1}}{\sum_{j} \sum_{i} c(j) n(j,i) Z_{i}}$$
(2)

where in Equation 1,  $\rho_e$ ,  $\rho$ , and  $m_p$  are the electron density (in electron/cc), mass density (in gm/cc), and mass of proton, respectively (=1.67×10<sup>-27</sup>kg). Atomic number and atomic mass of the *i*-th atom are represented by  $Z_i$  and  $A_i$ , respectively. c(j) is "the ratio of the (number of the *j*-th molecules/total number of molecules)" with c(j) = w(i)/M(j), where w(j) and M(j)are (weight/weight) concentration and molecular weight of the *j*-th component, respectively. In equation 2,  $Z_{eff}^{p}$  is the weighted average of the atomic number where p > 1.0 (here p=4.0) is an index in the exponent of  $Z_{i}$ , as is explained in Reference [12].



Figure 1. Schematic diagram of phantom (a) front view demonstrating the arrangement of test tube holders, (b) lateral view depicted by the photograph of the phantom in Figure 1 of Reference [10].

The operating voltages used were 80, 110, and 130 kVp with tube current (mAs) being equal to 135, 4.8 mm slice thickness, and H31s convolution kernel. These settings were used to scan the calibration samples which included (a) water in the phantom, (b) chemical compounds in the test tubes by 16-slice Siemens Somatom CT system. To this end, the water-filled test-tubes were successively replaced with those filled with methanol, glycerol, and potassium hydroxide solutions of known concentration. Each series of chemical compounds was scanned separately by the insertion of the test tubes containing different samples in the different test tube holders in the phantom.

Liquid samples are used due to their homogeneity. The chemicals that were selected for calibration included methanol, glycerol, and potassium hydroxide (KOH) which were obtained from Merck chemicals (methanol and glycerol with 99.9% purity). Furthermore, the density measurements were performed with a precision balance of  $\pm 0.001$  gm, density values and the calculated values of  $\rho_e$  had an accuracy of  $\pm 0.01\%$ . The ( $\rho_{er}$ ,  $Z_{eff}^x$ ) values of the calibration substances are demonstrated in Figure 2.

These samples were primarily selected due to their purity, ready availability, and ease of handling. Secondly, it was possible to prepare samples with a broad range of ( $\rho_e$ ,  $Z_{eff}$ ) values that resemble those found in the human body. Nonetheless, some limitations exist regarding the fulfillment of the second condition since nature does not allow the choices of ( $\rho_e$ ,  $Z_{eff}$ ) as may be desired by the calibration purpose. Therefore, we are limited by the values that are practically realizable which depend on the miscibility of substances, their densities, volumes of mixing, and molecular weights.



Figure 2. Variations of effective atomic number versus electron density of (a) methanol, (b) glycerol, and (c) potassium hydroxide (KOH) which were used as calibration samples. The electron density ( $\rho_e$ ) is expressed in units of  $10^{23}$ electrons per cc.

For the calculation of  $Z_{eff}$ , we used the photoelectric exponent to be x=4- the well-known case for a hydrogen-like atom, though various values of x are used in the literature.

For all computational purposes, the "corrected" HU values were employed which were calculated using the following formula:

$$HU_{corrected} = HU_s - HU_w \tag{3}$$

where  $HU_s$  and  $HU_w$  represent the HU values of the solution and water in the corresponding test-tubes, respectively.

# Method of data analysis

From the definition of HU (V), it follows:  $F(V) = 1 + \frac{HU(V)}{1000} = \left(\frac{\hat{\mu}(V)}{\hat{\mu}_{W}(V)}\right)$ (4)

where F(V) is calculated from the corrected HU(V) values as determined by Equation 3.  $\hat{\mu}(V)$  and  $\hat{\mu}_w(V)$  are the average attenuation coefficients of the substance and water, respectively, and the average was taken over the source spectrum of the x-ray and detector efficiency. As illustrated in Equation 4, F(V) is proportional to the average attenuation coefficients of the substance. For any energy (E) of the photon, the attenuation coefficient is obtained from:

$$\mu(E) = \alpha_0 f_{sc}(E) \rho_e + \beta_0 f_{ph}(E) \left[\rho_e Z_{eff}^{x}\right]$$
(5)

with

$$f_{sc}(E) = f_{coh}(E) + f_{incoh}(E)$$
(6)

where the suffixes "*coh*" and "*incoh*" refer to coherent (Rayleigh) and incoherent (Compton) parts, respectively. It is worthy to note that the contributions from both these types of scattering are dependent only on  $X=\rho_e$ , and there is NO dependence on  $Y=[\rho_e Z_{eff}^x]$ . On the other hand, the attenuation coefficient due to the photoelectric effect depends ONLY on Y. We have the well-known coefficients,  $\alpha_0= 66.62 \times 10^{-24}$  cm<sup>2</sup> = scattering cross-section for Thomson scattering and  $\beta_0$  =  $54.7578 \times 10^{-18}$  cm<sup>2</sup> = coefficient for the photoelectric cross-section for atomic hydrogen. In addition, absorption can exist at the K-edges of the atoms. These lie at13.6, 288.8, 401.6, and 532 eV for hydrogen, carbon, nitrogen, and oxygen, respectively. They are the most abundant elements in the human body, they are also the elements used in our calibration materials. We have also used a high  $Z_{eff}$  material, such as potassium hydroxide for which the K-edge for potassium lies at 3590-3670 eV [13]. As is widely known, x-ray tubes in CT machines emit an insignificant number of photons at these K-edge energies. Therefore, it is possible to parametrize attenuations the of x-ray the abovementioned atoms using equations 5 and 6 in the region of diagnostic x-rays employed in CT machines. This can also be verified from the NIST tables [14].

The attenuation coefficients are a sum of the abovementioned two terms presented in Equation 6. Thereafter, by averaging over the source spectrum (along with internal and external filtering) and the detector response for different photon energies, average attenuation coefficient detected by the CT machine is the sum of the averages of the above two quantities:  $\hat{\mu}(V) = \alpha_0 \hat{f}_{sc}(V)X + \beta_0 \hat{f}_{ph}(V)Y$  (7)

where  $\hat{\mu}(V)$  denotes the averages over source spectrum and detector response for an applied voltage V.

Thereafter, combining equations 4 and 7 yields: F(V)=a(V)X + b(V)Y (8) where  $a(V) = \propto_0 \hat{f}_{sc}(V)/\hat{\mu}_w(V)$  (8.1)

$$b(V) = \beta_0 \hat{f}_{nh}(V) / \hat{\mu}_w(V)$$
(8.2)

$$X = \rho_e \tag{8.3}$$

$$Y = \rho_e Z_{eff}^{x} \tag{8.4}$$

where  $\hat{f}_{sc}(V)$  and  $\hat{f}_{ph}(V)$  are the average  $f_{sc}(E)$  and  $f_{ph}(E)$  taken over the source spectrum. The quantities a(V) and b(V) are unknown since the source spectrum is not provided by the manufacturer. Independent measurements to find the source spectrum would be

highly demanding in terms of investments in infrastructure and human resources or computation using methods, such as Monte Carlo. In the absence of the knowledge of the source spectrum or the detector efficiency, a(V), b(V) will be found with the help of independent experiments by fitting the HU(V) data with (X, Y) for samples with known (X, Y) values. From these fits, we calculate the a(V) and b(V) by an iterative calibration procedure.

The method is used for the calculation of F(V) values of known substances from their HU(V) data and fit F(V) to a linear equation, such as equations 8 and 8.4 using the known (X,Y) values of these substances. This is the calibration part of the experiment from which several other predictions can follow about different procedures in diagnostics, dosimetry, treatment-planning, and radiation protection. For instance, if a(V) and b(V) are known, it will be possible to determine F(V) and HU(V) for any substance, given their  $X=\rho_e$  and  $Y=[\rho_e Z_{eff}^x]$  values. In the current study, it was also indicated that a(V) and b(V) values found for V=80, 130 kVp can be used for inversion to find  $X=\rho_e$  and  $Y=[\rho_e Z_{eff}^x]$  values with a high level of accuracy.

## Iterative algorithm for calibration

In the range of x-ray energies,  $f_{sc}(E) \approx 1-0.5$ ,  $f_{ph}(E) \approx (I_0/E)^{3.5} \approx 10^{-10}$ , with  $I_0 = 13.6$  eV was the ionization energy of hydrogen so that we expect  $b(V) \sim 10^{-5} a(V)$ . Therefore, in any data, the first term in Equation 6 is dominated by several orders of magnitude over the second one.

Therefore, we decided to follow an "iterative gradient search algorithm" to find the two unknowns, namely a(V) and b(V). This iterative gradient search method uses the data in the low Y regime to estimate a(V). This a(V) value is then fed to the data in the higher Y regime to determine b(V). Steps in this successive iterative process use feedback which is described below.

# Method of iteration

#### Zeroth-order approximation

It is known that for samples with low  $Z_{eff}$ , we can neglect the second term in Equation 7 involving Y; therefore, we can write approximately as the "0-th order step"

$$F(V) = a(V;0)X \tag{9.1}$$

which is used to find a(V; 0) by a linear least-square fit of the data. To find b(V), we use data with higher  $Z_{eff}$ (i.e., higher Y) and write as the "0-th order step" F'(V)=F(V) - a(V;0)X = b(V;0)Y (9.2)

where a(V; 0) is already found by the least square fit with Equation 9.1. Therefore, b(V; 0) can be found by making a linear least square fit between F'(V) and Y as illustrated in Equation 9.2. In the above expressions, the parameter "0" is used to indicate that these are the "zeroth" order approximations. These zeroth order calibrations can be assumed to be close to the real ones since a(V;0) is found with samples where scattering dominates and b(V;0) is found from data that are dominated by photoelectric absorption.

# Successive iterations

Successive iterations were employed to a(V) and b(V) to higher levels of accuracy. This is performed as follows. Firstly, we define F''(V; n) and F'(V; n) as: F''(V; n) = F(V) - b(V; n - 1)Y = a(V; n)X (10.1)

$$F'(V; n) = F(V) - b(V; n - 1)Y = a(V; n)X$$
(10.1)  
$$F'(V; n) = F(V) - a(V; n)X = b(V; n)Y$$
(10.2)

where a(V; n) and b(V; n) are the values of a(V) and b(V) obtained from the  $n^{th}$  iterative process. As illustrated in equations 10.1 and 10.2,  $n^{th}$  iteration uses the values of a(V; n-1) and b(V; n-1) that were found from the previous iteration. It is desired that the differences [a(V; n+1)-a(V; n)] and [b(V; n+1)-b(V; n)] become smaller and smaller as 'n' increases. The iteration can be terminated when these differences become insignificant. In the data obtained in the present study, it suffices to continue up to n=5 or 6. The iterative algorithm is summarised in the flow diagram presented in Figure 3. The goodness-of-fit is found using the F-test.



Figure 3. Flow chart for iterative algorithm to determine a(V) and b(V)

#### Application for CT inversion

When the above fits are found to be satisfactory in reproducing the F(80), F(130), they can be used to find the inversion formulae by inverting the two simultaneous equations, F(80) = a(80) X + b(80)Y and F(130) = a(130)X + b(130)Y to obtain:

$$X = a_{11}F(80) + a_{12}F(130) \tag{11.1}$$

$Y = a_{21}F(80) + a_{22}F(130)$	(11.2)
$a_{11} = b(130)/D$ ; $a_{12} = -b(80)/D$ ; $a_{21} = -a(a_{12})/D$ ; $a_$	$(130)/D; a_{22} =$
a(80)/D;	
D=b(130).a(80)-b(80).a(130)	(11.3)

Acceptability of the above inversion is further checked by the application of the F-test.

#### Results

The variations of  $Z_{eff}^x$  with  $\rho_e$  are depicted in Figure 2 demonstrating that there is no simple correlation between the two variables. The HU values for the water portion of the phantom indicated that (i) the accuracy of HU value (within ±3.2), (ii) the noise level in the image (less than 0.6% deviation from the baseline), and (iii) image uniformity (with less than ±2 HU) were within the acceptable limits. It is obvious that since the HU values for water were accurate within ±4, the F(V) values could have errors within ±0.004.

Table 1. Results of the 1<sup>st</sup> to 5<sup>th</sup> order of iteration for the Compton scattering and photoelectric coefficients as calculated based on the data with methanol and Potassium hydroxide. These were found by the least square fits of equations 8.1, 8.2, 9.1, and 9.2 at 80, 110, and 130 kVp. The quantities of X, Y are expressed in units of  $10^{23}$ /cm<sup>3</sup>.

Order	Coefficio scatterin	ent a(V; n) $g \times 10^{-1}$ (in	) of x-ray cm <sup>3</sup> )	Coefficie Photoele cm <sup>3</sup> )	ent b(V; ctric effect	n) of $\times 10^{-6}$ (in
V	80	110	130	80	110	130
$1^{st}$	3.0705	3.0782	3.0814	4.8184	3.2125	2.6224
$2^{nd}$	2.9222	2.9794	3.0007	5.466	3.6440	2.9748
3 <sup>rd</sup>	2.9023	2.9661	2.9898	5.5529	3.7020	3.0224
$4^{\text{th}}$	2.8996	2.9643	2.9884	5.5647	3.7099	3.0285
$5^{\text{th}}$	2.8993	2.9641	2.9882	5.5660	3.7108	3.0294



Figure 4. The least-square fit of F"(V; 5) versus  $X = \rho_e$  of methanol for the 5<sup>th</sup> order iteration. The coefficient of Compton scattering are a (80; 5)=0.28993±0.01108, a(110; 5)=0.29641±0.01934, a(130; 5)= 0.29882± 0.01400, with  $r_{80}^2=0.99$ ,  $r_{110}^2=0.99$ ,  $r_{130}^2=0.99$  at 80, 110, and 130kVp, respectively. It is found that p= P ( $r^{2} \ge r_{obs}^2$ )<<0.01. Therefore, the confidence levels in the fits were found to be above 99.9% for all the above cases. The quantities a(V;5) are expressed in cm<sup>3</sup>.



Figure 5. The least-square fit of F'(V; 5) versus  $Y = [\rho_e Z_{eff}^x]$  of Potassium hydroxide for the 5<sup>th</sup> order iteration, with x=4.0. The coefficients of photoelectric absorption are b(80;5)= 5.5660\pm0.6350]\times10^{-6}, b(110;5)= [3.7108\pm0.5521]\times10^{-6}, b(130;5)= [3.0294\pm0.5260]\times10^{-6}, respectively, with  $r^2_{s0}=0.99$ ,  $r^2_{110}=0.99$ ,  $r^2_{130}=0.99$  at 80, 110, and 130kVp, respectively. It is found that p=  $P(r^2 \ge r^2_{obs}) <<0.01$ . Therefore, the confidence levels in the fits were found to be above 99.9% for all the above cases. The quantities b (V;5) are expressed in cm<sup>3</sup>.

# Coefficients of x-ray scattering and photoelectric absorption

Based on the data, iteration up to n=5 is found to provide sufficient convergence as indicated in Table 1. The least-square fits of x-ray scattering and photoelectric coefficients for the n=5 level of the iteration are displayed in figures 4 and 5.

The coefficients of x-ray scattering (*a*) and photoelectric absorption (*b*) as obtained from the 5<sup>th</sup> order iteration (presented in Table 1) were used to calculate  $F_{cal}(V)$  of methanol, glycerol, and potassium hydroxide solutions. It is worthy to note that while methanol and Potassium hydroxide were the calibration materials, glycerol solutions were test *materials* that were not used for calibration purposes. These fits were further tested with *Fisher's F-test* and yielded p<0.001 in all the cases. The results of the *F*-test are presented below (in Table 2).

Figure 2 displays the values of  $(\rho_e, Z_{eff}^x)$  which were used in the calibration. In Table 3, the HU(V) and F(V)values are displayed that were obtained from the observation with the CT machine and the comparison between the F(V) obtained by Equation 8 and a(V) and b(V) values presented in Table 2.

Table 2. Goodness of fit for F(V) which is fitted against Equation 6 for different values of V (in kVp). Number of data points: n=24, number of variables k=2. We then have degrees of freedom,  $df_1$ =k-1=1,  $df_2$ =n-k=22. The quantities a(V) and b(V) are expressed in units of cm<sup>3</sup>.

kVp	a(V)	b(V)×10-6	F	р
80	0.28993	5.5660	1621	< 0.001
110	0.29541	3.7108	1038	< 0.001
130	0.29882	3.0294	865	< 0.001



Table 3. The observed HU(V) at 80, 110, and 130 kVp, as well as F(80), F(110), and F(130) calculated by Equation 8 and those determined by the coefficients a(V) and b(V) of 5<sup>th</sup> order of iterative.

material	Con.	HU80	HU110	HU130	Fobs 80	Fcal80	Fobs 110	Fcal110	Fobs 30	Fcal130
Methanol	5	-15	-12	-12	0.985	0.989	0.988	0.987	0.988	0.991
Methanol	10	-22	-21	-20	0.978	0.978	0.979	0.976	0.980	0.980
Methanol	15	-30	-28	-27	0.970	0.970	0.972	0.969	0.973	0.973
Methanol	20	-38	-35	-35	0.962	0.960	0.965	0.959	0.965	0.963
Methanol	25	-46	-43	-41	0.954	0.949	0.957	0.949	0.959	0.953
Methanol	30	-55	-52	-50	0.945	0.937	0.948	0.937	0.950	0.941
Methanol	35	-65	-61	-59	0.935	0.929	0.939	0.929	0.941	0.933
Methanol	40	-73	-70	-69	0.927	0.920	0.930	0.920	0.931	0.924
Glycerol	5	6	6	10	1.006	1.046	1.006	1.044	1.010	1.048
Glycerol	10	13	16	18	1.013	1.059	1.016	1.057	1.018	1.061
Glycerol	15	26	28	29	1.026	1.065	1.028	1.063	1.029	1.067
Glycerol	20	39	41	42	1.039	1.070	1.041	1.069	1.042	1.073
Glycerol	25	44	50	51	1.044	1.077	1.050	1.076	1.051	1.081
Glycerol	30	57	61	61	1.057	1.085	1.061	1.084	1.061	1.089
Glycerol	35	69	69	72	1.069	1.086	1.069	1.086	1.072	1.091
Glycerol	40	84	87	92	1.084	1.110	1.087	1.109	1.092	1.114
Potassium hydroxide	5	104	81	71	1.104	1.131	1.081	1.103	1.071	1.098
Potassium hydroxide	10	212	171	152	1.212	1.215	1.171	1.161	1.152	1.147
Potassium hydroxide	15	317	243	217	1.317	1.365	1.243	1.281	1.217	1.256
Potassium hydroxide	20	439	335	298	1.439	1.474	1.335	1.361	1.298	1.325
Potassium hydroxide	25	574	434	386	1.574	1.562	1.434	1.419	1.386	1.373
Potassium hydroxide	30	732	554	492	1.732	1.705	1.554	1.527	1.492	1.469
Potassium hydroxide	35	848	642	568	1.848	1.857	1.642	1.642	1.568	1.570
Potassium hydroxide	40	971	733	647	1.971	1.992	1.733	1.740	1.647	1.655

Table 4. Goodness of fit for X and Y which are fitted against equations 12.1 and 12.2. Number of data points: n=24, number of variables k=2. We then have degrees of freedom,  $df_1=k-1=1$ ,  $df_2=n-k=22$ .

Eq. No.	a <sub>11</sub>	a <sub>12</sub>	a <sub>21</sub>	a <sub>22</sub>	F	р
12.1	-3.8102	7.0433	-	-	550	< 0.001
12.2	-	-	375873	-364656	19460	< 0.001

As displayed in Table 3, the observed and the calculated values of F(V) are within 5% in all of the cases. Therefore, F(80) and F(130) can be used to obtain the inversion as provided by the least square fit:  $X = a_{11}F(80) + a_{12}F(130) = X'$  (12.1)  $Y = a_{21}F(80) + a_{22}F(130) = Y'$  (12.2)

With  $df_1=1$ ,  $df_2=22$ , *F*-test for these inversions yield the corresponding goodness of fit results as depicted in Table 4.

The quantities of X and Y are material properties of the system. These quantities as calculated from F(80) and F(130) data are expected to have a satisfactory correlation with the observed F(110) values. With the substitution of these calculated values (i.e., X, Y) in Equation 7 and using a(110) and b(110) as presented in Table 2, the goodness of fit yields P<0.001 signifying that the fit has above 99.9% confidence. This illustrates the effectiveness of this method in the inversion of F(80) and F(130) data for the determination of the material properties (X, Y) as required by DECT inversion and the use of these calculated quantities for determining other physical quantities of the system(e.g., F(110)). It

was further found that the ratio  $[F(V)calculated/F(V)_{actual}]$  lies within 1.01±0.20 providing accuracy within 3%.



Figure 6. Actual chemical characteristic of methanol, glycerol, and Potassium hydroxide with 5 to 40% weight by weight concentrations, including (a)  $Z_{\rm eff}$  and (b)  $\rho_e$ , as compared to the calculated ones by DECT inversion

Figure 6 displays a scatter diagram of the values of  $(\rho_e, Z_{eff})$  as obtained from equations 12.1 and 12.2 with the actual values. Both graphs are illustrated to be straight lines with unit gradient. This demonstrates that the equations 12.1 and 12.2 can be employed for DECT inversion for the accurate determination of  $(\rho_e, Z_{eff})$  values.

# Discussion

From the fundamentals of the theory, the HU values of a substance must satisfy Equation 8 where a(V) and b(V) are the coefficients for x-ray scattering and the photoelectric effect. Such a fit describes a plane whose slopes are presented by  $a = (\partial F / \partial X)_Y$  and  $b = (\partial F / \partial Y)_X$ [15]. In the present iterative parameter search, "a" is initially found from the region with aX >> bY while b is obtained from the region where aX < bY. This signifies that the determination of only one unknown parameter is found in the region where it is dominated with *minimum* interference from the other. These approximations are fine-tuned by the iterative equations, including equations 9.1, 9.2, 10.1, and 10.2, which combine F(V)' s dependences on both X and Y. This yields a good fit as indicated by the F-test pointing to the accuracy of the method.

This accuracy in a(V) and b(V) determination was also checked by fitting  $[F(V) / \rho_e] = a(V) + [b(V) \times Z_{eff}^x];$ therefore, the values of a(V) and b(V) were obtained by Sklearn package in Python. The values of a(V) and b(V)obtained from the iterative method differ from those found by the abovementioned package by only 2%. In summary, the present result can be discarded with a high risk of abandoning an acceptable model (note the Fvalues and the p values in tables 2 and 5) when the acceptability is presented by the "standard packages". In order to arrive at these satisfactory results, it is important that the calibration samples be properly selected so that the two terms in Equation 5 do not subsume each other. This implies that the data must contain sufficient points in the regions where the first term dominates and also in the points where the second term in Equation 5 dominates. If this is not the case, unphysical results can occur as observed in our trials. Consequently, in our iterative method, gradient searches were performed independently by estimating the gradients in regions where one of them dominates over the other.

The coefficients a(V) and b(V) can be employed in various situations. They can be readily used to calculate the F(V) values and the linear attenuation coefficients if the ( $\rho_e$ ,  $Z_{eff}$ ) values of the scanned materials are known. On the contrary, equations 12.1 and 12.2 can be used to determine the ( $\rho_e$ ,  $Z_{eff}$ ) values of any substance from the experimentally determined HU(80) and HU(130). This is the step that is utilized for DECT inversion in different studies. These estimates are also of paramount importance for radiation dosimetry and treatment planning. As is widely known, different organs have different chemical compositions. The radiation dose distributions in these organs can be calculated from a(V) and b(V) values of the CT machine and using the known chemical compositions ( $\rho_{e}$ ,  $Z_{eff}$ ) of the organs in the body. In the photoelectric effect, the absorbed photon can cause "damages", no matter how small, by "disturbing" the charge distributions in the atoms. The x-ray scattering part determines the redistribution of the x-ray photon flux and the risk of its penetration into different organs. These issues are important in both dosimetry and treatment planning and in calculating attenuation maps that can be used for attenuation corrections in Positron Emission Computed Tomography or PET data [16].

## Conclusion

As evidenced by the obtained result, the iterative gradient search algorithm which was employed in the present research is reliable and converges in a few steps (e.g., five steps in the present case). The accurate prediction of coefficients of x-ray scattering and photoelectric effects and calibration of CT machines is feasible by the utilization of this process on the data obtained from phantom-based observations. It naturally follows that these results can be used to calculate organ dose for human organs with known chemical characteristics. In addition, calibration-inversion of DECT systems may be possible by knowing the coefficients of x-ray scattering and the photoelectric effect. DECT inversion may use these inversion coefficients as a useful tool for tissue characterization.

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