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Methodology for attainment of density and effective atomic number through dual energy technique using microtomographic images

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HIGHLIGHTS

- Dual energy technique is promising for identification of distribution of minerals.
- A feasible methodology of dual energy in analysis of tomographic images was sought.
- The dual energy technique is efficient for density and atomic number identification.
- Simulation showed that the proposed methodology agrees with theoretical data.
- Nondestructive characterization of distribution of density and chemical composition.

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ABSTRACT

Dual energy technique for computerized microtomography shows itself as a promising method for identification of mineralogy on geological samples of heterogeneous composition. It can also assist with differentiating very similar objects regarding the attenuation coefficient, which are usually not separable during image processing and analysis of microtomographic data. Therefore, the development of a feasible and applicable methodology of dual energy in the analysis of microtomographic images was sought.

1. Introduction

The combination of chemical composition and density from a sample yields the attenuation coefficient. This condition is a challenge in understanding the distribution of heterogeneous composition, throughout geological samples, in microtomographic images, because it does not establish, per se, if observed variations of color in grayscale images are due to differences in density, chemical composition, or some combination of the two. Still, if contributions of density and chemical composition can be resolved, a powerful tool for nondestructive characterization of the internal distribution of density and chemical composition of any sample will be achieved.

One problem is that the density and chemical composition are not attainable for any microtomographic system through conventional methods since there is not, a priori, a sole combination of those parameters for specific energies or energy spectra, i.e., a range of energies. This problem, however, can be solved using data obtained from two distinct X-ray spectra, i.e., two different ranges of energies, hence the use of the dual energy computed microtomography technique (μCT-DE) (Tsuchiyama et al., 2013).

The application of μCT-DE technique is usually based in the ascertainment of the relative contributions of photoelectric absorption and Compton scattering in the total attenuation coefficient (Eq. 1) (Remeysen and Swennen, 2008):

$$\mu_{m(E)} = \mu_{l(E)}/\rho = \alpha_{(E)} + \beta_{(E)} Z_{ef}^{3.8} \quad (1)$$

where μ_m is the mass attenuation coefficient and μ_l is the linear attenuation coefficient.

The α and β constants are energy dependent, i.e., they change according to the interaction of the X-rays when passing through the sample. Since it is a polychromatic source, the resulting mean

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energy will change according to the sample and, likewise, the α and β variables. Therefore this relationship is better represented by a monochromatic X-ray, although it can be extended to polychromatic X-rays by means, e.g., of mean energy, or effective energy.

μCT-DE technique allows the obtainment of two or more linear equations, for each chosen energy, so that through, e.g., the mathematical method of linear regression, the linear and angular constants α and β, respectively, of a linear equation of the form $y=\beta x+\alpha$ can be attained.

All of this data enables a calibration of a microtomographic system, i.e., to find meaningful and standard information regarding the objective of the technique, which is density and effective atomic number. Any sample tomographed under the same conditions of acquisition, except the two chosen energies of the X-ray source, can be studied for further knowledge of its density and effective atomic number (Van Geet et al., 2000) by the following equations:

$$\rho = \frac{\beta_h \mu_l - \beta_l \mu_h}{\beta_h \alpha_l - \beta_l \alpha_h} \tag{2}$$

$$Z_{ef} = \sqrt[3.8]{\frac{\alpha_l \mu_h - \alpha_h \mu_l}{\beta_h \mu_l - \beta_l \mu_h}} \tag{3}$$

where ρ is the density of the analyzed material or sample; β_l and β_h are angular constants for low and high chosen energies, respectively; α_l and α_h are linear constants for low and high chosen energies, respectively; μ_l and μ_h are the linear attenuation coefficients for low and high chosen energies, respectively.

Z_{ef} is the effective atomic number of the analyzed material or sample, defined by:

$$Z_{ef} = \left(\sum_i^N f_i Z_i^{3.8} \right)^{1/3.8} \tag{4}$$

where f_i is the molecular percentage of the element found in the sample.

The objective of this work was to develop and implement a methodology to calibrate a μCT system into a μCT-DE system. Its applications allow distinguishing small variations in chemical composition and density, which cannot be observed in a conventional grayscale tomographic image. It can also be used to obtain the effective atomic number and density of any sample of unknown composition and, eventually, separate images by mineral composition.

2. Methodology

The methodology was divided in three main steps: the validation of the proposed methodology of μCT-DE technique through a simulation using tabulated theoretical values of density, atomic number and attenuation coefficients for chemical elements of the periodic table (Cesareo, 2000; Chantler et al., 1995); the evaluation of the X-ray tube spectrum regarding its effective energy by interaction on a certified aluminum sphere; and the application of the methodology for calibration of the system using geological samples and minerals of known effective atomic number and density.

The microtomographic system used in this work to study the dual energy technique was the microtomograph, 1173 model, from Skyscan-Bruker®. This system consists of: an X-ray tube of tungsten (W) anode with maximum capacity of operation on 130 kV tension and 8 W power; a flat-panel detector of 2240 × 2240 pixels in its matrix; minimum focal spot size of 5 μm; maximum resolution of 10 μm; and a micropositioning stage, in XYZ direction, for samples.

Table 1
Acquisition parameters.

Parameters	Values
Tension (kV)	80/130
Current (μA)	100/61
Matrix (pixels)	2240 × 2240
Pixel size (μm)	10
Angular step (deg)	0.5
Number of frames	5
Filter (mm)	0.15 / 0.50 Cu

Table 1 shows acquisition parameters used in the study and implementation of the methodology of μCT-DE.

The energy of the system is related to the capacity of the X-ray to pass through a sample. Higher energies are able to go through denser objects, as lower energies are able to go through less dense objects. It is of much importance to choose an adequate energy for each studied sample, since it will affect the contrast and quality of the final image. The current is proportional to the number of photons, or X-rays, which exit the X-ray source towards the sample and the detector. A higher current helps in statistical data of the incident radiation, but it can also increase noise on the final image due to scattering. The detector matrix is connected to the image quality and resolution. A higher matrix allows for more detailed information, i.e., higher resolution on the final image of the sample. The pixel size is directly connected to the spatial resolution of the system. It represents the ability to solve and differentiate all objects on an image, i.e., the smallest structure, if it is an object, or the smallest separation between objects, if it is a void, that can be recognized in the image. The angular step is the angle between each acquired projection. The number of frames refers to the number of images taken to compose the final projection image, as to raise the signal to noise ratio and, hence, improve the final image quality. The physical and metallic filters are used to absorb and attenuate the lower energy photons, increasing the effective energy of the X-ray spectrum, and reducing the intensity of undesirable effects in the final image such as beam-hardening (Jovanović et al., 2013).

2.1. Simulation

The proof and validation of the μCT-DE technique was made using tabulated attenuation coefficients for pure, chemical elements of known effective atomic number and density from the periodic table, for two chosen energies (Cesareo, 2000). α and β, from Eq. (1), were obtained through linear regression of the mass attenuation coefficient and atomic number of the pure elements. The choice of which energies to use to verify the methodology through simulation is irrelevant, since the methodology is expected to work with any two different energies, provided that the energies and all acquisition parameters remain constant, aside from the minimum and maximum values of attenuation coefficients during reconstruction procedure. Therefore, this step was made with 100 and 150 kV energies.

Table 2 shows all pure chemical elements used for the simulation of dual energy technique, as well as its calibration parameters, such as density, atomic number and attenuation coefficient. The elements used in this calibration are the ones that are most commonly found on minerals and geological samples.

The use of random elements from the periodic table allows evaluation of the simulated calibration, to ensure the methodology works with any choice of pure elements. In this case, the elements used to validate the proposed simulation were vanadium (V), potassium (K) and sodium (Na). It is important to warn that it was noticed that the dual energy technique does not give reliable