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Effective atomic number and density determination of rocks by X-ray microtomography

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ABSTRACT

Microtomography, as a non-destructive technique, has become an important tool in studies of internal properties of materials. Recently, interest using this methodology in characterizing the samples with respect to their compositions, especially rocks, has grown. Two physical properties, density and effective atomic number, are important in determining the composition of rocks. In this work, six samples of materials with densities that varied from 2.42 to 6.84 g/cm^3 and effective atomic numbers from 15.0 to 77.3 were studied. The measurements were made using a SkyScan-Bruker 1172 microtomography apparatus operating in voltages at 50, 60, 70, 80, 90 and 100 kV with a resolution of 13.1 μm. Through micro-CT images, an average gray scale was calculated for the samples and correlation studies of this value with the density and the effective atomic number of samples were made. Linear fits were obtained for each energy value. The obtained functions were tested with samples of Amazonite, Gabbro, Sandstone and Sodalite.

1. Introduction

X-ray tomography was developed in the 1970s for medical applications (Landis and Keane, 2010). A few years later, this methodology was being applied in studies of rocks (Atanasio et al., 2010; Baker et al., 2012), reservoir rocks (Appoloni et al., 2007; Marques et al., 2011; Fernandes et al., 2012), materials structures (Moreira et al., 2010; Nagata et al., 2011) and biological samples (Mizutani and Suzuki, 2012). In the area of applications in studies of rocks, microtomography is a methodology able to get 2D images of the internal structures of the rocks, pore size and the distribution of pore size (Oliveira et al., 2012). Also 3D images of samples can be rendered to study the connectivity between the pores and analyze the spatial distribution of the different phases of a rock, if this occurs. In recent years, interest has increased in the characterization of rocks by their chemical composition (Remeysen and Swennen, 2008; Koroteev et al., 2011). There are many studies that seek to characterize rocks by their density and effective atomic number using the technique of dual energy (Yasdi and Esmaeilnia, 2003; Duliu et al., 2009; Miller et al., 2013; Tsuchiyama et al., 2013). This technique consists of making two scans at two different voltages and the results are analyzed simultaneously. This is not the methodology employed in this work. Another possible technique such as X-ray Fluorescence Computed Tomography (XFCT) is more complex and very expensive compared with the methodology proposed in this paper. We have been working since 2010 determining the chemical composition of samples making only one scan (Jussiani, 2012; Jussiani and Appoloni, 2013).

Microtomography is based on attenuation of X-rays which pass through a sample. This attenuation is detected by a CCD camera (detector) and from projections at different angles and through mathematical models (Feldkamp et al., 1984) it is possible to determine the attenuation of the radiation in the smallest area of the sample element (pixel) or in 3D images, the smallest sample volume (voxel). The attenuation coefficients are shown in images with 256 gray scale, which are distributed among the elements of pixel/voxel with the highest and lowest radiation attenuation.

2. Theory

When a polychromatic radiation goes through an inhomogeneous material, the relationship between the incident and the transmitted radiation is given by the equation:

$$I = \int_0^{E_{max}} I_0(E) \exp\left[-\int_0^x \mu'(E,x)\,dx\right] dE \quad (1)$$

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where I is the intensity of transmitted X-rays, I_0 is the intensity of the incident X-rays that depends on the energy and μ' is the linear attenuation coefficient that depend on the position x and the energy E.

Two important factors determine the intensity of the radiation attenuation: density (ρ) and effective atomic number (Z_{eff}). These physical properties are fundamental in studies of the interaction of radiation with matter, as in the photoelectric and Compton effects (Mees et al., 2003). The photoelectric effect occurs when the incident radiation is completely absorbed by an electron from the atom, which is ejected. This occurs mainly with electrons from K-shell. In this layer, the cross section of the photoelectric effect depends on Z^5. The Compton effect is the inelastic scattering of radiation with matter. The cross-section in this case has a linear dependence on Z. Thus, the total probability of interaction of X-rays with matter is

$$\sigma = \phi_{photo} + Z\sigma_c \quad (2)$$

where σ is the total probability of interaction, ϕ_{photo} is the cross section of the photoelectric effect, σ_c is the cross section of the Compton scattering and Z is the atomic number (in mixtures should be used Z_{eff}). Multiplying the equation by the density of atoms, N, we get the probability of interaction per unit length:

$$\mu = N\sigma = \sigma\left(\frac{N_a \rho}{A}\right) \quad (3)$$

with N_a Avogadro's number, ρ is density of the material and A is molecular weight.

The density of a material can be determined experimentally by making the ratio of its mass by the volume of liquid displaced when the sample is placed in water.

The calculation of the effective atomic number of a material is given by the equation (Murty, 1965):

$$Z_{eff} = \sqrt[2{,}94]{f_1 \times (Z_1)^{2{,}94} + f_2 \times (Z_2)^{2{,}94} + f_3 \times (Z_3)^{2{,}94} + \cdots} \quad (4)$$

where Z_{eff} is the effective atomic number of the sample, f_n is the fraction of the total number of electrons associated with each element of atomic number Z_n.

3. Materials and methods

3.1. Materials

Rock samples were measured with a microtomography model SkyScan-Bruker 1172. Samples were placed one over the other to be measured together (Fig. 1). The microtomography has an X-ray tube with a tungsten anode. The operating voltage of the equipment may vary from 20 to 100 kV, current 0–250 μA, both values associated to provide a maximum power of 10 W. The detection is done by a CCD camera with a maximum resolution of 11 MP. The spatial resolution is determined by some parameters such as pixel size, the distance from the source to the sample and the distance from the sample to the CCD camera. Six Samples were studied to verify the possibility to be used as standard samples (Table 1). They had a mean diameter of 6 mm and mean height of 5 mm. Table 2 shows the acquisition parameters used in this work. SkyScan and NRecon software were used for acquisition and processing of data (SKYSCAN, 2005). To calculate the average gray scale of the samples Imago and Excel softwares were used (Fernandes et al., 1998).

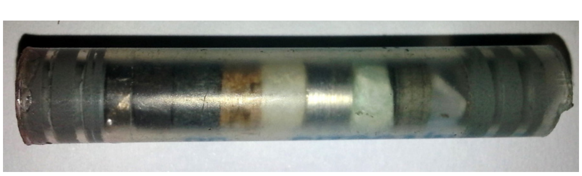

Fig. 1. Sample holder.

Table 1
Densities and effective atomic numbers of the samples studied.

Samples	Gravimetric density (g/cm^3)	Theoretical Z_{eff}
Slate	2.46 ± 0.26	10.9
Aluminum	2.52 ± 0.27	13.0
White marble	2.85 ± 0.32	13.1
Fluorite	2.88 ± 0.25	16.6
Hematite	4.95 ± 0.77	22.9
Galena	6.84 ± 0.55	77.3

Table 2
Acquisition parameters and physical characteristics of the samples.

Voltage (kV)	100/90/80/70/60/50
Current (μA)	100/112/124/141/167/201
Resolution (μm)	13.1
Filter	Al
Exposure time (ms)	2000
Angular step (°)	0.4
Frames	3
Grid size (pixels)	2000 × 1336

3.2. Methods

Measurements were performed from 50 to 100 kV (always at maximum power) with a resolution of 13.1 μm.

It was not possible to determine a linear relationship between the average gray scale of the samples with their effective atomic number and density parameters when individual reconstructions were used (Fig. 2). The reconstruction parameters are computational tools that aid in the reduction of artifacts of the micro-CT images. The two main artifacts in the images are beam hardening and ring artifacts. Beam hardening occurs due to the absorption of low energy X-rays at the edge of the sample. Thus, the software interprets this region as an area of high attenuation, leaving it whiter than the center of the sample (see Fig. 3). Ring artifacts appear due to a problem in the detection of a one pixel in CCD camera. As the sample is rotated, concentric rings appear in the images.

A relationship between densities and effective atomic numbers with the average gray scale can only be obtained when a single set of parameters reconstruction for all samples is used. The

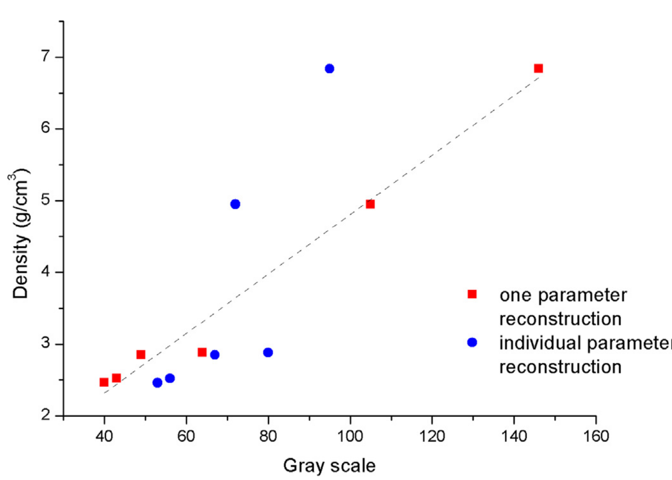

Fig. 2. Graph showing that a linear relationship exists between the density and the average shade of gray of the samples only when the reconstruction parameters are equal for the samples (dashed line).