



How Does the Soil Chemical Composition Affect the Mass Attenuation Coefficient? A Study Using Computer Simulation to Understand the Radiation-Soil Interaction Processes

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Abstract

In the last few decades, a lot of research has focused on the radiation interaction with complex materials such as soil. The mass attenuation coefficient (μ) is important to analyze the different physical properties of porous media. For this reason, it is important to understand how μ varies as a function of the chemical composition of porous materials. This study analyzes the influence of the chemical composition on μ , from 1 to 1500keV, using the XCOM computer simulation code. Five types of soil, containing variable proportions of SiO_2 , Al_2O_3 , Fe_2O_3 , and TiO_2 , were evaluated. The results showed that the influence of each of the partial effects (photoelectric, coherent, and incoherent scattering), in μ values, occurred from their dependence on the atomic number (Z), with greater Z influence in low energies. A detailed analysis of the influence of the chemical composition considering the oxides individually is also presented. In addition, this paper brings a comprehensive description of the methodology employed for the measurements of the radiation interaction main effects and it can also be used to teach physics applied courses in areas such as modern physics, dosimetry, and radiation protection, among others.

Keywords XCOM · Radiation interaction · Photoelectric effect · Coherent and incoherent scattering · Oxides

1 Introduction

Porous media such as soils are natural and complex materials characterized by different chemical compositions in terms of minerals and oxides. Some of the major oxides found in the soils are SiO_2 , Al_2O_3 , Fe_2O_3 , and TiO_2 , among others in lower concentrations [1, 2]. The analysis of physical parameters related to the chemical composition is important due to its influence in the soil texture and, consequently, in the soil structure. Differences in the soil oxide content might affect the way the radiation interacts with this porous system [3]. For example, soils with oxide percentages containing

chemical elements of higher atomic number (e.g., Fe_2O_3 and TiO_2) tend to attenuate the radiation more intensely in relation to the soils that are mainly composed of oxides that include chemical elements of lower atomic number (e.g., SiO_2 and Al_2O_3).

The study of the radiation interaction with matter is interesting in different areas of knowledge [4]. The characterization of compound materials such as medication, polymers, ceramic, metallic alloys, soils and rocks, and chemical solutions regarding radiation interaction is of great interest in the area of radiation physics [5–7]. For the soil and rock cases, the knowledge of the way with which the radiation interacts has great environmental importance. Composite materials such as soils can be employed for radiation shielding purposes, and the knowledge of radiation properties is of prime relevance.

The most important physical parameters to evaluate radiation absorption and scattering are the linear attenuation coefficient (k) and the mass attenuation coefficient (μ) [1]. The k represents the probability of a photon being attenuated by the unit of length, which depends on the photon energy, chemical composition, and density of the attenuating material [8]. The mass attenuation coefficient is for example

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widely utilized in the photon penetration and energy deposition calculations in biological shielding materials [5].

In the area of environmental physics applied to the study of porous media such as soil, it is necessary to understand how photons interact with this medium and what is the dependence of this interaction on the chemical composition. This understanding is important because several physical properties of the soil might be obtained from the measurements of the attenuation coefficient, such as solute retention, bulk density, hydraulic conductivity, and porosity, among others [8–10].

Processes based on the analysis of X-ray or gamma-ray computed tomography are also directly related to the way the radiation interacts with the medium, since tomographic units are generated from the attenuation coefficients of the object being analyzed [11, 12]. For this reason, it is important to obtain representative determinations of μ and understand the factors that affect the radiation interaction with the matter such as the photoelectric effect, coherent and incoherent scattering and the pair production effect [13].

There are many studies in the scientific literature about the effect of the material chemical composition on μ values as those of Medhat et al. [1], Manohara et al. [4], Ferreira et al. [9], Mudahar et al. [14], Cesareo et al. [15], Alam et al. [16], Han and Demir [17], Trunova et al. [18], Medhat and Pires [19], Taqi and Khalil [20], Kucuk et al. [21], and Prandel et al. [22], to cite some of them. Most of these investigations employed experimental measurements or calculations of μ using computer codes such as XCOM or Monte Carlo simulation methods. However, what is observed is

that many studies do not explore in detail how different soil oxides influence partial and total μ values. Previous studies on evaluating the soil elemental composition effect in partial and total μ are still scarce. Thus, this paper presents for the first time a detailed analysis of the influence of the major soil oxides in the mass attenuation coefficient.

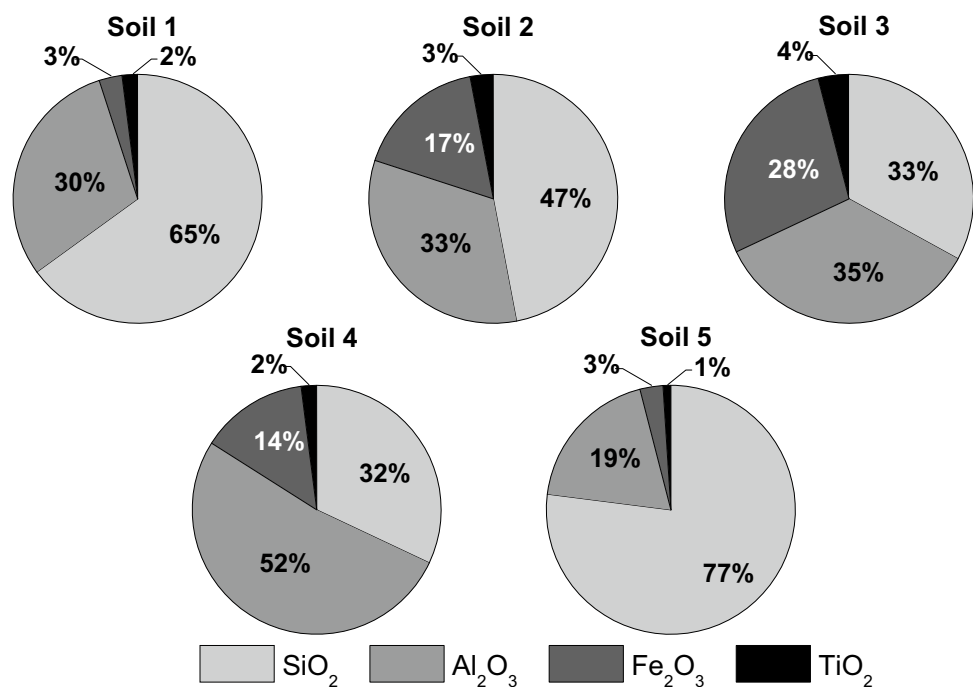
The main aim of this study is to analyze the influence of the chemical composition, mainly the four oxides that are most commonly found in tropical soils (SiO_2 , Al_2O_3 , Fe_2O_3 and TiO_2), to determine μ in the energy band from 1 to 1500keV. To calculate μ , the XCOM computer code was employed [23].

2 Materials and Methods

To evaluate the influence of the chemical composition in μ values, five different types of soils were selected, regarding their oxide content (Fig. 1). The chemical composition of the four first soils (Soils 1 to 4) were obtained based on the study by Medhat et al. [1], while the fifth (Soil 5) was based on the study put forward by Pires et al. [7].

Since this study aims to analyze the influence of the chemical composition in the attenuation properties of the soils, full oxide composition values were obtained for the four major oxides usually found in tropical soils (SiO_2 , Al_2O_3 , Fe_2O_3 , and TiO_2) through rounding. In the cases where the sum of the four oxides did not result in 100%, the residual value was added for SiO_2 .

Fig. 1 Composition of the soils under study as a function of the four major oxides most commonly found in tropical soils (Soils 1–5)



The μ values were determined by using the XCOM computer code (Version 1.5), which gathers information from a data base of attenuation coefficients [23]. This program enables μ determination for pure and compound elements or mixtures with atomic number (Z) varying from 1 to 100 in the energy band from 1 to 100GeV. The μ (cm^2g^{-1}) value of a compound or mixture is given by [24]

$$\mu = \sum_i W_i \mu_i \tag{1}$$

where μ_i is the mass attenuation coefficient of the i th term. For compounds and mixtures, the weight fraction W_i do i th term is written as

$$W_i = \frac{n_i A_i}{\sum_j n_j A_j} \tag{2}$$

where A_i is the atomic weight of the i -th element and n_i is the number of formula units.

When photons interact with a certain material, different interaction partial events occur, which contribute to the μ total value:

$$\mu = \mu_C + \mu_{PE} + \mu_{IC} + \mu_{PP} \tag{3}$$

where μ_C , μ_{PE} , μ_{IC} , and μ_{PP} represent, respectively, the partial attenuation coefficients referring to the following effects: coherent scattering (Rayleigh), photoelectric effect, incoherent scattering (Compton effect), and pair production. The partial interaction effects are directly related to their atomic cross-sections ($\text{cm}^2\text{atom}^{-1}$) [25, 26]:

$$\mu_{(IC,PE,PP)} = \frac{N_A}{A} \sigma_{(IC,PE,PP)} \tag{4}$$

$$\mu_C \sim \frac{Z}{(h\nu)^2} \tag{5}$$

where N_A is the Avogadro’s number, A is atomic mass, Z is the atomic number, and $h\nu$ is the photon energy. The terms σ_{IC} , σ_{PE} , and σ_{PP} are the cross-sections for the different interaction effects. The values of each cross-section are dependent on the values of Z and the incident photon energy (Table 1).

Unlike what occurs in attenuation experimental measurements using X-ray or gamma-ray, the theoretical analysis of μ using the XCOM enables the evaluation of the different processes of the radiation interaction with matter [23]. The probability of occurrence of each one of the radiation attenuation partial effects as a function of the energy and atomic numbers of the substances is presented in Fig. 2.

Dotted and continuous lines in Fig. 2a indicate the energy bands and Z values where each of the effects is predominant. The hatched region represents the region analyzed in this

Table 1 Dependence of the process of radiation interaction with matter on the atomic number (Z) and photon energy (E) (adapted from Appoloni et al. [27])

Process	Z dependence	Dominant energy region
Coherent scattering	Z^{2-3}	$< 30\text{keV}$
Photoelectric effect	Z^{4-5}	$< 30\text{keV}$
Incoherent scattering	Linear	$150\text{keV} < E < 3\text{MeV}$
Pair production:		
Nuclear field	Z^2	$> 50\text{MeV}$
Electron field	Linear	

study, which is between the elements iron (Fe) and oxygen (O), in the energy band between 1 and 1500keV. Figure 2 b shows the percentage, in relation to the total attenuation, with which each interaction process contributes to the total μ value as a function of the incident photon energy. The μ dependence on the incident photon energy, as well as the individual contributions of each interaction process of the radiation with matter are presented in Fig. 2c. Table 2 shows the weight fraction of the chemical elements found in the soils under analysis. This result was also obtained using the XCOM.

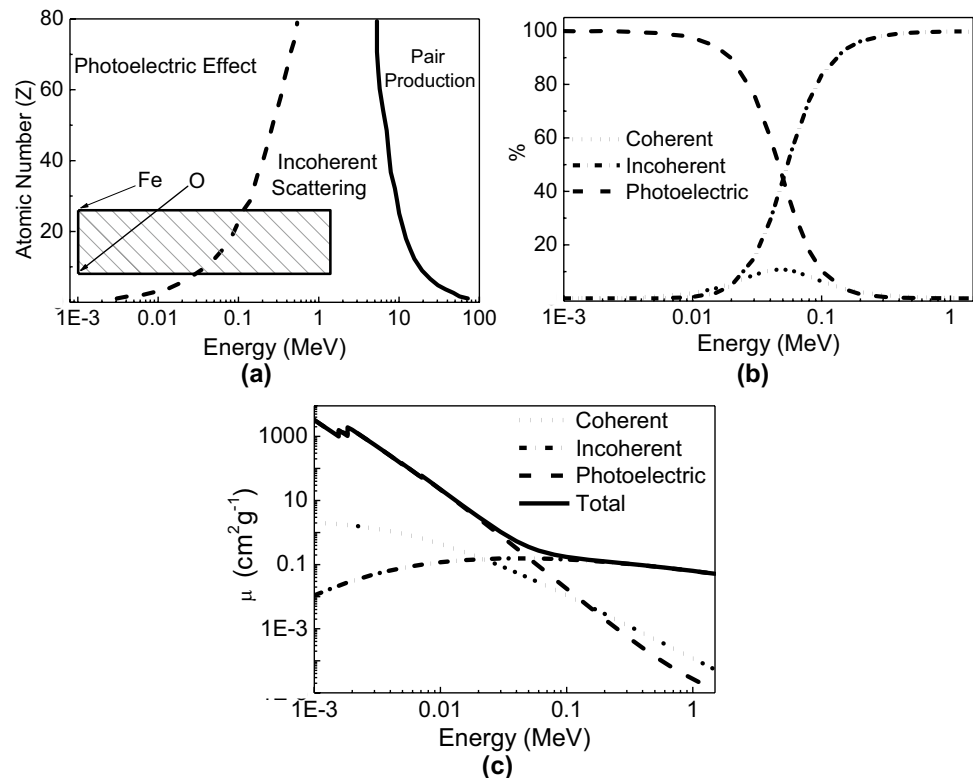
In this study, four photon additional energies were selected referring to the radiation sources of ^{241}Am (59.54keV), ^{133}Ba (356keV), ^{137}Cs (661 keV), and ^{60}Co (1.33 MeV). It seems relevant to emphasize that the energy band selected is due to the usual values of energies found in the X-ray tomography equipment and the most used radiation sources in experimental studies involving porous media such as soil (we also highlight that no experimental measures were carried out with these radiation sources or any tomographic equipment in the present study) [28, 29].

3 Results and Discussion

Figure 3 shows partial and total μ values as a function of energy, while Figs. 4 to 7 present the correlations between partial and total μ of the soils as a function of the partial and total μ of each one of the oxides found in the soils under investigation. The μ values of the oxides were also calculated using the XCOM, by selecting the compound materials and the same energy band and additional energies.

When analyzing the way the partial effects affect the total mass attenuation coefficient, the photoelectric effect is expected to predominate in the μ value in low energies, while with the increase in the photon energy, the incoherent scattering and the pair production effects start to influence μ values more significantly [25, 26]. Figure 3, as expected, shows greater influence of the photoelectric effect followed by the coherent and incoherent scattering, respectively, as a function

Fig. 2 **a** Predominance of the different effects of the radiation interaction with matter as a function of atomic number (Z) and photon energy (E). **b** Contribution of each partial effect to the total value of the mass attenuation coefficient (μ) as a function of the photon energy. **c** Variation of μ as a function of energy regarding partial effects and total μ . The results of **b**, **c** refer to soil 1



of the gradual increase in energy. Regarding the photoelectric effect and the coherent scattering, the greater influence of these effects is mainly noticed in the regions of lower energies ($E < 10\text{keV}$) of the soils investigated. The influence of the incoherent scattering becomes more relevant in the intermediary energy regions ($E > 100\text{keV}$) regarding total μ (Table 1).

It seems relevant to highlight that the results for the pair production effect are not presented in this study due to the energy band and additional energies selected. Very high energies are not usually used in porous systems studies, especially in measurements carried out in laboratory, and for this reason, the influence of the pair production effect in total μ might be neglected.

The dominance of each one of the effects might be explained from the Z dependence on the partial cross-sections, a sequence is observed that progresses from Z^{4-5} to a linear

dependence on Z , for the different effects (Table 1). Based on the results presented, no significant differences were observed in the behavior of total and partial curves (different effects) between the soils under study (Fig. 3).

With the increase in the photon energy, μ values decrease up to the intermediary energy values, such as the ones analyzed in this study [21]. Figure 4 shows the graphs of correlation between the μ of the soils and the μ of the oxides found, regarding coherent scattering. In lower energies (higher μ values), the coherent scattering is more sensitive to the soil chemical composition. This is evidenced by the greater separation of values for the different soils. Regarding high energies (lower μ values) the coherent scattering as well as the chemical composition become less important. It seems relevant to mention that high energies, in this case, represent intermediary energies when working with a photon energy band that includes the pair production effect.

The greater separation of μ values is due to the amount (weight fraction) of chemical elements with higher Z values present in the soils investigated (in this case Fe and Ti that show, respectively, $Z = 26$ and $Z = 22$) (Table 2). In this study, the following (decreasing) order was observed: Soils 3, 2, 4, 1, and 5 (overlap of the 1 and 5). These soils presented the following amounts of Fe + Ti: 22% (3), 14% (2), 11% (4), 3% (1), and 3% (5). Therefore, the straight line 1:1 for Fe_2O_3 and TiO_2 is closer to the Soil 3 straight line, while the straight line 1:1 for Al_2O_3 and SiO_2 is closer to Soils 1 and 5, regarding coherent scattering.

Table 2 Weight fraction of the chemical elements constituting the four main oxides found in the soils under study

Atomic number (Z)	Fraction by weight				
	Soil 1	Soil 2	Soil 3	Soil 4	Soil 5
$O(Z = 8)$	0.51	0.47	0.44	0.46	0.51
$Al(Z = 13)$	0.16	0.17	0.19	0.28	0.10
$Si(Z = 14)$	0.30	0.22	0.15	0.15	0.36
$Ti(Z = 22)$	0.01	0.02	0.02	0.01	0.01
$Fe(Z = 26)$	0.02	0.12	0.20	0.10	0.02

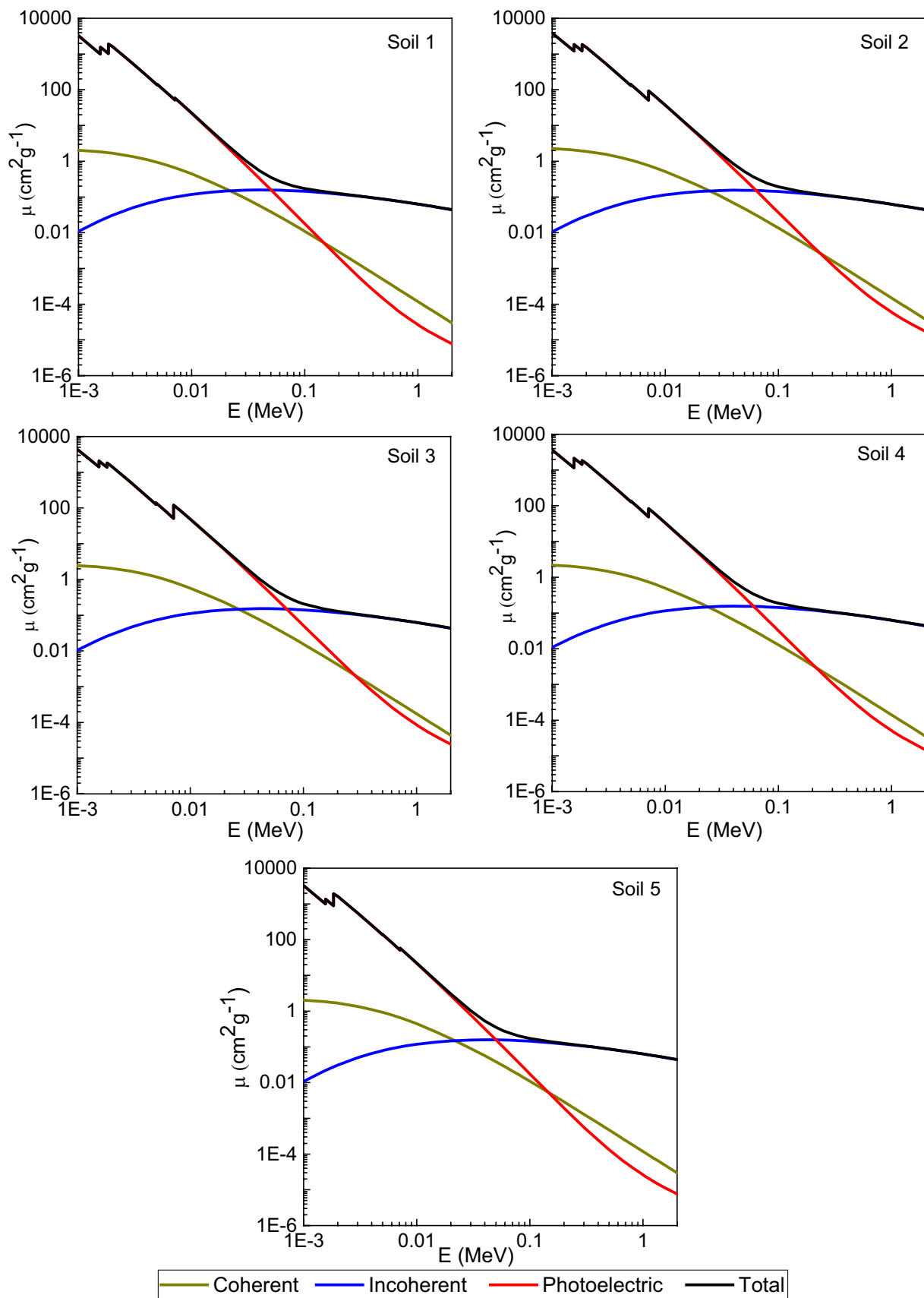
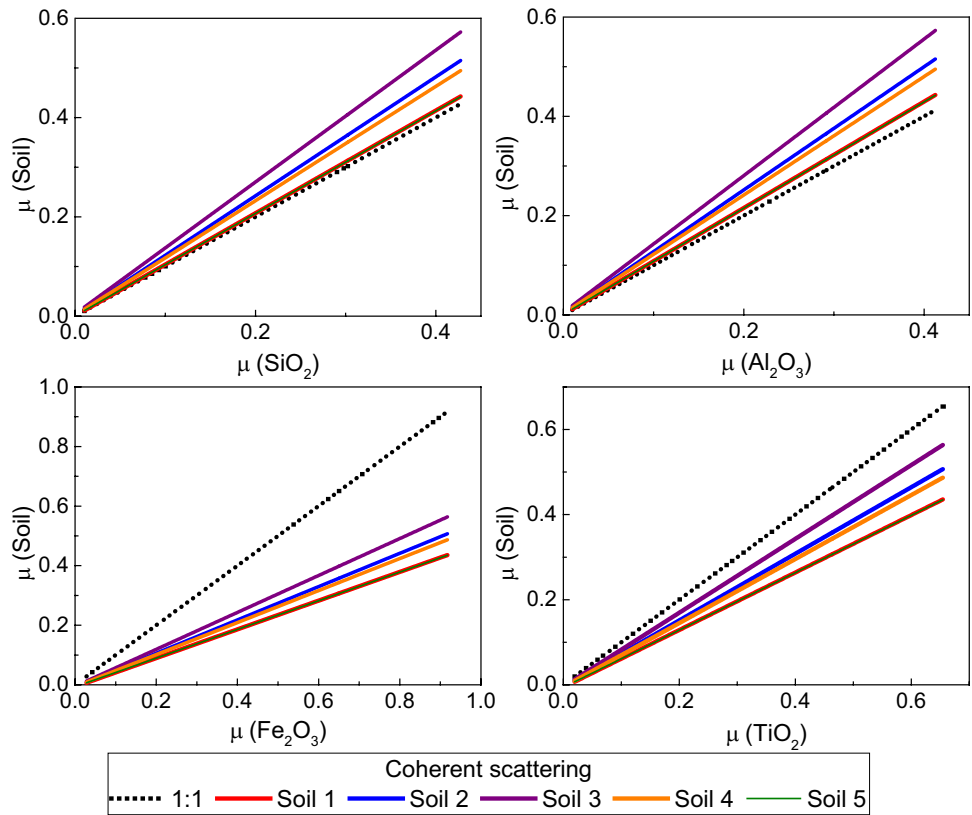


Fig. 3 Mass attenuation coefficient for the coherent and incoherent scattering effects and photoelectric effect of the 5 soils under study

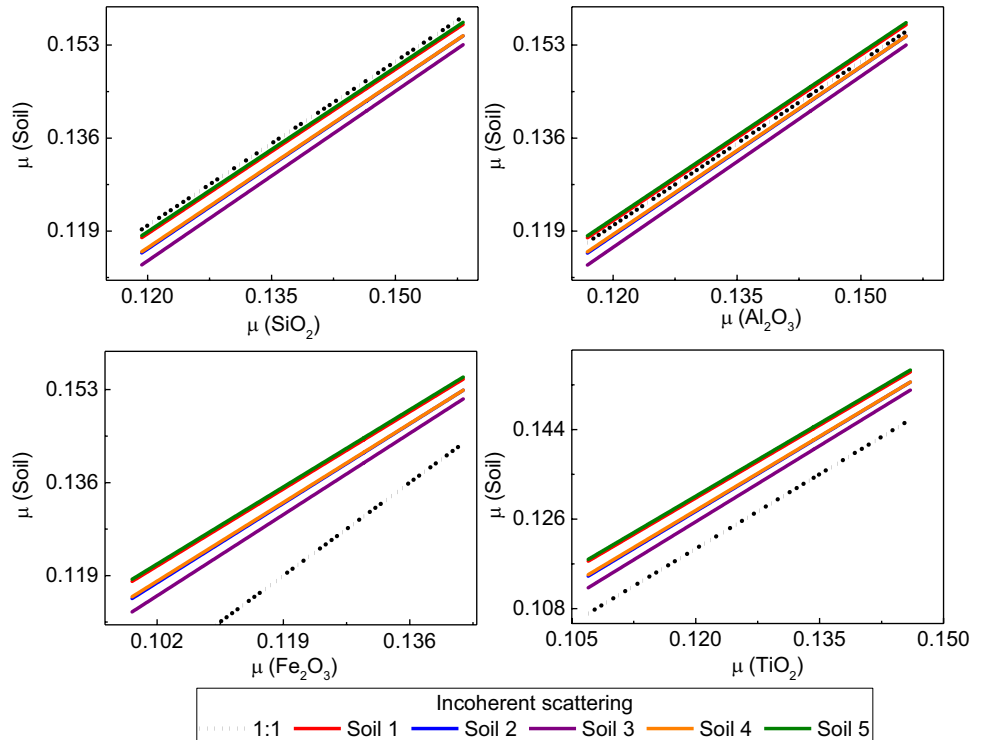
Fig. 4 Correlation between the mass attenuation coefficients for the coherent scattering effect of the 5 soils as a function of the 4 major oxides. Soils 1 and 5 show an overlap of the adjustment straight lines in the four correlations presented



The correlation between μ values for the soils and oxides found regarding the incoherent scattering is presented in Fig. 5. As for the incoherent scattering, a linear dependence

on Z is noticed, since the μ values, in the energy region where this effect predominates are approximately constant [1]. In the incoherent scattering, the following (decreasing)

Fig. 5 Correlation between the mass attenuation coefficients for the incoherent scattering effect of the 5 soils as a function of the 4 major oxides found. Soils 1 and 5 show overlapped adjustment straight lines in the four correlations presented



sequence was observed: Soils 5, 1, 4, 2, and 3. The amount of Si + Al explains the differences observed between the soils, with the following percentages: 46% (5), 46% (1), 43% (4), 39% (2), and 34% (3) (Table 2).

The results obtained from the soils with higher Si + Al contents (Soils 1 and 5) were closer to the straight line 1:1, when correlated to the μ values for SiO₂ and Al₂O₃. However, soils with lower amounts of these chemical elements and higher Fe and Ti content presented underestimated attenuation values in relation to the SiO₂ and Al₂O₃ oxide attenuation. Therefore, the lower the amounts of Si and Al in the soils are, the farther from the straight line 1:1 the adjustment straight lines are when the correlation of SiO₂ and Al₂O₃ is analyzed. Regarding the soils with higher Fe and Ti content (Soils 3, 2 and 4), when correlated to the attenuation due to Fe₂O₃ and TiO₂, greater proximity is observed of the adjustment straight lines for these soils in relation to the straight line 1:1.

When the photoelectric effect is analyzed (Fig. 6), μ values are strongly influenced by the soil chemical composition in the low energy band (higher μ values), evidenced by the greater separation between the adjustment straight lines of the different soils. Regarding the higher energies studied (lower μ values), a decrease in the importance of the photoelectric effect in the μ values is observed, with a tendency to show values close to zero. The photoelectric effect is highly influenced by the chemical composition of

the soil, due to its cross-section being strongly dependent on Z (Table 1) [30]. The sharp fall with the energy variation is explained by the dependence on the inverse of the energy for the photoelectric effect ($E^{3.5}$) [25, 26]. The straight lines that were closer such as Soils 4 and 2, in the incoherent and coherent scatterings, start to present greater separation, mainly due to the higher amount of Fe + Ti (Soil 2: 14% and Soil 4: 11%) in these two soils.

When analyzing the adjustment straight lines, regarding SiO₂ and Al₂O₃, the μ straight lines for Soils 1 and 5 are close to the straight line 1:1, which is directly related to the amount of the elements Si and Al in those soils. The soils with the lowest Si and Al amounts tended to present overestimated μ values, due to the lower influence of these chemical elements. On the other hand, when the relation between the attenuation due to the Fe₂O₃ and TiO₂ oxides and μ for the photoelectric effect is analyzed, the adjustment straight lines of the soils with higher amounts of the elements Fe and Ti tend to remain closer to the straight line 1:1. The fact that greater influence of the elements with higher Z was observed in the photoelectric effect explains the distancing of the adjustment straight lines of the different soils in relation to the straight line 1:1 for Fe₂O₃ and TiO₂.

Figure 7 presents the existing relation between total μ for the different soils and μ for the major oxides under study. A very similar behavior was observed in the photoelectric

Fig. 6 Correlation between the mass attenuation coefficients for the photoelectric effect of the 5 soils as a function of the 4 major oxides. Soils 1 and 5 show an overlap of their adjustment straight lines in the four correlations presented

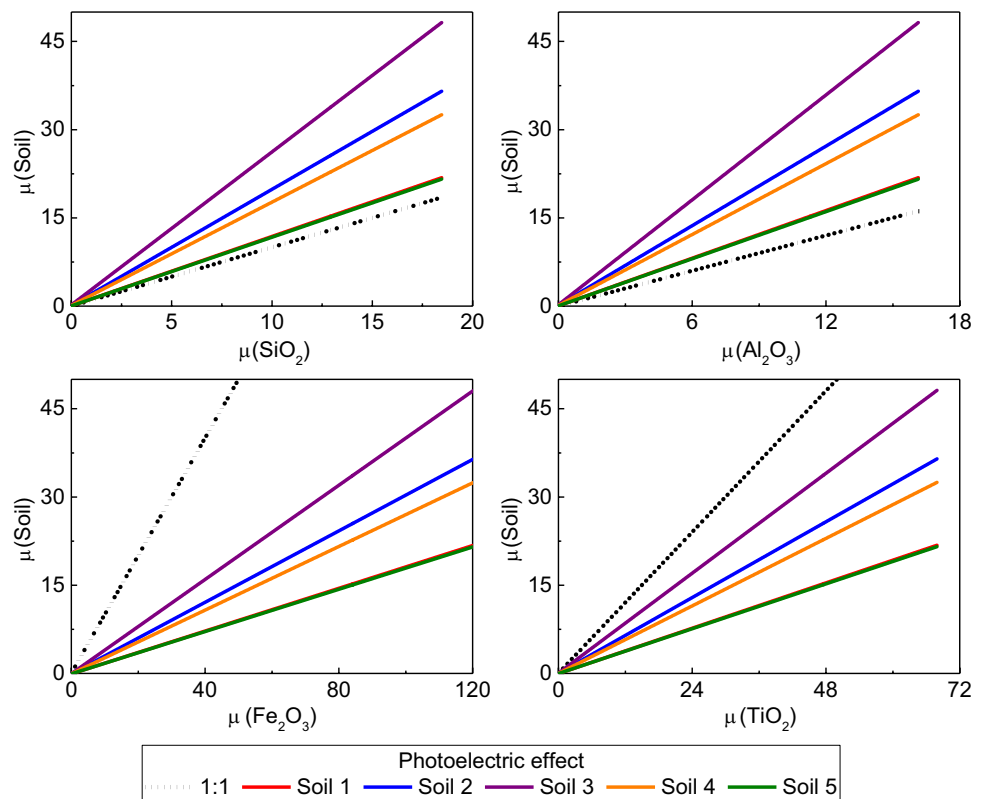
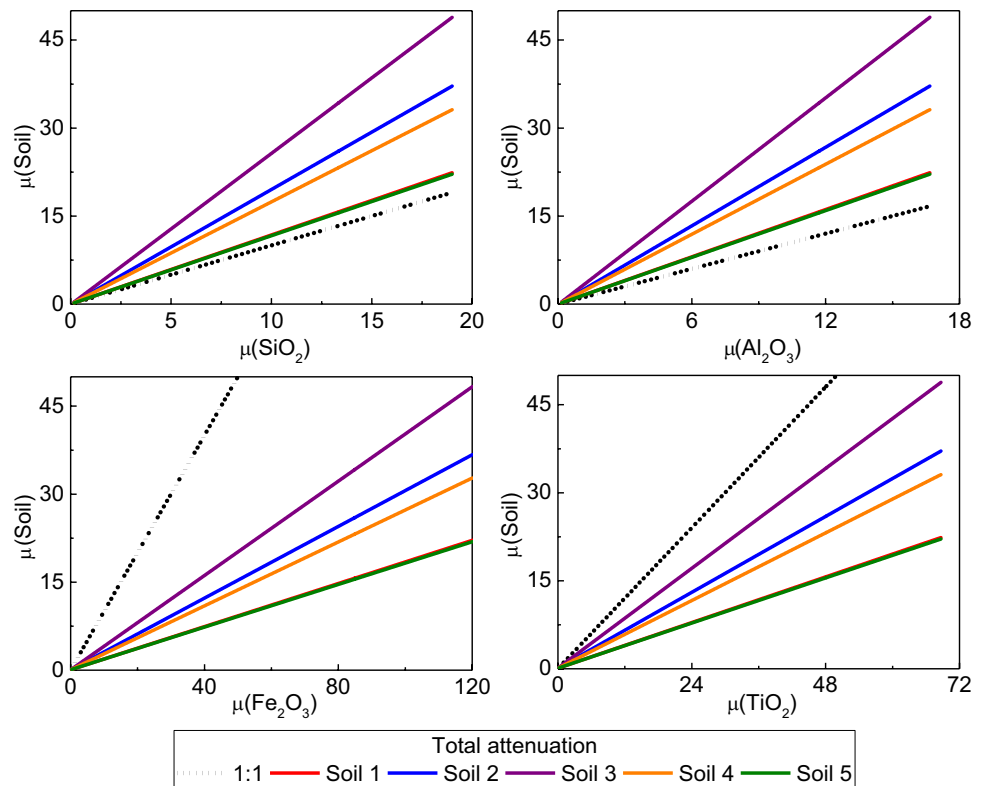


Fig. 7 Correlation between the total mass attenuation coefficients of the 5 soils as a function of the major 4 oxides found in the soils. Soils 1 and 5 show an overlap of their adjustment straight lines in the four correlations presented



effect results, in the energy band used in this study (Fig. 6). This shows that the photoelectric effect along with the coherent scattering present great influence in the results, mainly regarding lower energies. This can be evidenced by the comparison of the attenuation magnitudes due to the photoelectric effect, mainly in the low energy band, in relation to the magnitude of the remaining effects (Fig. 3). In higher energies, the influence of the incoherent scattering is also observed in the results obtained (Fig. 5).

The results presented in this study show that the possibility of the use of accurate theoretical cross-sections for complex compounds, like soils, can allow a detailed analysis of the behavior of radiation interaction processes, such as those related to the partial photon interaction effects (photoelectric effect, coherent and incoherent scatterings, and pair production). The knowledge of the way with which radiation interacts with soil is of great importance for understanding many of their physical properties as well as for studying the radiation absorption properties of the soils focusing on their future use as radiation shielding materials.

4 Conclusions

The results presented here involved the computational simulation of the mass attenuation coefficient using the XCOM program, which has been widely employed in the radiation

physics field due to its ease of use and accessibility. This work presented a detailed analysis of the influence of the main soil oxides on the values of the mass attenuation coefficient in the energy band between 1 and 1500 keV. This study presented as an unprecedented result the analysis of the effect of each oxide on the partial and total attenuation coefficients in comparison with the total oxide composition of each soil. Thus, it was possible to demonstrate the impact of each oxide on the attenuation properties of the soils. Another important result of this study was to show for the first time the influence of photon energy on the correlation between each oxide and the total oxide composition of each soil studied.

The results showed that in low energy bands, the photoelectric effect was the main factor of the attenuation; however, the coherent scattering also contributed to a lesser extent, in all soils investigated. The photoelectric effect is also the effect that was seen to be the most sensitive to the soil chemical composition, mainly in relation to Fe and Ti contents. In energies over 100 keV, the incoherent scattering became predominant in the radiation interaction in all soils, presenting a linear dependence on Z .

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Author Contribution M.A. Camargo: Formal analysis, Data Curation, Methodology, Writing—Original Draft. K.S. Kodum: Formal analysis, Data Curation, Methodology, Writing—Original Draft. L.F. Pires: Conceptualization, Data Curation, Writing—Original Draft.

Availability of Data and Material Not applicable.

Code Availability Not applicable.

Declarations

Conflict of Interest The authors declare no competing interests.

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