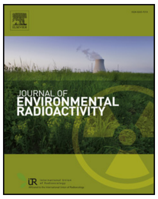
Journal of Environmental Radioactivity 192 (2018) 105–116

Contents lists available at ScienceDirect

Journal of Environmental Radioactivity

journal homepage: www.elsevier.com/locate/jenvrad



Investigating the potentialities of Monte Carlo simulation for assessing soil water content via proximal gamma-ray spectroscopy

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ARTICLE INFO

Keywords:
Proximal gamma-ray spectroscopy
Soil water content
Mass attenuation coefficient
GEANT4
Gamma-ray spectra reconstruction
NaI spectrometer

ABSTRACT

Proximal gamma-ray spectroscopy recently emerged as a promising technique for non-stop monitoring of soil water content with possible applications in the field of precision farming. The potentialities of the method are investigated by means of Monte Carlo simulations applied to the reconstruction of gamma-ray spectra collected by a NaI scintillation detector permanently installed at an agricultural experimental site. A two steps simulation strategy based on a geometrical translational invariance is developed. The strengths of this approach are the reduction of computational time with respect to a direct source-detector simulation, the reconstruction of ^{40}K, ^{232}Th and ^{238}U fundamental spectra, the customization in relation to different experimental scenarios and the investigation of effects due to individual variables for sensitivity studies. The reliability of the simulation is effectively validated against an experimental measurement with known soil water content and radionuclides abundances. The relation between soil water content and gamma signal is theoretically derived and applied to a Monte Carlo synthetic calibration performed with the specific soil composition of the experimental site. Ready to use general formulae and simulated coefficients for the estimation of soil water content are also provided adopting standard soil compositions. Linear regressions between input and output soil water contents, inferred from simulated ^{40}K and ^{208}Tl gamma signals, provide excellent results demonstrating the capability of the proposed method in estimating soil water content with an average uncertainty < 1%.

1. Introduction

Starting from its primary applications to mineral exploration and geological prospecting, gamma-ray spectrometry entered the field of applied geoscience as a highly effective technique for retrieving, at different spatial resolutions, geochemical information on the basis of the distribution of radionuclides in the environment. Although early developments focused on mapping gamma radiation emitted from terrestrial radioisotopes (i.e. ^{40}K and daughter products of the ^{238}U and ^{232}Th decay chains) for the identification of rare earth ores or other mineral commodities (Bristow, 1983; Killeen, 1963; Mero, 1960; Ward, 1981), progressively the exceptional capabilities of radiometric measurements in estimating soil properties have been demonstrated (Beamish, 2015; Mahmood et al., 2013; Wilford et al., 1997; Wilford and Minty, 2006). In particular, promising applications regard soil texture (Heggemann et al., 2017; Viscarra Rossel et al., 2007), clay content (Coulouma et al., 2016; Priori et al., 2013; Van der Klooster et al., 2011), cadmium contamination (Söderström and Eriksson, 2013), pH, organic carbon and plant available potassium (Dierke and Werban, 2013; Pracilio et al., 2006).

In the panorama of environmental variables affecting radiometric measurements, water content and bulk density are the most crucial factors. As water has 1.11 times as many electrons per gram compared to most soils, water is 1.11 times as effective in attenuating gamma-radiation compared to typical soils (Grasty, 1997). The expected high sensitivity of gamma spectroscopy to soil water content has triggered numerous studies which addressed a broad range of applications including soil classification (Beamish, 2013, 2014), radon flux mapping (Manohar et al., 2013; Szegvary et al., 2007) and snow water equivalent assessment (Carroll and Carroll, 1989; Peck and Bissell, 1973). Nevertheless, the potentialities of the method for monitoring soil moisture dynamics have been not fully explored yet (Bogena et al., 2015; Pereira, 2011), especially in the field of proximal sensing, which is foreseen to be an efficient strategy for filling the existing gap between

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Abbreviations: Photon Field Building, (PFB); Gamma Spectrum Reconstruction, (GSR); Photon Field Layer, (PFL); Full Spectrum Analysis - Non Negative Least Squares, (FSA-NNLS)

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https://doi.org/10.1016/j.jenvrad.2018.06.001
Received 23 March 2018; Received in revised form 22 May 2018; Accepted 2 June 2018

punctual measurements, generally provided by in situ electromagnetic sensors (Walker et al., 2004), and remote measurements, typically performed by satellites (Brocca et al., 2017; Zeng et al., 2016).

Although in the last decades proximal gamma-ray spectroscopy experienced a boost in terms of technological and spectral analysis developments, current radiometric data processing concerning the specific topic of soil moisture assessment is typically based on first order analytical models (Carroll, 1981; Grasty, 1997; Loijens, 1980). These methods lack however a custom approach able to integrate individual site characteristics to distinct experimental set up features. In this perspective, Monte Carlo simulations can overcome the limits of analytical solutions, which generally address the description of the sole unscattered gamma-ray flux, by providing information on the entire gamma spectra (Allyson and Sanderson, 1998; Androulakaki et al., 2016; Vlastou et al., 2006). In a Monte Carlo simulation all parameters can be separately controlled and uncertainties coming from temporary variations in the experimental conditions can be excluded, which is particularly relevant in relation to calibration procedures and feasibility studies (Chirosca et al., 2013; De Groot et al., 2009; Van der Graaf et al., 2011). This peculiarity makes the methodology highly versatile in terms of input boundary conditions and extraordinarily effective in both investigating the effects of individual variables (e.g. for sensitivity studies) and in the calibration of different source-detector systems (e.g. permanent stations, carborne based platforms).

The focus of this paper is investigating by means of Monte Carlo simulations the potentialities of proximal gamma-ray spectroscopy applied to the estimation of soil water content in precision agriculture. After providing depth and lateral horizons of proximal gamma-ray spectroscopy in Section 2, we present in Section 3 a strategy which allows to tackle the challenge of simulating gamma spectra generated by a homogeneous infinite medium. A two-step simulation algorithm based on a gamma photon path translational invariance is developed which is subdivided into a Photon Field Building (PFB) procedure followed by a Gamma Spectrum Reconstruction (GSR) inside the detector. In Section 4 the methodology is validated against gamma measurements acquired at a test field in the framework of a precision agriculture experiment. In Section 5 ready-to-use formulae for inferring soil water content from proximal gamma-ray spectroscopy measurements are provided and the reliability of the method is assessed by means of an internal validation test. Finally, Section 6 summarizes the main results of the work.

2. Spatial horizons of proximal gamma-ray spectroscopy

Proximal gamma-ray spectroscopy investigates high energy gamma radiation produced in the decays of ^{40}K and daughter products of the ^{238}U and ^{232}Th decay chains, which are the only naturally occurring radionuclides producing gamma radiation of sufficient energy and intensity to be measured in the framework of in-situ surveys. Since each gamma decay has a specific emission energy, it is possible to recognize distinctive structures (photopeaks) in a gamma spectrum, which allow for the quantification of ^{40}K, ^{238}U and ^{232}Th abundances in the soil source. The integrated numbers of events inside the energy ranges associated to the main photopeaks (IAEA, 2003) are typically adopted for determining the corresponding counts per second (cps) which are related to ^{40}K, ^{238}U and ^{232}Th activities in the soil by some sensitivity calibration factors. While ^{208}Tl (^{232}Th decay chain) and ^{40}K are distributed solely in the soil, gamma radiation produced by the decay of ^{214}Bi (^{238}U decay chain) comes both from ^{214}Bi in the soil and from ^{214}Bi in the atmosphere originated by the decay of ^{222}Rn gas exhaled from rocks and soils.

The number of net counts recorded in the photopeak centered at the gamma emission energy E by a detector placed at height h scales with the gamma photon flux $\Phi(h)$, which can be written as follows, assuming an infinite half-space soil volume source, a homogeneous radionuclide concentration and homogeneous soil and air materials (Feng et al., 2009):

$$\Phi(h) = \frac{A_V P_\gamma}{2\mu_s(E)} \int_0^{\pi/2} \sin\theta e^{-\frac{\mu_a(E)h}{\cos\theta}} d\theta \tag{1}$$

where A_V is the unit volume activity in Bq/m^3, P_γ is the γ-ray intensity in number of gammas per Bq, $\mu_s(E)$ and $\mu_a(E)$ are the linear attenuation coefficients in m^{-1} of soil and air, respectively, and θ is the polar angle between the detector vertical symmetry axis and one radioactive unit element in the source. Linear attenuation coefficients μ define the probability P_0 that a gamma travels a distance d in a given material without suffering any interaction and are generally expressed as the product of the mass attenuation coefficients μ/ρ (m^2/kg) (which depend only on the material composition and on gamma energy) times the material density ρ (kg/m^3):

$$P_0(E) = e^{-\mu(E)d} = e^{-\left(\frac{\mu}{\rho}(E)\right)\rho d} \tag{2}$$

Eq. (2) is what governs gamma photon survival in traversing a given material as photon attenuation is respectively positively and negatively correlated to material density and photon energy. This is the key for understanding the lateral and vertical horizons of proximal gamma-ray spectroscopy.

The vertical field of view of a gamma-ray detector placed at height h can be estimated on the basis of the gamma photon flux produced within a soil thickness t, which can be written according to Eq. (3), where the notation is simplified for the implicit gamma energy dependence (Feng et al., 2009):

$$\Phi(h) = \frac{A_V P_\gamma}{2\mu_s} \int_0^{\pi/2} \sin\theta e^{-\frac{\mu_a h}{\cos\theta}} \left[1 - e^{-\frac{\mu_s t}{\cos\theta}}\right] d\theta \tag{3}$$

The cumulative contribution to the unscattered gamma photon flux as function of soil depth has a steeper profile for decreasing gamma energy (Fig. 1a) and for increasing soil density (Fig. 1b). Considering a [1.2–1.8] g/cm^3 typical range of soil densities, 95% of the unscattered gamma flux at the soil surface is produced within the first [19–28] cm for ^{40}K gamma photons (E = 1.46 MeV) and within the first [24–36] cm for ^{208}Tl gamma photons (E = 2.61 MeV) (Table 1).

The horizontal field of view of a gamma-ray detector placed at height h can be estimated on the basis of the gamma photon flux produced within a cone of radius r and opening angle 2θ* (Feng et al., 2009):

$$\Phi(h) = \frac{A_V P_\gamma}{2\mu_s} \int_0^{\theta*} \sin\theta e^{-\frac{\mu_a h}{\cos\theta}} \left[1 - e^{-\mu_s\left(\frac{r}{\sin\theta} - \frac{h}{\cos\theta}\right)}\right] d\theta \tag{4}$$

In the height range of proximal surveys (~few meters), the cumulative contribution to the unscattered flux as function of the cone radius is slightly influenced by gamma energy (Fig. 2a), while it sensibly changes for different heights above the ground (Fig. 2b). By lifting a detector from 1 m to 10 m height the radius from which 95% of the unscattered flux is produced increases from ~15 m to ~85 m (Table 2). The differential contribution to the unscattered gamma photon flux originated by concentric hollow cylinders centered at the detector vertical axis also changes with the detector height. By increasing the detector height, the hollow cylinder providing the highest contribution is progressively farther from the detector vertical axis (Fig. 3).

Gamma photon flux attenuation for increasing height is directly connected to the acquisition time which is needed for attaining a target counting statistics (Table 2): by increasing the detector height from 1 m to 10 m, the acquisition time needs to be extended by approximately 20% in order to measure the same number of events in a given energy range.

Summarizing, proximal gamma-ray spectroscopy has in principle the power of being sensitive to the physico-chemical properties of the first 30 cm of soil in an area wide fractions of hectares. The application