

Modeling of the setup for carbon analysis of soil sample

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Abstract

Accurate determining the concentration of carbon in soil today remains an important task for various fields of science. The special role of soil in food production, as well as its participation in regulating the chemical composition of the atmosphere, makes it necessary to research it.

Chemical methods are commonly used to determine carbon concentration in soil, but they require specific preparations. Nuclear physics methods are promising for measuring carbon concentration in soil, and mobile installations that perform neutron gamma analysis on instantaneous gamma-quanta in the field are being developed.

As part of the TANGRA International Collaboration (LNF JINR, Dubna), a method for determining carbon in soil is being developed through the study of fast neutron scattering. This work focuses on computer modeling of one of the possible configurations of the installation to develop data processing methods obtained during measurements.

The object of the study

Soil is a complex, polyfunctional, and multi-component multiphase structural system formed in the surface layer of weathered rocks. It is a composite of mountain rocks, organisms, climate, relief, and time [1]. The average content of chemical elements in the soil is presented in Table 1.

Chemical element	O	Si	Al	Fe	Mg	C	Ca	K
% content	49.00	33.00	7.13	3.80	2.10	2.00	1.37	1.36

Table 1. Average content of chemical elements in soils by weight % (A.P. Vinogradov, 1950) [2]

Neutron-gamma analysis in fast neutrons

Currently, the determination of carbon concentration in soil using neutron-gamma analysis on fast neutrons is considered promising. This method is based on neutron irradiation of the material and analysis of γ -ray spectra emitted as a result of neutron-nuclear reactions. The system used for such an analysis consists of a neutron source, γ -detectors, and a data acquisition system. One possible configuration of such a setup is shown in Fig. 1.

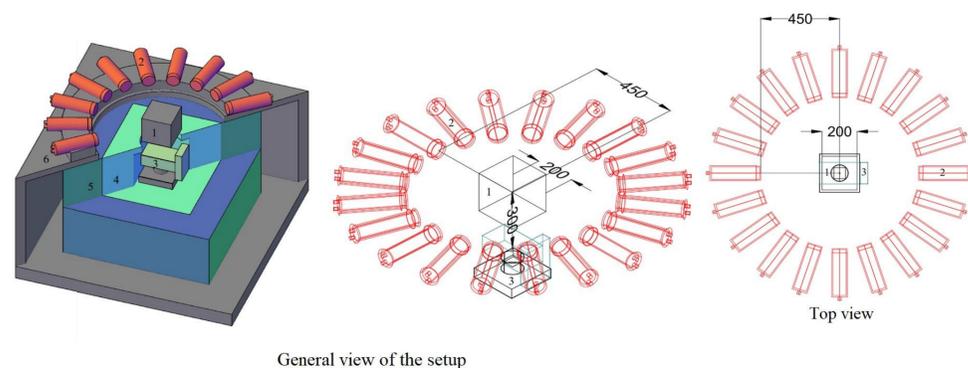


Fig. 1 Simulated setup. 1 - sample, 2 - BGO gamma detector, 3 - ING-27 neutron generator, 4, 5 - combined shielding, 6 - instrument housing. Dimensions are given in mm

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The calculations presented in this work were performed using the GEANT4 software package [3]. In this study, the QGSP_BIC_HP physics list recommended by the Geant4 developers for modeling systems using neutrons with energies less than 20 MeV was used. A cube consisting of O, Si, Al, Fe, C and H, in proportion shown in table 1, with a density of 1.2 g/cm³, was chosen as the model soil sample. Figure 2 shows the simulated gamma spectrum of the soil material, where peaks are visible predominantly corresponding to reactions on O, Si, and Al.

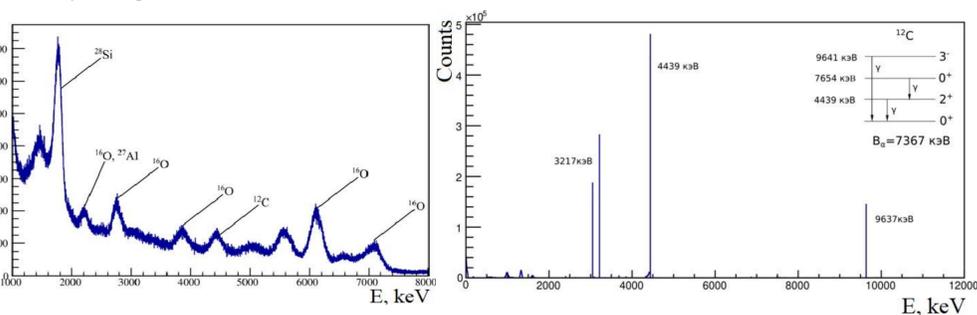


Fig. 2 Model γ spectrum of soil.

Fig. 3 The spectrum of γ -rays from ¹²C

To determine the carbon concentration, the peak with an energy of 4439 keV can be used. In the simulation, 10⁹ tagged neutrons were launched, which corresponds to approximately 1.5 minutes of operation of the ING-27 generator at full intensity of 5x10⁷ n/s and a tagged neutron flux of about 10⁷ n/s.

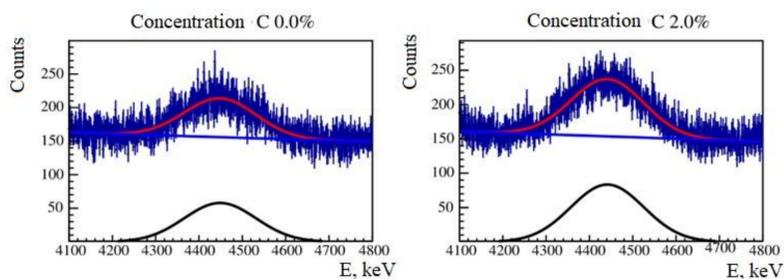


Fig. 4 Approximated gamma spectra at carbon concentrations of 0% and 2%

The challenges of modeling neutron-gamma analysis in Geant4

Developers of the Geant4 software package indicate that results regarding the generation of gamma-rays during neutron irradiation of a sample should always be questioned.

In particular, it has been found that the cross-sections for the production of gamma-rays associated with the transition of nuclei from excited states do not correspond to experimental values.

The data obtained from modeling the interaction of 10⁷ tagged neutrons with a sample of size 1x1x0.5 cm³ and density of 1200 kg/m³, consisting of ¹²C, ¹⁶O, ⁵⁶Fe, ²⁷Al, and ²⁸Si, are presented in Table 2.

Sample and its characteristics	Energy of the characteristic peak, keV	Experimental cross sections [2] σ ,mb	FENDL-1, σ ,mb	The values of the cross sections calculated from the simulation, mb
¹² C	3215			193
	4439	187.0 \pm 7.5	184	304
	9638			97
¹⁶ O	2732	38.0 \pm 3.9	62.2	111
	6129	148 \pm 10	173.0	199
⁵⁶ Fe	412	32.5 \pm 2.4		1348
	847	621 \pm 29		373
	1239	290 \pm 16		42
²⁷ Al	844			84
	1015			188
	2212	145 \pm 10		148
²⁸ Si	586	41 \pm 10		96
	1780	403 \pm 18	442	215
	2839	59.0 \pm 6.7	70	48

Table 2. Data obtained from modeling the interaction of 10⁷ tagged neutrons

Currently, it seems most reasonable to perform calculations of the distribution of neutrons and gamma-rays separately.

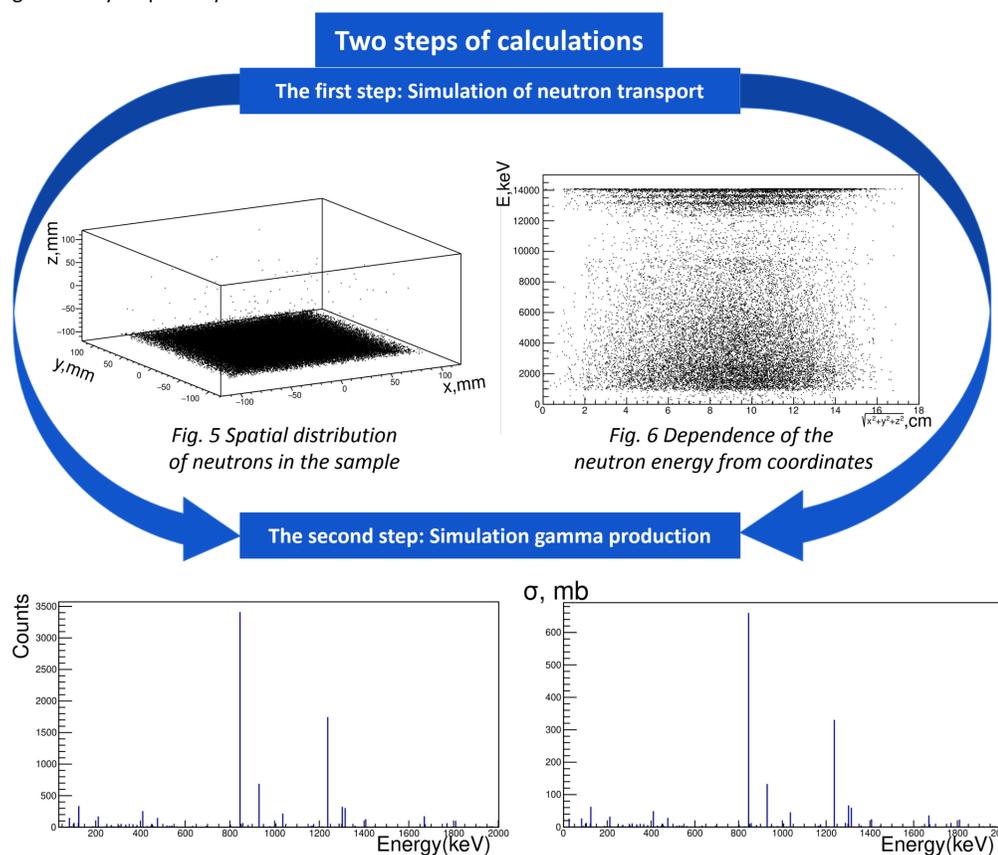


Fig. 7 Model γ spectrum of ⁵⁶Fe

Fig. 8 Dependence of the cross section of the energy of gamma transitions for ⁵⁶Fe

Reference

[1] G. D. Belitsina. Soil science. Higher School. M., 1988.

[2] A. Kavetskiy, G. Yakubova, S. A. Prior et al.//AppliedRadiationandIsotopes. 2019. V. 150, p. 127-134. <https://doi.org/10.1016/j.apradiso.2019.05.028>

[3] Geant4 v. 10.01, p. 2. https://geant4.web.cern.ch/support/download_archive?page=3.