



Fluka simulation of PGNAA system for determining heavy metal pollution in the soil sample

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Abstract. This study presented a self-designed prompt gamma neutron activation analysis (PGNAA) model and used Fluka simulation to simulate the heavy metals (Mn, Cu, Hg, Ni, Cr, Pb) in soil samples. The relationship between the prompt γ -ray yield of each heavy metal and soil thickness, content of heavy metals in the soil, and source distance was obtained. Simulation results show that the prompt γ -ray yield of each heavy metal increases with the increase in soil thickness and reaches saturation at 18 cm. The greater the proportion of heavy metals in the soil, the greater the prompt γ -ray yield. The highest content is approximately 3%, and the change in distance between the neutron source and soil sample does not affect the prompt γ -ray yield of heavy metals.

Keywords: PGNAA • Fluka • Heavy metal • Prompt gamma-ray yield

Introduction

Prompt gamma neutron activation analysis (PGNAA) is a fast-growing multinuclear method with a fast detection speed and simple data processing and is non-destructive and does not require sampling. It reduces complex intermediate links and experimental errors. PGNAA is widely used in oil logging, environmental samples, mining, and detection of explosives [1–18].

Heavy metals (Mn, Cu, Hg, Ni, Cr, Pb) in the soil are easily accumulated and converted into toxic compounds because they cannot be decomposed by microorganisms, which endanger human health through the food chain and threaten the growth of plants. Thus, detecting the content of heavy metals in the soil has attracted considerable attention in environmental monitoring. At present, most systems for detecting heavy metals in the soil are complicated to operate and are not portable, and these disadvantages can be overcome through PGNAA. However, PGNAA has not been applied in soil heavy metal detection. In this study, Fluka simulation was conducted to investigate the influencing factors between the neutron source and samples through a self-designed PGNAA model. The relationships between soil heavy metal concentration and soil thickness and between neutron capture γ -ray yield and sample thickness and purity of main elements, such as Mn, Cu, Hg, Ni, Cr, and Pb, in soil samples were evaluated. A rough analysis model of soil samples was optimized based on the change relationship to provide a theoretical basis for the analysis of soil environmental pollution.

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Received: 22 April 2019
Accepted: 13 January 2020

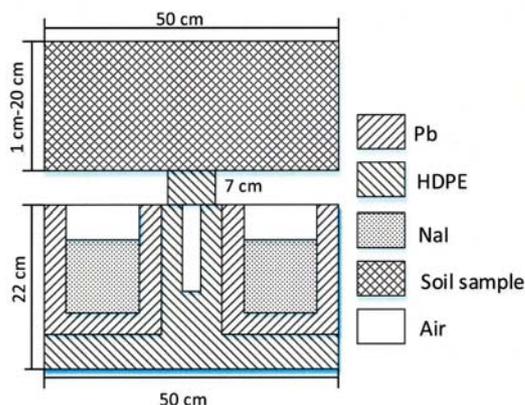


Fig. 1. PGNAA simulation model.

Materials and methods

Simulation model

The simulation model is shown in Fig. 1. The bottom of the model was a polyethylene (PE) with 50 cm diameter and 22 cm length to reduce the neutron source and make the thermal neutrons uniform in the sample. The inner center of high-density polyethylene (HDPE) had a cavity with 0.25 cm radius and 10 cm length for placing a ^{252}Cf neutron source with an emissivity of $2.3 \times 10^{12} \text{ s}^{-1}\cdot\text{g}^{-1}$. Four NaI(Tl) detectors with diameter $12.8 \text{ cm} \times 12.8 \text{ cm}$ were placed around the neutron source circumference and HDPE with a distance of 9 cm from the sample chamber for recording PNGAA gamma rays

Table 1. Parameters of each element with different heavy metal contents

Heavy metal content [%]	Density [g/cm^3]						Mass fraction of each element in the soil [%]						
	Hg	Mn	Ni	Cu	Pb	Cr	O	Si	Al	Fe	C	H	
0.00	1.2500	1.2500	1.2500	1.2500	1.2500	1.2500	68.43	20.25	7.16	2.34	1.23	0.59	
0.01	1.2515	1.2514	1.2515	1.2515	1.2515	1.2514	68.42	20.25	7.16	2.34	1.23	0.59	
0.10	1.2525	1.2524	1.2524	1.2524	1.2525	1.2524	68.36	20.23	7.15	2.34	1.23	0.59	
1.00	1.2628	1.2618	1.2622	1.2622	1.2626	1.2618	67.75	20.05	7.08	2.32	1.22	0.58	
2.00	1.2745	1.2724	1.2732	1.2733	1.2740	1.2724	67.06	19.85	7.02	2.29	1.21	0.58	
3.00	1.2864	1.2832	1.2845	1.2843	1.2857	1.2831	66.38	19.64	6.95	2.27	1.19	0.57	
4.00	1.2985	1.2941	1.2959	1.2959	1.2975	1.2941	65.69	19.44	6.87	2.24	1.18	0.57	
5.00	1.3109	1.3053	1.3075	1.3076	1.3096	1.3052	65.01	19.24	6.80	2.22	1.17	0.56	

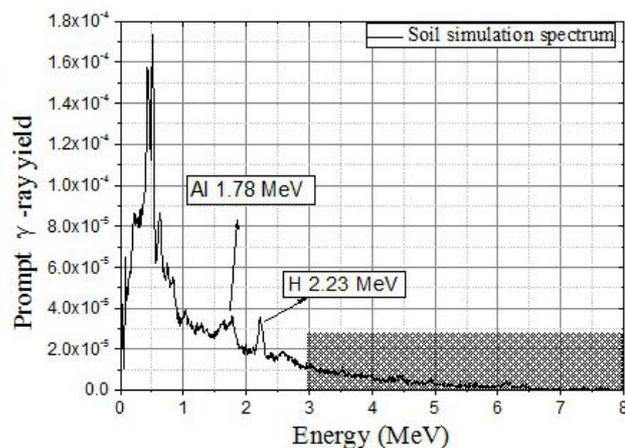


Fig. 2. Prompt γ -ray yield of soil sample.

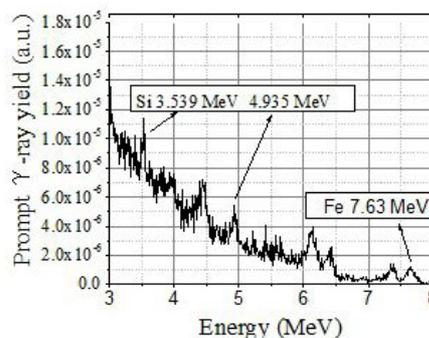
Table 2. Characteristic γ -rays energy and cross-sections

Heavy metal	Characteristic γ -rays energy [MeV]	Cross-section [barns]
Hg	0.08	0.0093
Mn	7.25	–
Ni	1.35	0.0036
Cu	0.97	0.0054
Pb	7.37	0.0319
Cr	0.75	0.0030

reflected from the sample. All detectors were wrapped with 5 cm-thick lead. HDPE with 2 cm radius and 7 cm length was placed between the sample and HDPE to reduce the neutron source. The diameter of the sample chamber was 50 cm, and the thickness of the sample chamber varied from 0 cm to 20 cm.

Methods

Fluka program was used to find the best simulation parameters by changing the source distance, thickness of soil samples, and the proportion of heavy metals in soil samples. The neutron source was a homogenous ^{252}Cf point source with an emissivity of $2.3 \times 10^{12} \text{ s}^{-1}\cdot\text{g}^{-1}$. A Watt fission energy spectrum model was used to describe the spontaneous fission spectrum. The parameters of each element in the soil are given in Table 1 with different heavy metal contents, and characteristic γ -rays energy and cross-sections are given in Table 2.



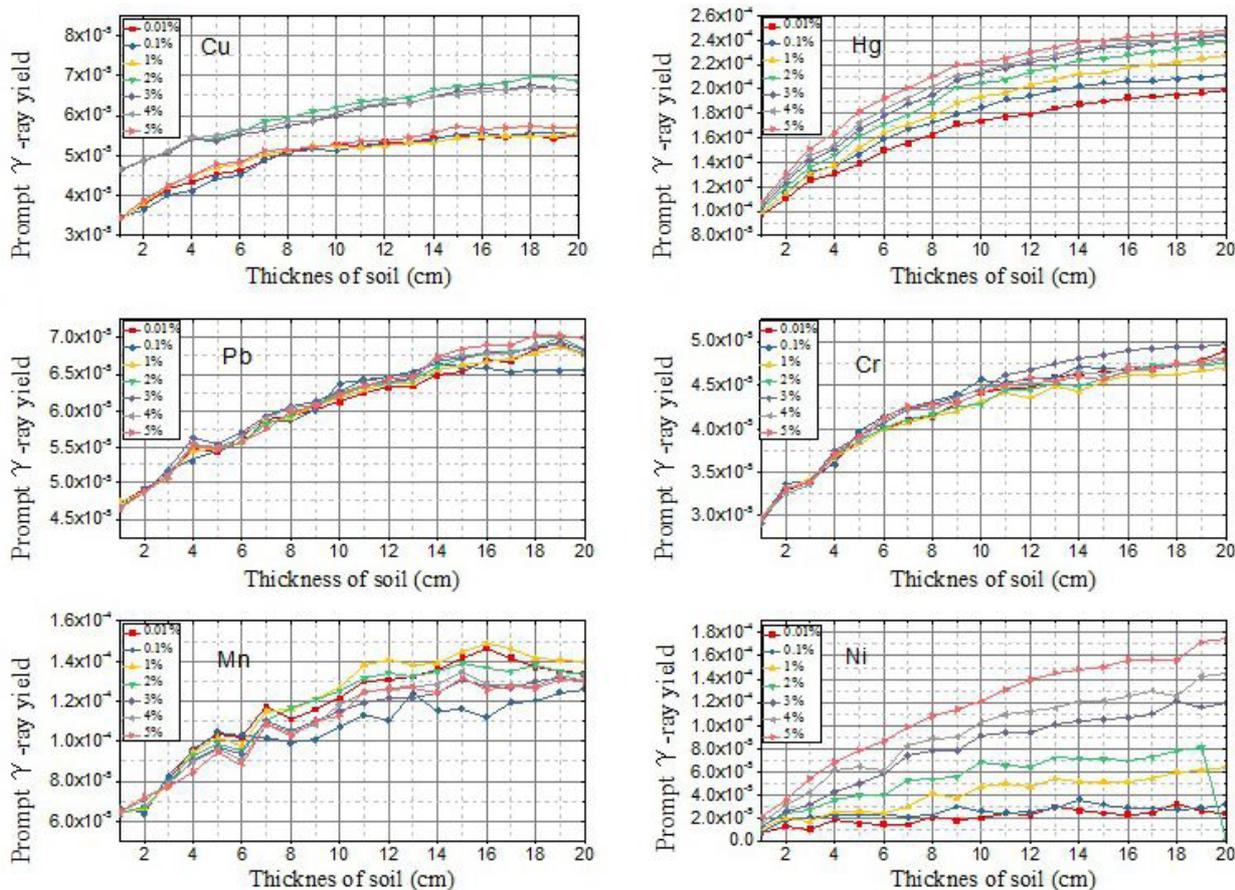


Fig. 3. Soil sample thickness.

Results and discussion

Pure soil PGNAA simulation

The soil was simulated to obtain the gamma line of the PNGAA characteristic when no heavy metal existed in the soil, as shown in Fig. 2.

Figure 2 shows that the prompt γ -ray peaks corresponding to aluminium, hydrogen, silicon, and iron are 1.78, 2.23, and 7.63 MeV. Silicon produces prompt γ -rays with several different energies, and the most significant γ -rays are 3.539 MeV and 4.935 MeV.

Sample thickness simulation

Soil thickness was changed from 1 cm to 20 cm, and the concentration gradients of six heavy metal elements were simulated, which were 0.01, 0.1, 1, 2, 3, 4, and 5%, respectively, as shown in Fig. 3.

Figure 3 shows that the gamma yield of prompt gamma rays at different contents of heavy metals, such as Cu, Hg, Pb, and Cr, increases with the increase in soil thickness, and the maximum value appears at a certain soil thickness position. The prompt γ -ray yield of heavy metals fluctuates and decreases when the maximum value is reached. As shown in the comprehensive diagram, each heavy metal can reach its maximum value at 18 cm soil thickness.

Simulation of the proportion of heavy metals in the soil

Soil thickness was set to 18 cm, and the relationship between the content of six heavy metals in the soil and prompt γ -ray yield was simulated.

Figure 4 shows that the prompt γ -ray yield of Cu reaches its maximum value when its proportion in the soil reaches 2%. The greater the proportion of Hg in the soil, the greater the prompt γ -ray yield. The prompt γ -ray yield of Pb reaches its maximum value and decreases when its proportion in the soil reaches 1% and 2%. The prompt γ -ray yield of Mn reaches its maximum value when its proportion in the soil reaches 5%. The prompt γ -ray yield of Ni

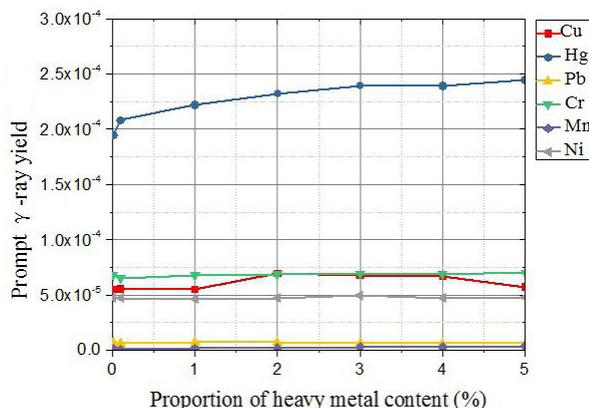


Fig. 4. Proportion of heavy metals in the soil.

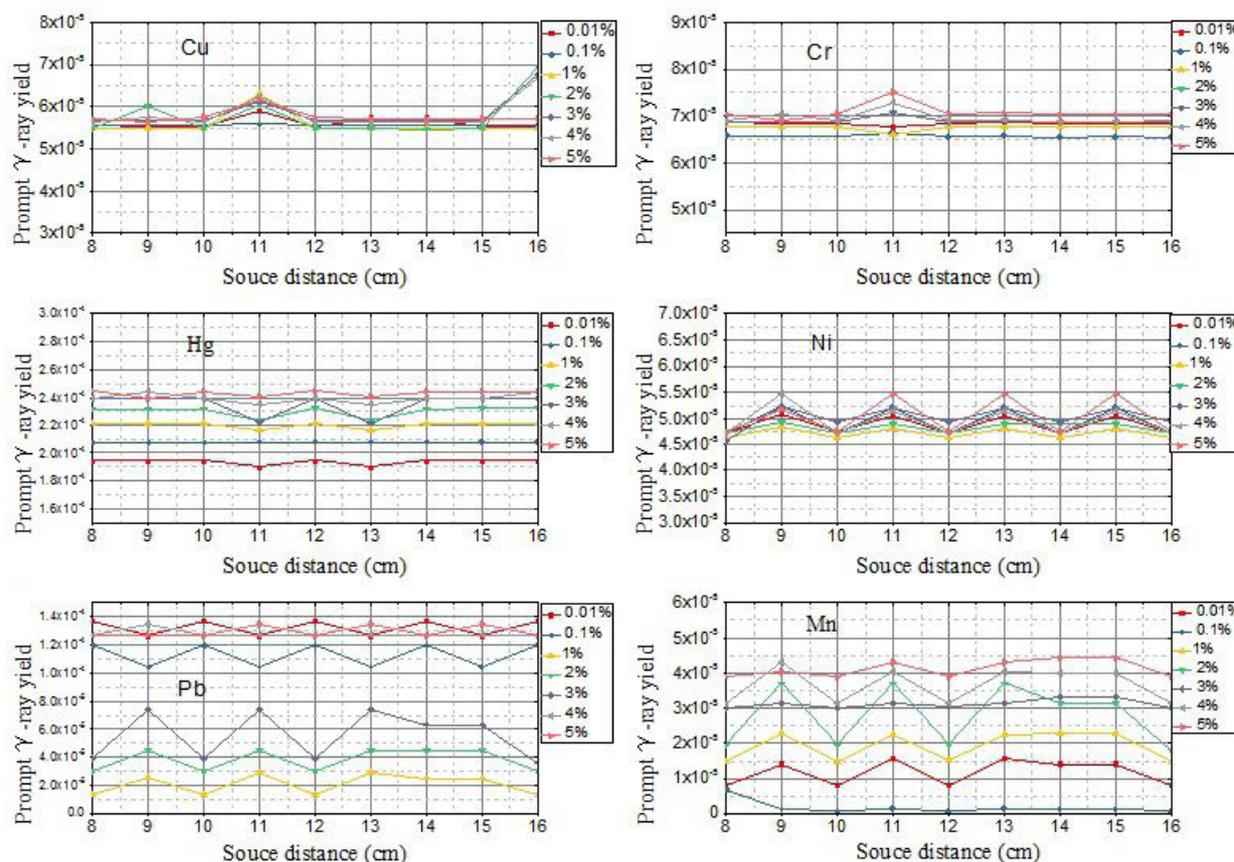


Fig. 5. Source distance.

reaches its maximum value when its proportion in the soil reaches 3%. Considering the relationship between the content ratio of the above various elements and prompt γ -ray yield and the actual situation of the environment, the prompt γ -ray yield of various metals is saturated and decreases when their proportion is 3%.

Relationship between gamma yield and source distance of characteristic gamma rays of heavy metal elements

Soil thickness was set to 18 cm. The neutron source and soil sample were simulated to determine their relationship. The results are shown in Fig. 5.

Figure 5 shows the variation in prompt γ -ray yield of each heavy metal by changing the distance between the source and the sample at different concentrations. As shown in Fig. 5, the prompt γ -ray yield of each heavy metal fluctuates with the change in distance and tends to be balanced. Therefore, the distance between the source and the soil sample affects the prompt γ -ray yield of heavy metals.

Conclusion

Six heavy metals, namely, Mn, Cu, Hg, Ni, Cr, and Pb, in the soil have different γ -ray yield values received by the detector under different soil thicknesses. The soil thickness is set to 18 cm after

comprehensively considering various elements. The higher the proportion of heavy metals, such as Mn, Cu, Hg, Ni, Cr, and Pb, in the soil, the higher the prompt γ -ray yield of various metals. However, the prompt γ -ray production of elements is approximately 3%. The prompt γ -ray production reaches its maximum value, that is, it reaches saturation and shows a downward trend. Changing the distance between the source and soil sample does not affect the prompt γ -ray yield of heavy metals.

Acknowledgments. This work was supported by the National Natural Science Foundation of China (41774120), the Sichuan Science and Technology Program (2018TJPT0008, 2019YFG0430), and the Science and Technology Program of Sichuan Education Department (17ZA0023).

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