Bulgarian Chemical Communications, Volume 49, Number 4, (pp. 874 – 878) 2017

Study of the possibility of using IXRF technique to detect the elements present in dust using Monte Carlo N Particles

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Received November 15, 2016; Accepted April 12, 2017

Detecting heavy metals present in soil and dust as a major factor of environmental pollution has got a particular importance. An experimental (laboratory) method based on energy-dispersive X-ray fluorescence (EDXRF) technique was utilized so far to detect the elements. In this research, the Monte Carlo method based on the EDXRF technique was used to detect the elements. MCNPX2.7 code is based on Monte Carlo calculations and is able to trace 32 particles including photons within the range of X-rays and γ-rays. In this paper, the outcomes of multi-source EDXRF simulation technique were compared with the experimental results. The comparison shows that multi-source EDXRF technique(IXRF) is able to detect the percentage of elements present in soil and dust with a high compatibility.

Keywords: IXRF; Elements; Dust; EDXRF; Multi Source; MCNPX; Detection.

INTRODUCTION

Detecting the elements present in soil and the percentage of each component has got a particular importance from the aspect of agriculture, environmental pollution, agrology and mines discovery [1]. Different methods based on chemical decomposition and physical methods have been used for this purpose so far [2]. The most important chemical method CMB (Chemical Mass Balance) is not really capable of detecting dust and soil elements as the major pollution source [2]. The most efficient method is EDXRF which is a fast non-destructive method in which an X-ray system mostly of electron strip type isutilized [2]. EDXRF is being applied for detection of the elements present in soil [3-7]. MCNPX is a multi-task nuclear code offering the possibility of tracing a characteristic X-ray emission spectrum produced by collision of energetic photons, which is an atomic process. Accuracy of MCNPX code to detect the percentage of brass alloy has been investigated and verified byT.Trojek and T. Ćechák [7]. In this research the possibility of using MCNPX with three radioactive sources, *viz.*^{55}Fe(5.9 KeV), ^{241}Am(26.4, 59.6KeV) and ^{57}Co(122KeV), to detect the elements present in soil by the three source EDXRF method (IXRF)was studied.

MATERIALS AND METHODS

Purpose of the present research is the detection of the elements present in soil with the use of Monte Carlo N Particles (MCNPX) which is based on particles transportation using the Monte Carlo method. Soil is a combination of Cu, Al, Ca, Co, Cr, Fe, K, Mn, Na, Ni, Pb, Rb, Si, Sr, Ti, V, Y, Zn, and Zr, each having its own specific X-ray spectrum. The energy emitted from the K layer is brought in Table 1 [9].

Ordinary soil contains different elements, most of which are in the Z≤50 range, however polluted soils and dust particles might have different elements in the range of 0≤Z≤100. So far, one X-ray source has always been used for detection of the elements present in soil [10, 11]. Since each source emits X-rays with its particular energy spectrum, and the need for energy is to some extent higher than the atomic layer energy difference, so in order to precisely detect different elements, different sources are required. In this research, an attempt was made to use more than one source for detection of the elements present in soil and dust. Before producing any device, a fabrication feasibility study is needed. Atomic and nuclear codes are the best options for a fabrication feasibility study and MCNP is a credible nuclear code. This research was performed with the use of MCNP code in three phases, in each of which, acharacteristic X-ray spectrum was obtained. In the first phase, γ-ray energy produced by three sources of ^{55}Fe(5.9KeV), ^{241}Am(26.4, 59.6KeV) and ^{57}Co(122KeV), was radiated separately to each element present in the soil. Then in the second phase, the elements included in a typical soil with certain percentages were separately irradiated by ^{55}Fe(5.9KeV), ^{241}Am(26.4, 59.6KeV) and ^{57}Co(122KeV). In the third phase, a radioactive source in form of a combination of ^{55}Fe(5.9KeV), ^{241}Am(26.4, 59.6KeV) and ^{57}Co(122KeV) sources irradiated the soil. The characteristic X-ray energy

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spectrum in all three phases can be obtained in MCNP code with the use of tallies F_1 and F_2 in the specific input file of each phase. The input file description will be given in the following. The probability of emission in each energy range for each particle can be obtained with the use of MCNPX code and an input file was written for this purpose. An overview of the defined geometry in the input file is illustrated in Fig.1.

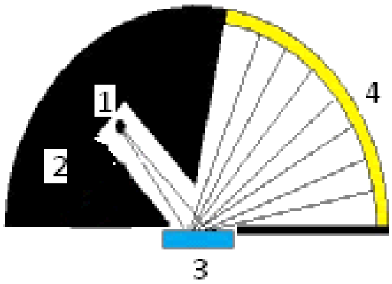

Fig. 1. The geometry considered in the simulation

In this geometry cell no.1 shows the point source with certain activity for sources with^{55}Fe(5.9KeV),^{241}Am(26.4,59.6KeV) and^{57}Co (122KeV) energies, cell no.2 shows the source cover, cell no.3 shows the considered material (target) with optimal calculated thickness in each mode and for dimensions 2×2cm^2, and cell no.4 shows a special shell defined as a detector. After radiation, the X-ray fluorescence spectrum will reach the internal surface of the cylindrical shell. Tally F_1 will provide the characteristic X-ray spectrum received by the detector. The number of particles wasconsidered 108 in order to reach below 1% error. Splitting and Russian Roulette methods were used to reduce variance, increase FOM and uniform SLOP in the output file of MCNPX. The percentage of elements presentin a typical soil according to [9] is shown in Table 1.

RESULTS

Chemistry

The results of this simulation which wasdone in three phases with the use of tally $F_1$are reported below. First, the characteristic X-ray spectrum of each element present in the soil, which was separately irradiated by γ-rays produced by three different sources of ^{55} Fe(5.9KeV), ^{241}Am(26.4,59.6KeV) and ^{57}Co(122KeV) was obtained and the results are shown in Table 1.

The comparison of theoretical and experimental results of Table 1 shows that MCNPX code has the capability of detecting each element separately with the use of EDXRF technique.

The soil with the mentioned element percentages in Table 1, was irradiated by different sources and the obtained EDXRF spectrum with the use of tally $F_1$is shown in Figures 2 to 5.

The results show that ^{55}Fe(5.9KeV) can detect the elements in the $Z \leq 23$ range, whereas ^{241}Am(26.4,59.6KeV) is more appropriate to detect the elements in the $22 \leq Z \leq 40$ range.

Also, ^{57}Co(122KeV) is better for detection of heavy elements like lead. Eventually the X-ray spectrum of soil with the use of a composed sourc e produced by ^{241}Am(59.6KeV), ^{55}Fe(5.9KeV) and ^{57}Co(122KeV)with different percentages which

Table1. The emission energy of K layer for elements in dust

Elements	K_α		K_β		Percent
	Experimental	MCNPX	Experimental	MCNPX	
Na	1.04	1.02	------	------	0.00755
Al	1.48	1.47	------	------	0.21326
Si	1.74	1.73	------	------	0.7024
K	3.31	3.38	------	------	0.04806
Ca	3.69	3.66	4.01	3.99	0.00247
Ti	4.5	4.5	4.93	4.91	0.00293
V	4.95	5.02	5.42	5.40	0.000133
Cr	5.41	5.4	5.94	5.91	0.000901
Mn	5.89	5.85	6.49	6.45	0.000926
Fe	6.4	6.36	7.05	7.02	0.0197
Co	6.93	6.88	7.64	7.61	0.0000123
Ni	7.48	7.5	8.26	8.24	0.000049
Cu	8.04	8.00	8.90	8.89	0.0000256
Zn	8.63	8.61	9.57	9.60	0.000133
Rb	13.39	13.4	14.96	14.92	0.00117
Sr	14.16	14.12	15.83	15.80	0.000102
Y	14.95	14.92	16.73	16.72	0.0002118
Zr	15.77	15.74	17.67	17.65	0.00005198
Pb	74.96	75.02	84.93	85.10	0.000225

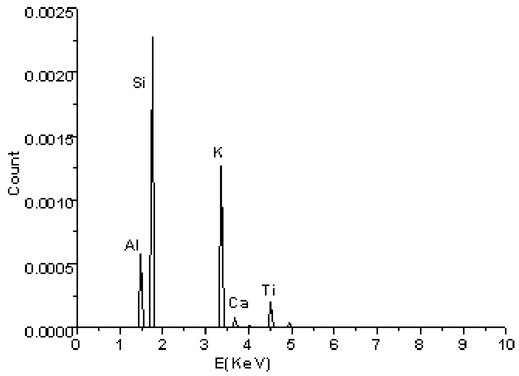

Fig. 2. The X-ray spectrum ofa dust target at 5.9KeV (^{55}Fe source)

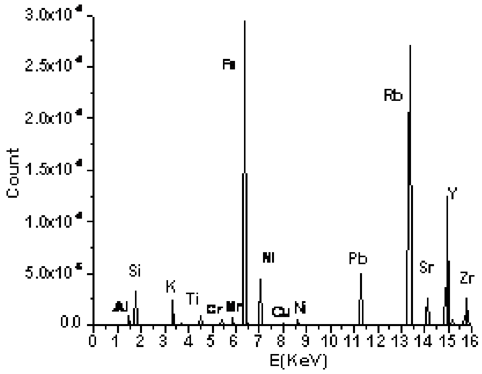

Fig. 3. The X-ray spectrum of adust target at 26.4KeV (^{241}Am source)

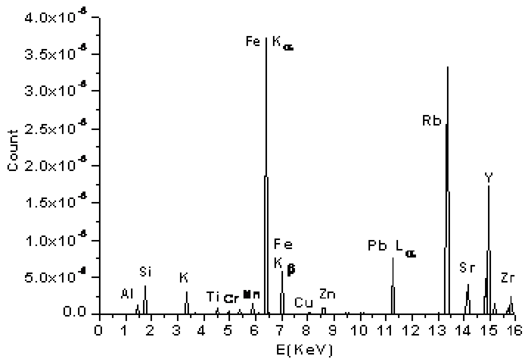

Fig. 4. The X-ray spectrum of adust target at 59.6KeV (^{241}Am source)

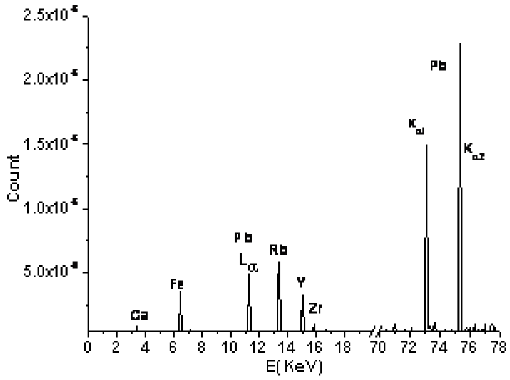

Fig. 5. The X-ray spectrum of adust target at 122KeV (^{57}Co source)

have been obtained from MCNPX simulation code is according to figures 6 to 9. In these figures source percentages have changed and the related spectrum wasobtained accordingly. As can be seen in the figures and table 1, the spectrumshape depends on source percentages and percentage of the elements present in the compound. Comparing the detected elements by the multi-source EDXRF method(IXRF) with the presentresults for the elements in the soil shows that the introduced method is well able to detect the elements present in soil. Meanwhile, percentages of the elements obtained by this technique have a good compatibility with the percentages in soil. Percentage of elements in each mode is obtained according to the proportion of characteristic X-ray intensity in the compound to characteristic X-ray intensity obtained for the pure element. Afterwards, according to percentages of reported elements presentin soil, the material of cell 1 was positioned by (2) and the EDXRF spectrum related to element admixture in soil was obtained (Figures 2 to 5).

M_1 card for the considered soil in MCNPX code is brought in Table 1. After executing the code, the obtained spectrum by the defined detector in MCNPX code with the three above mentioned sources is produced, which is shown in Figures 6 to 9.

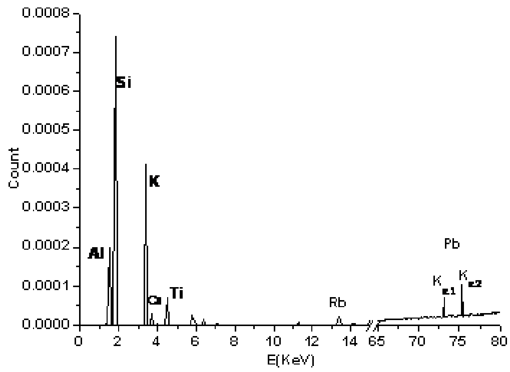

Fig. 6. The X-ray spectrum of adust target at 5.9, 59.6, 122Kev equal percent (^{55}Fe, ^{241}Am, ^{57}Co source)

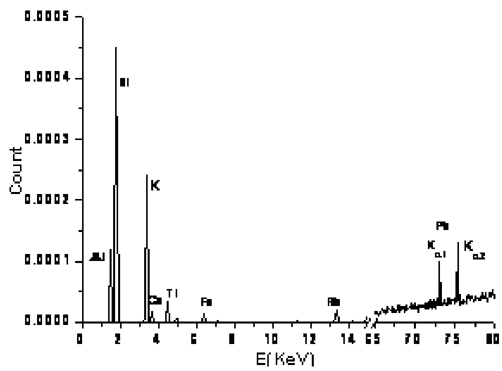

Fig. 7. The X-ray spectrum of adust target at 5.9, 59.6, 122Kev 20,25,55 percent, respectively (^{55}Fe, ^{241}Am, ^{57}Co source)

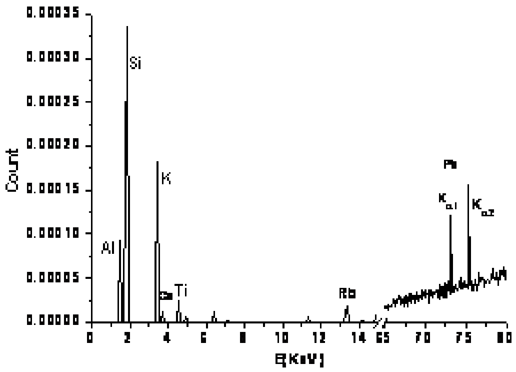

Fig. 8. The X-ray spectrum of a dust target at 5.9, 59.6, 122Kev 15,25,60 percent, respectively (^{55}Fe, ^{241}Am, ^{57}Co source)

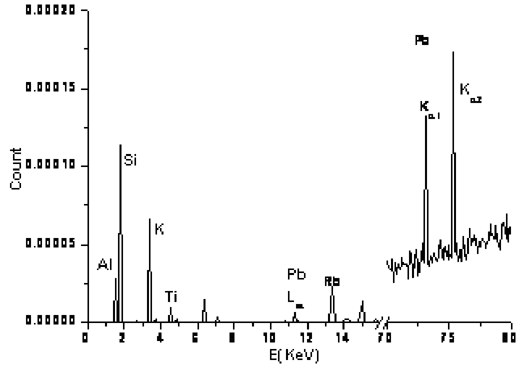

Fig. 9. The X-ray spectrum of a dust target at 5.9, 59.6, 122Kev 5,30,60 percent, respectively (^{55}Fe, ^{241}Am, ^{57}Co source)

CONCLUSIONS

One-source EDXRF technique is one of the most important techniques applied for detection of soil elements. In order to detect heavy elements present in soil with higher precision, the multi-source EDXRF(IXRF) technique wasintroduced in this research. To investigate functionality of the proposed technique, MCNPX nuclear code wasutilized. Initially, the accuracy of the code in element detection was investigated and verified. Research outcomes show that in using sources of^{55}Fe(5.9KeV) ^{241}Am(26.4KeV), ^{241}Am(59.6KeV) and also ^{60}Co(1173KeV) , for detection of soil elements within the $Z \leq 23$, $23 \leq Z \leq 40$ and $Z \geq 40$ ranges, ^{55}Fe(5.9KeV), ^{241}Am(26.4,59.6KeV) and ^{60}Co(1173KeV) are appropriate, respectively. The reason of using three experimental sources is demonstrated by comparing the figures obtained with the code with the experimental results. The results show that the source with lower energy ^{55}Fe(5.9KeV), is appropriate for extraction of element spectra with atomic numbers between 11 and 19;the source (^{241}Am(26.4, 59.6KeV) is better for atomic numbers between 19 and 40 and the energetic source (^{60}Co1173, 1331KeV) is appropriate for detection of heavy metals like lead.The reason for this is the dependency of absorption cross-section and dispersion to energy.

Afterwards, with the use of IXRF technique, the emitted X-ray spectrum characteristic for the soil was obtained. The comparison between the results for the spectrum obtained by MCNPX with the experimental results, done by J. A. Bearden [9], shows that the IXRF technique has a good capability in detecting the elements present in soil with high precision.

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ИЗСЛЕДВАНЕ НА ВЪЗМОЖНОСТИТЕ НА IXRF-ТЕХНИКА ЗА ОТКРИВАНЕТО НА ЕЛЕМЕНТИ В ПРАХ ПО МЕТОДА МОНТЕ-КАРЛО N ЧАСТИЦИ

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Постъпила на 15 ноември, 2016 г.; приета на 12 април, 2017 г.

(Резюме)

Откриването на тежки метали в почви и прах е важен фактор в изследването на замърсяването на околната среда. Досега за тази цел се използва лабораторен метод, основан на енерго-дисперсионна рентгенова флуоресценция (EDX-RF). За откриването на тези елементи в настоящето изследване се предлага методът Монте-Карло, основан на EDX-RF-техника. Кодът MCNPX2.7 се основава на Монте-Карло изчисления и е способен за трасиране на 32 частици (включително на фотони) в обхвата на рентгенови и γ-лъчи. В настоящата работа са сравнени резултатите на много-източникова симулация EDX-RF-техника (IXRF)с опитни резултати. Сравнението показва, че IXRF е в състояние да се открие процентното съдържание на елементите, налични в почвата и праха с голяма корелация.